OCRWM	DESIGN CALCULATION OR ANALYSIS COVER SHEET	1. QA: QA 2. Page: 1

3. System:	4. Document Identifier:
Uncanistered Spent Nuclear Fuel	CAL-DSU-NU-000007 REV 00B

5. Title:
Isotopic Model for Commercial SNF Burnup Credit

6. Group:
Criticality

7. Document Status Designation:
☒ Preliminary ☐ Final ☐ Cancelled

8. Notes/Comments:

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1) ECN-001, DATED 07/27/2005

Attachments:	Total Number of Pages:
I	4
II	4
III	8
IV (Compact Disk Attachment)	N/A

RECORD OF REVISIONS

9. No.	10. Reason For Revision	11. Total # of Pgs.	12. Last Pg. #	13. Originator (Print/Sign/Date)	14. Checker (Print/Sign/Date)	15. QER (Print/Sign/Date)	16. Approved/Accepted (Print/Sign)	17. Date
00A	Initial Issue. Supercedes MDL-DSU-NU-00001 REV 00 and ICN 01, Errata. Data for BWR SNF were added and changes are too extensive to use change bars.	100	III-8	Alan H. Wells Jason E. Huffer	John Scaglione	D.J. Tunney	Daniel A. Thomas	
00B	Document revised to address DOE LP-6.1Q review comments. Pages 1 and 15 contain only revised text. Attachment IV was copied over from previous revision (00A), but had no modifications.	100	III-8	J.M. Scaglione John M. Scaglione 11/17/2004	A.A. Alsaed aaalsaed 11/17/04	W.N. Dockery W.N. Dockery 17 NOV 2004	W.E. Hutchins W.E. Hutchins	17 NOV 04

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EXECUTIVE SUMMARY

Disposal Criticality Analysis Methodology Topical Report[1] describes a methodology for performing postclosure criticality analyses within the repository at Yucca Mountain, Nevada. An important component of the postclosure criticality analysis is the calculation of conservative isotopic concentrations for spent nuclear fuel. This report documents the isotopic calculation methodology. The isotopic calculation methodology is shown to be conservative based upon current data for pressurized water reactor and boiling water reactor spent nuclear fuel.

The isotopic calculation methodology is to be used for conservatively calculating isotopic concentrations for criticality calculations for commercial spent nuclear fuel waste forms. The isotopic calculation methodology uses the SAS2H control module of the SCALE code system to apply the transition matrix method along with a nuclear data library to solve the transmutation and radioactive decay equations that describe the isotopic changes as fuel is irradiated in a reactor. Bounding parameters are chosen to ensure that the calculated reactivity of spent nuclear fuel is conservative. Radiochemical assay data or commercial reactor critical data are used to test the bounding parameter set to ensure that they produce conservative reactivity results for the enrichment and burnup ranges. The isotopic calculation methodology also provides the isotopic component of the critical limit, as required in *Disposal Criticality Analysis Methodology Topical Report*[1]. The use of conservative, bounding parameters ensures that the Δk_{ISO} term of the critical limit equation is zero, indicating that no additional isotopic term is needed.

This report addresses two open items from *Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0*[2]. The open items are as follows:

> Open Item 11: "The DOE is required to develop an acceptable methodology for establishing bias and uncertainties for the isotopic depletion model."
>
> Open Item 15: "The DOE is required to include the isotopic bias and uncertainties as part of Δk_c, if not included as isotopic correction factors."

This report provides additional data for an item addressed elsewhere:

> Open Item 7: "The DOE must demonstrate the adequacy of using one-dimensional calculations to capture three-dimensional neutron spectrum effects in their point-depletion calculation or use two/three dimensional calculations for determining the neutron spectra during the depletion cycles to be used in the depletion analyses."

This report provides a description of the isotopic calculations and the demonstration that the bounding parameters that were chosen are indeed conservative, and determines the range of applicability of the calculations.

[1] YMP (Yucca Mountain Site Characterization Project) 2003. *Disposal Criticality Analysis Methodology Topical Report.* YMP/TR-004Q, Rev. 02.

[2] Reamer, C.W. 2000. "Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0." Letter from C.W. Reamer (NRC) to S.J. Brocoum (DOE/YMSCO), June 26, 2000, with enclosure.

Based on applicable pressurized water reactor and boiling water reactor experimental results from commercial reactor critical and radiochemical assays, this report concludes that the bounding parameters produce conservative calculations of the isotopic contents of pressurized water reactor and boiling water reactor spent nuclear fuel.

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ACRONYMS

B & W	Babcock & Wilcox
BWR	boiling water reactor
CRC	commercial reactor critical
CRWMS	Civilian Radioactive Waste Management System
CSCI	Computer Software Configuration Item
DTN	data tracking number
ENDF	evaluated nuclear data file
FEPs	features, events, and processes
GE	General Electric
GWd/MTU	gigawatt-day per metric ton of uranium
LWR	light water reactor
M&O	Management and Operating Contractor
MW/MTU	megawatt per metric ton of uranium
PC	personal computer
psia	pound per square inch absolute
PWR	pressurized water reactor
RCA	radiochemical assay
SNF	spent nuclear fuel
STN	Software Tracking Number

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1. PURPOSE

The purpose of this report is to demonstrate a process for selecting bounding depletion parameters, show that they are conservative for pressurized water reactor (PWR) and boiling water reactor (BWR) spent nuclear fuel (SNF), and establish the range of burnup for which the parameters are conservative. The general range of applicability is for commercial light water reactor (LWR) SNF with initial enrichments between 2.0 and 5.0 weight percent ^{235}U and burnups between 10 and 50 gigawatt-day per metric ton of uranium (GWd/MTU).

The *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003) presents an approach to the methodology for evaluating potential criticality situations in the geological repository. As stated in the referenced topical report, the detailed methodology for performing the disposal criticality analyses will be documented in model reports. Many of the models developed in support of the topical report differ from the definition of models as given in the Office of Civilian Radioactive Waste Management procedure AP-SIII.10Q, *Models*, in that they are procedural, rather than mathematical. These model reports document the detailed methodology necessary to implement the approach presented in the *Disposal Criticality Analysis Methodology Topical Report* and provide calculations utilizing the methodology. Thus, the governing procedure for this type of report is AP-3.12Q, *Design Calculations and Analyses*. The *Isotopic Model for Commercial SNF Burnup Credit* is of this latter type, providing a procedure to evaluate the criticality potential of in-package and external configurations.

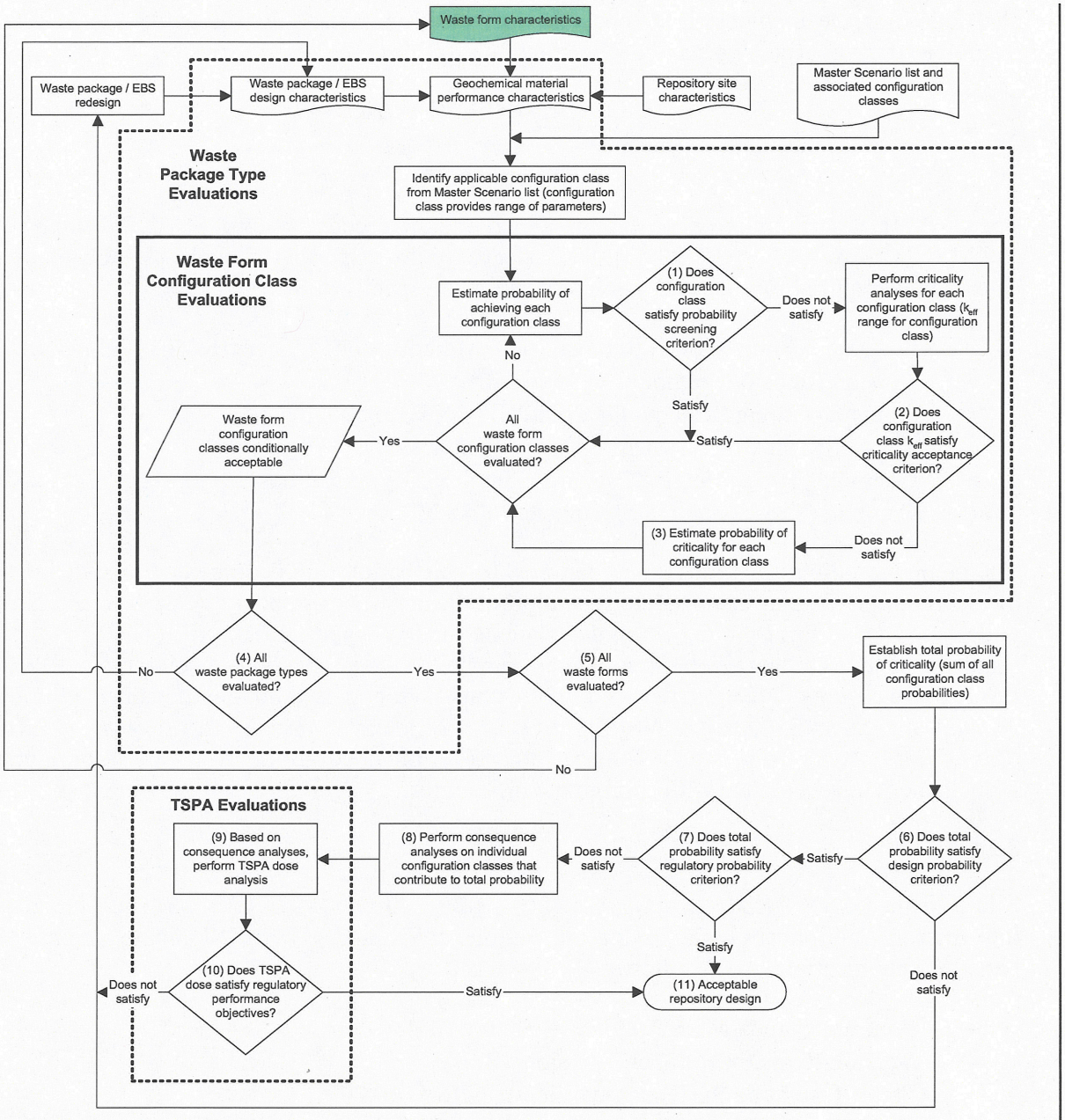
Throughout the remainder of the document the term "isotopic model" will refer to the overall process of establishing bounding isotopic concentrations with respect to criticality applications. The isotopic model is a component of the methodology presented in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003). How the isotopic model fits into the overall disposal criticality analysis methodology is illustrated in Figure 1. The specific methodology steps related to the isotopic model are highlighted in Figure 1. The isotopic model will not provide a direct input to the total system performance assessment for license application. Parameters that describe the fuel and its environment in the reactor are used to calculate the isotopic concentration of SNF. A method was developed for confirming that bounding parameters for isotopic calculations are conservative. Isotopic concentrations calculated using the conservative, bounding parameters are used in generating waste form characteristics, which are used as input parameters to evaluate the criticality potential of the waste form configurations.

This calculation confirms that bounding parameters are only shown to be conservative for PWR SNF and older, simpler BWR SNF including 6×6, 7×7, and 8×8 assemblies but are inconclusive for modern 9×9 assemblies, such as the General Electric (GE)-11, which are more complex. Modern BWR assembly types contain substantial quantities of gadolinium burnable absorbers that control the initial reactivity of the high enrichment needed to achieve long cycle lengths. Such assemblies may also contain a range of enrichments of several percent, and these different enrichments and strong absorbers cause strong flux gradients between rods that exceed the capabilities of the one-dimensional computer code used for this report. Older assembly types have simpler enrichment lattice arrangements and do not show such strong gradients, and are thus adequately modeled by the one-dimensional computer code.

This report addresses specific open items 7, 11, and 15 from *Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0* (Reamer 2000, Section 4) which are as follows:

> Open Item 7–"The DOE must demonstrate the adequacy of using one-dimensional calculations to capture three-dimensional neutron spectrum effects in their point-depletion calculation or use two/three dimensional calculations for determining the neutron spectra during the depletion cycles to be used in the depletion analyses." (Addressed in Section 6.3)
>
> Open Item 11–"The DOE is required to develop an acceptable methodology for establishing bias and uncertainties for the isotopic depletion model." (Addressed in Sections 6.1 and 6.2)
>
> Open Item 15–"The DOE is required to include the isotopic bias and uncertainties as part of Δk_c, if not included as isotopic correction factors." (Addressed in Section 6)

This report provides the Δk_{ISO} isotopic value required by the *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Section 3.5.3.2.5). The method for confirming that the bounding parameters of the isotopic calculation are conservative causes the Δk_{ISO} isotopic value to be greater than or equal to zero, which is set to zero. Thus, there is no need for an additional correction to the critical limit equation in the *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Eq. 3-1). Results from this report will also be used as input to analyses evaluating the criticality potential of internal waste package loading curves and for use in the criticality features, events, and processes (FEPs) screening analyses.



Source: YMP 2003, Figure 3-1.

Figure 1. Disposal Criticality Analysis Methodology

2. QUALITY ASSURANCE

Development of this analysis and the supporting activities have been determined to be subject to the Yucca Mountain Project's quality assurance program (DOE 2004) in Section 8 of *Technical Work Plan for: Criticality Department Work Packages ACRM01 and NSN002* (BSC 2004e). Approved procedures identified in the technical work plan (BSC 2004e, Section 4) have been used to conduct and document the activities described in this analysis. The technical work plan

also identifies the methods used to control the electronic management of data (BSC 2004e, Section 8) during the analysis and documentation activities.

3. USE OF SOFTWARE

3.1 SAS2H

The SAS2H control module of the baselined modular code system SCALE Version 4.4A (SCALE V.4.4A, STN: 10129-4.4A-00) was used to perform the fuel assembly depletion calculations required for this evaluation. The software specifications are as follows:

- Program Name: SAS2H of the SCALE Modular Code System (STN: 10129-4.4A-00)
- Version/Revision Number: Version 4.4A
- Status/Operating System: Qualified/HP-UX B.10.20
- Software Tracking Number (STN): 10129-4.4A-00
- Computer Type: Hewlett Packard 9000 Series Workstations
- Computer Processing Unit Number: 700887

The input and output files for the various SAS2H calculations are documented in Attachment II of this report so that an independent repetition of the software use could be performed. SAS2H is designed to perform the depletion calculations for PWR and BWR SNF. The SAS2H code sequence of SCALE that was used is (1) appropriate for the application of commercial PWR and BWR fuel assembly depletion, (2) used only within the range of validation documented in *Users Manual for SCALE-4.4A* (CRWMS M&O 2000a) and *Validation Test Report (VTR) for SCALE-4.4A* (CRWMS M&O 2000b), and (3) obtained from Software Configuration Management in accordance with appropriate procedures.

3.2 MCNP

The baselined MCNP code (MCNP V.4B2LV, CSCI: 30033-V4B2LV) was used to calculate the neutron multiplication factor for the various PWR and BWR SNF compositions. The software specifications are as follows:

- Program Name: MCNP (CSCI: 30033-V4B2LV)
- Version/Revision Number: Version 4B2LV
- Status/Operating System: Qualified/HP-UX B.10.20
- Computer Software Configuration Item (CSCI) Number: 30033-V4B2LV
- Computer Type: Hewlett Packard 9000 Series Workstations
- Computer Processing Unit Number: 700887

The input and output files for the various MCNP calculations are documented in Attachment II of this report so that an independent repetition of the software use may be performed. MCNP is designed to perform criticality and shielding calculations, such as the criticality calculations for irradiated fuel required for this report. The MCNP software used was (1) appropriate for the application of multiplication factor calculations for PWR and BWR SNF, (2) used only within the range of validation documented throughout *Software Qualification Report for MCNP Version 4B2, A General Monte Carlo N-Particle Transport Code* (CRWMS M&O 1998b) and

MCNP-A General Monte Carlo N-Particle Transport Code (Briesmeister 1997), and (3) obtained from Software Configuration Management in accordance with appropriate procedures.

3.3 EXCEL

- Title: Excel
- Version/Revision Number: Microsoft® Excel 2000 SP-3
- Computer Processing Unit Number: Software is installed on a DELL OptiPlex GX260 personal computer (PC), Civilian Radioactive Waste Management System (CRWMS) Management and Operating Contractor (M&O) Tag Number 152395, running Microsoft Windows 2000, Service Pack 4.

Microsoft Excel for Windows, Version 2000 SP-3, is used in calculations and analysis to manipulate the inputs using standard mathematical expressions and operations. It is also used to tabulate and chart results. The user-defined formulas, inputs, and results are documented in sufficient detail to allow an independent repetition of computations. Thus, Microsoft Excel is used only as a worksheet and not as a software routine. Microsoft Excel 2000 SP-3 is an exempt software product in accordance with LP-SI.11Q-BSC, *Software Management*, Section 2.0.

The spreadsheet files for the Excel calculations are documented in Attachment IV. The files in Attachment IV are such that an independent repetition of the software use may be performed.

3.4 MATHCAD

- Title: Mathcad
- Version/Revision Number: Mathsoft Engineering and Education, Inc. Mathcad® 11 Version 2a
- Computer Processing Unit Number: Software is installed on a DELL OptiPlex GX260 PC, CRWMS M&O Tag Number 152395, running Microsoft Windows 2000, Service Pack 4.

Mathcad® for Windows 2000, Version 11.2a, is a problem solving environment used in calculations and analysis. It is also used to tabulate results and evaluate mathematical expressions. The user-defined expressions, inputs, and results are documented in sufficient detail to allow an independent repetition of computations. Thus, Mathcad® is used as a worksheet and not as a software routine. Mathcad 2001 Version 11.2a is an exempt software product in accordance with LP-SI.11Q-BSC, *Software Management*, Section 2.0.

The input and output files for the various Mathcad® calculations are documented in Attachment IV. The calculation files in Attachment IV are such that an independent repetition of the software use may be performed.

4. INPUT PARAMETERS

The following data tracking number (DTN) was used for representing material properties:

- DTN: MO0003RIB00071.000, Physical and Chemical Characteristics of Alloy 22.

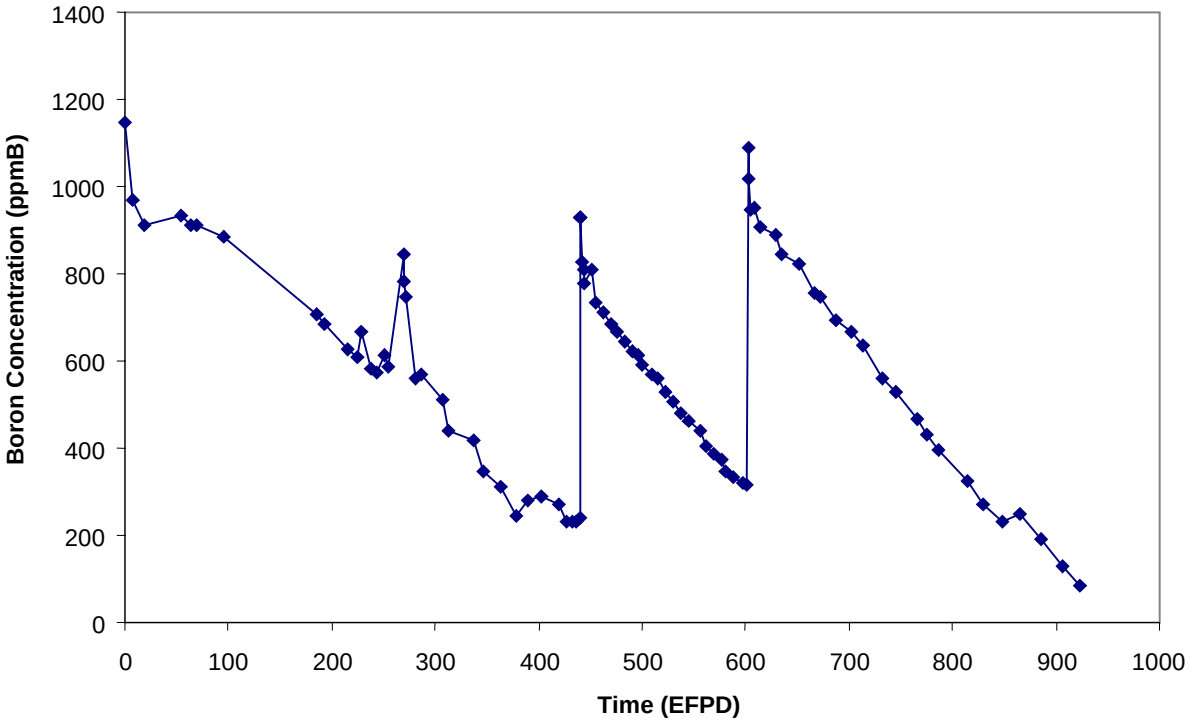
The following reference sources were used for material specifications:

- *Corrosion* (ASM International 1987)
- *Properties and Selection: Nonferrous Alloys and Special-Purpose Materials, Specific Metals and Alloys* (ASM International 1990)
- *Standard Specification for Heat-Resisting Chromium and Chromium-Nickel Stainless Steel Plate, Sheet, and Strip for Pressure Vessels* (ASTM A 240/A 240M-03b, 2003)
- *Standard Specification for Wrought Zirconium Alloy Seamless Tubes for Nuclear Reactor Fuel Cladding* (ASTM B 811-97, 2000)
- *Standard Practice for Preparing, Cleaning, and Evaluating Corrosion Test Specimens* (ASTM G 1-90, 1999)
- *Practical Handbook of Materials Science* (Lynch 1989)

Additional input parameters are provided in Section 7, where they are used to derive values needed for the computer inputs.

4.1 NOMINAL PWR BORON LETDOWN AND NOMINAL BWR CONTROL BLADE HISTORIES

The nominal PWR boron letdown information comes from Crystal River Unit 3 and is presented in Table 1 and illustrated in Figure 2. This boron letdown curve is for an early PWR reactor design, but is appropriate for the range of enrichments and burnups investigated. The longer cycle lengths required to attain burnups higher than 50 GWd/MTU use higher boron concentrations; hence the bounding parameters are limited to a maximum of 50 GWd/MTU (assembly average burnup).



NOTE: EFPD = effective full-power days; ppmB = parts per million boron by mass.

Figure 2. Boron Letdown Curve

Table 1. Boron Letdown Data for Crystal River Unit 3 Cycles 1 Through 3

Cycle 1A		Cycle 1B		Cycle 2		Cycle 3	
EFPD	**ppmB**	**EFPD**	**ppmB**	**EFPD**	**ppmB**	**EFPD**	**ppmB**
0.0	1147	269.4	843	0.6	930	0.7	1090
7.2	968	269.8	783	0.8	930	2.0	1020
18.6	912	272.0	748	0.9	930	4.0	947
55.2	934	280.2	558	2.1	826	6.7	951
63.8	909	287.2	571	3.0	809	12.6	908
69.9	909	306.2	513	4.4	778	26.8	891
94.9	884	313.2	441	11.4	809	32.6	843
184.7	705	337.2	419	15.8	735	50.7	822
192.3	683	345.7	346	22.5	709	66.0	757
216.0	627	364.2	309	29.3	683	69.9	746
224.8	610	377.6	246	35.3	666	85.0	692
228.5	666	389.5	279	42.3	644	100.2	666
238.0	584	401.7	290	50.0	623	111.2	636
244.0	575	419.3	272	55.8	614	130.5	562
250.8	614	427.1	229	60.8	592	143.8	528
254.7	588	431.8	231	69.1	571	163.9	467
—	—	437.1	229	75.2	558	174.0	432
—	—	440.1	242	83.1	528	184.2	394
—	—	—	—	89.8	506	212.9	324
—	—	—	—	97.8	480	227.5	272
—	—	—	—	104.7	463	246.4	229
—	—	—	—	116.4	441	262.9	250
—	—	—	—	122.5	406	283.8	190
—	—	—	—	129.1	385	304.0	130
—	—	—	—	135.9	372	322.0	86
—	—	—	—	139.9	346	—	—
—	—	—	—	148.6	333	—	—
—	—	—	—	156.4	320	—	—
—	—	—	—	161.4	316	—	—

NOTE: EFPD = effective full-power days; ppmB = parts per million boron by mass.

Source: Punatar 2001, pp. 4-238 to 4-240.

The operating history for Grand Gulf Unit 1, assembly C16, node 3, statepoint 15 (Wimmer 2004, p. 106) was chosen as representative of the nominal history because it has a relatively high burnup compared to the other Grand Gulf assemblies. Note that this assembly is an 8×8 design, but the operating history is independent of the fuel design so it can be applied to the 7×7 design chosen for the bounding parameter case. The operating history is provided in Table 2.

Table 2. BWR Nominal Operating History

Burn Step	Blade Position	Power	Time	Down	Burnup
1	Out	8.8332	68.833	0	2840.00
2	Out	8.8332	68.833	0	2840.00
3	Out	8.8332	68.833	0	2840.00
4	Out	7.7277	66.453	0	2398.66
5	Out	7.7277	66.453	0	2398.66
6	Out	7.7277	66.453	994	2398.66
7	In	5.7660	4.01	425	108.00
8	In	7.1702	69.48	205	2326.99
9	Out	9.0448	53.967	0	2279.98
10	Out	9.0448	53.967	0	2279.98
11	In	9.0448	53.967	0	2279.98
12	Out	7.4959	61.653	0	2158.65
13	Out	7.4959	61.653	0	2158.65
14	Out	7.4959	61.653	0	2158.65
15	Out	6.5874	26.78	1340	824.00
16	Out	7.5203	16.54	273	581.00
17	Out	7.5817	65.865	0	2332.52
18	Out	7.5817	65.865	114	2332.52
19	Out	7.9623	17.02	85	633.00
20	Out	7.1065	38.29	185	1271.00
21	Out	6.5574	68.415	0	2095.49
22	Out	6.5574	68.415	0	2095.49
23	Out	6.5574	68.415	0	2095.49
24	Out	6.5574	68.415	0	2095.49
25	Out	6.5574	71.077	1825	2177.03
		35.68 MW/MTU Average	1401.3 Days		50000 MWd/MTU

NOTE: MW/MTU = megawatt per metric ton of uranium; MWd/MTU = megawatt-day per metric ton of uranium.

Source: Wimmer 2004, p. 135, file N550.out.

Note that the power history shown in Table 2 has an average of 35.68 MW/MTU over the time period given. The entry "Power" in the table is based on the mass used by SAS2H as specified in the input: 214.09 kgU. The number of burnup steps has been increased to provide the necessary burnup, which is normalized to 50 GWd/MTU. Power has been adjusted as necessary to provide the desired burnup with the burnup time fixed.

4.2 GENERIC LWR FUEL ASSEMBLY DEPLETION PARAMETERS

The following parameters are nominal for PWR fuel assemblies. They provide the nominal parameter set to be used as the baseline for comparison for the determination of the conservatism of the bounding parameters. These representative parameters are taken from *Summary Report of Commercial Reactor Criticality Data for Crystal River Unit 3* (Punatar 2001) for Crystal River Unit 3, assembly A8, node 9 and are actual values for this assembly.

- Fuel temperature, 861.3 K (Punatar 2001)
- Moderator temperature, 579.8 K (CRWMS M&O 2000a, Table 5.5.2 for 2200 psia based on a density of 0.7556 g/cm^3) (Punatar 2001)
- Density, 0.7556 g/cm^3, homogenized density for spacers and moderator (Punatar 2001)
- Average specific power, 43.0 MW/MTU, selected to allow high burnups analyzed in this report to be achieved in typical reactor operating cycles. The actual power history would not allow a burnup of 40 GWd/MTU in the time of operation.
- Moderator boron concentration values are presented in Figure 2 and were linearly interpolated from the nominal values specified in Table 1 (Punatar 2001).

Similar parameters are used for BWR fuel assemblies. They provide the nominal parameter set to be used as the baseline for comparison for the determination of the conservatism of the bounding parameters.

- Fuel temperature, 1000 K, a typical fuel pellet temperature (Wimmer 2004, p. 107)
- Moderator temperature, 560.7 K (Wimmer 2004, p. 17)
- Density, 0.43 g/cm^3, length-averaged value (Wimmer 2004, p. 17)
- Average specific power, 35.68 MW/MTU, selected to allow high burnups analyzed in this report to be achieved in typical reactor operating cycles
- No gadolinium rods integral to generic 7×7 BWR assembly. Control blades fully inserted for three time periods of irradiation history of assembly, as shown in the time history of Table 2.

4.3 PARAMETERS USED

The following is a listing of various parameters that were used in demonstrating the conservatism of the bounding parameters:

- Commercial reactor critical (CRC) input from *Summary Report of Commercial Reactor Critical Analyses Performed for the Disposal Criticality Analysis Methodology* (CRWMS M&O 1998c)

- Radiochemical assay (RCA) input from *Calculation of Isotopic Bias and Uncertainty for PWR Spent Nuclear Fuel* (BSC 2002a) and *Calculation of Isotopic Bias and Uncertainty for BWR SNF* (BSC 2003a)

- Depletion parameters for demonstrating bounding parameter selection from *PWR Depletion Parameter Sensitivity Evaluation* (BSC 2001) and *BWR Depletion Parameter Sensitivity Evaluation* (Anderson 2003).

5. ASSUMPTIONS

The following assumptions are made by this report:

5.1 LIMITING PWR FUEL ASSEMBLY

Assumption: It is assumed that the Babcock & Wilcox (B & W) 15×15 Mk-B2 assembly design is representative of all PWR SNF and is the most limiting PWR fuel assembly design.

Rationale: A previous analysis for the BR-100 transportation cask established the B & W 15×15 fuel assembly as one of the most reactive fuel assembly designs (B & W Fuel Company 1991, p. II 6-6).

Confirmation: This assumption does not require further confirmation, because k_{eff} is dependent upon the global behavior of the neutron population and not localized behavior. Geometric details of the fuel design do not have a strong effect.

Usage: This assumption is used in Section 7.1.

5.2 BORON LETDOWN CURVE

Assumption: The Crystal River Unit 3 boron letdown curve is representative of PWR SNF.

Rationale: The basis for this assumption is that the dissolved boron required to provide excess reactivity control is more dependent upon assembly enrichment than the details of the fuel design.

Confirmation: This assumption does not require further confirmation because it is only used as a nominal letdown curve that actually comes from Crystal River Unit 3 cycles; any boron letdown curve could have been used.

Usage: This assumption is used in Section 7.1.

5.3 CRC PWR DATA

Assumption: It is assumed that the CRC PWR data set (CRWMS M&O 1998c) is an adequate statistical representation of PWR reactor designs.

Rationale: Forty-one startups or restarts were analyzed for four different PWRs. The basis for this assumption is that the details of reactor design do not have a strong effect on reactivity.

Confirmation: This assumption does not require further confirmation because the CRC data set follows a normal distribution and contains enough data points to allow a 95/95 confidence interval.

Usage: This assumption is used in Section 6.1.

5.4 SYSTEMATIC ERROR

Assumption: It is assumed that the systematic error is the same in k_{eff} calculations for both reactor and waste package environmental conditions.

Rationale: The basis for this assumption is that the systematic error proceeds from the resonance cross section treatment (principally ^{238}U) in the evaluated nuclear data file (ENDF).

Confirmation: This assumption does not require further confirmation because the resonance cross sections used in the CRCs are chosen from ENDF to match the reactor temperatures when available. The resonance cross sections used in the waste package calculations are at room temperature conditions, which are the most reactive. Thus, differences in the temperatures between the reactor and waste package environments are conservatively accounted for.

Usage: This assumption is used in Section 7.

5.5 CONSERVATIVE CONTROL BLADE INSERTION USED

Assumption: It is assumed that the GE 7×7 assembly design without gadolinium rods, but with control blades inserted for the final 15 GWd/MTU of burnup, produces conservative results for all BWR SNF.

Rationale: The basis for this assumption is that the 15 GWd/MTU blade insertion is shown to produce a higher discharge reactivity than gadolinium rods in Wimmer (2004, Section 5.1.1.5, p. 17).

Confirmation: This assumption does not require further confirmation because of the conservatism ensured by the 15 GWd/MTU blade insertion.

Usage: This assumption is used in Section 7.1.

5.6 CRC BWR DATA

Assumption: It is assumed that the CRC BWR data set (Saglam 2004) is an adequate statistical representation of BWR reactor designs.

Rationale: Sixteen startups or restarts were analyzed for one reactor design. The basis for this assumption is that the details of reactor design do not have a strong effect on reactivity.

Confirmation: This assumption does not require further confirmation because the CRC pooled (BWR and PWR) data set follows a normal distribution and contains enough data points to allow a 95/95 confidence interval.

Usage: This assumption is used in Section 6.1.

6. CALCULATIONS

When representing the behavior of commercial SNF, credit is sought for the reduced reactivity associated with the net depletion of fissile isotopes and the creation of neutron-absorbing isotopes, a process that begins when a commercial nuclear reactor is first operated at power. This period includes the time that the fuel was in a reactor and exposed to a high neutron flux (in a power production mode), the downtime between irradiation cycles, and the cooling time after it was removed from the reactor. Taking credit for the reduced reactivity associated with this change in fuel material composition is known as burnup credit. Burnup is a measure of the amount of exposure or energy produced for a nuclear fuel assembly, usually expressed in units of GWd/MTU initially loaded into the assembly. Thus, burnup credit accounts for the reduced reactivity potential of a fuel assembly and varies with the fuel burnup, cooling time, the initial enrichment of fissile material in the fuel, and the availability of individual isotopes based on degradation analyses.

A list of corroborating or supporting data or information used in the calculation, along with their sources, is provided in Table 3.

Table 3. Supporting Information and Sources

Description	Source
PWR depletion parameter sensitivity study	BSC 2001
PWR disposal criticality analysis methodology	YMP 2003
PWR CRC analyses results	CRWMS M&O 1998c
PWR isotopic bias and uncertainty study, and RCA information summary	BSC 2002a
PWR code-to-code comparison study	BSC 2002b
PWR representative assembly characteristics	Punatar 2001, DOE 1992, Larsen et al. 1976
General reference to laboratory critical experiments	CRWMS M&O 1999a
General reference to criticality model	BSC 2003b
BWR depletion parameter sensitivity study	Anderson 2003
BWR CRC criticality analyses results	Saglam 2003
BWR isotopic bias and uncertainty study	BSC 2003a
Isotopic generation and confirmation of the BWR application model	Wimmer 2004
Comparisons of RCA data to SAS2H calculations	BSC 2003c

This report demonstrates that the bounding depletion parameters are conservative for PWR and BWR SNF and obtains the range of burnup for which the parameters are conservative. The general range of applicability is for commercial LWR SNF with initial enrichments between 2.0 and 5.0 weight percent ^{235}U and burnups between 10 and 50 GWd/MTU.

Conservative calculations of isotopic concentrations are ensured by choosing bounding parameters for the fuel irradiation. A study of the effects of varying parameters for PWR fuel irradiation (BSC 2001) was used to guide the choice of bounding parameter values for the following:

- UO_2 fuel pellet temperature
- Moderator temperature
- Specific power
- Moderator boron concentration.

A study of the effects of varying parameters for BWR fuel irradiation (Anderson 2003) was used to guide the choice of bounding parameter values for the following:

- UO_2 fuel pellet temperature
- Moderator temperature and density
- Specific power
- Gadolinium concentration.

This report provides a means for testing the chosen parameters for conservatism. Bounding depletion parameters were chosen based upon sensitivity studies, and then tested for conservatism. Either CRC or RCA data, or both, may be used to generate the isotopic contribution used for the conservatism test procedure. The conservatism test procedure ensures that the isotopic bias (Δk_{ISO} as shown in Equation 3-1 in Section 3.5.3.2.5 of *Disposal Criticality Analysis Methodology Topical Report* [YMP 2003]) will be zero or positive (indicating an overprediction in k_{eff}), which is then set to zero.

$$CL(x) = f(x) - \Delta k_{EROA} - \Delta k_{ISO} - \Delta k_m \quad \text{(Eq. 1)}$$

where

$CL(x)$ = the critical limit function determined by the criticality model (BSC 2003b)
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
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.

Isotopic concentrations were calculated using the SAS2H code sequence (10129-4.4A-00) and k_{eff} values were calculated (using the calculated isotopics) using the MCNP computer code (3033 V4B2LV). The k_{eff} calculations are based on taking credit for burnup with a subset of the total isotopes present in commercial SNF defined as the principal isotopes, identified in Table 4.

Table 4. Principal Isotopes for Commercial SNF Burnup Credit

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

Source: YMP 2003, Table 3-1, p. 3-30.

A comparison of the k_{eff} was performed for nominal (real-world) SAS2H parameter values and the example bounding values in order to determine the magnitude of conservatism caused by use of the bounding values. The conservatism thus instilled in the isotopic concentrations was then confirmed by a comparison to the overall bias and uncertainty of the SAS2H and MCNP codes as determined through CRC and RCA studies (CRWMS M&O 1998c; BSC 2002a; Saglam 2004; BSC 2003a). Further, a code-to-code comparison of PWR calculations was previously performed in *Summary Report of Code to Code Comparisons Performed for the Disposal Criticality Analysis Methodology* (BSC 2002b) to ensure that code-dependent issues had been addressed.

Using bounding depletion parameters for the generation of SNF assembly isotopics will ensure conservative criticality calculations for LWR SNF in any desired waste package for both preclosure and postclosure. LWR SNF with initial enrichments between 2.0 and 5.0 weight percent ^{235}U, and burnups between 10 and 50 GWd/MTU were evaluated. PWR burnable absorbers are simply another depletion parameter for the isotopic calculation as shown in Section 6.4.6. Separate sets of PWR bounding depletion parameters may be chosen with and without burnable absorbers, or alternatively a single set including burnable absorbers could be chosen.

The k_{eff} calculations were performed using continuous-energy neutron cross section libraries from *Selection of MCNP Cross Section Libraries* (CRWMS M&O 1998a, pp. 61 to 66). The results reported from the MCNP calculations were the combined average values of k_{eff} from three estimates (collision, absorption, and track length) listed in the final generation summary in the MCNP output. In order to evaluate the change in reactivity associated with the varied depletion parameters, a representative 21-PWR waste package configuration (illustrated in Attachment I) and a representative 44-BWR waste package configuration (BSC 2004a; BSC 2004b; BSC 2004c; BSC 2004d) illustrated in file att2.zip of Attachment IV were used. The 21-PWR and 44-BWR waste package configurations provide a basis for comparison of nominal and conservative calculations. This provides a Δk that is not sensitive to minor design changes to the fuel basket structures of the waste package. Thus the calculations for PWRs have not been revised to reflect updates to the 21-PWR design and the sketches provided in Attachment I are the versions used for the calculation. The BWR calculations used the drawings current at the time of issuance of this report. The PWR fuel assembly design was represented in detail using specifications for the B & W 15×15 assembly (Punatar 2001) and the BWR design was represented using specifications for the GE 7×7 assembly (DOE 1992, Larsen et al. 1976).

6.1 COMMERCIAL REACTOR CRITICAL BENCHMARKS

Conventional criticality benchmarks for fresh, unirradiated LWR fuel assemblies typically consist of subcritical measurements of k_{eff} for an array of fuel rods in a known configuration. The fuel rods are manufactured to tightly controlled specifications for materials and dimensions. The isotopic constituents of fresh fuel assemblies are well known and typically consist of enriched uranium without plutonium or fission products. The end result of a critical benchmark experiment is to accurately know the positions of the fuel rods in the critical array plus all of the other conditions that affect fuel reactivity, such as water level, temperature, and the concentration of dissolved boron (if boron is used in the experiment). The reactivity, or k_{eff}, of the experiment is dependent upon the relative probability that a neutron will be captured by ^{235}U, cause fission, and contribute to the nuclear chain reaction. Neutrons that are captured by other isotopes, such as ^{238}U or the structural materials of the fuel, disappear from the chain reaction. The relative probabilities of capture are a measure of what is called the macroscopic capture cross sections of the fuel and moderator. The macroscopic cross section (Σ [cm^{-1}]) of an isotope is the product of the number density (isotopic concentration, N [atoms/cm^3]) and the microscopic cross section (σ, measured in barns [10^{-24} cm^2/atom]) as shown in Equation 2.

$$\Sigma = N \cdot \sigma \qquad \text{(Eq. 2)}$$

Since the isotopic constituents of the fuel and moderator are well-known in critical benchmark experiments, the accuracy of the microscopic cross section is tested directly and the experiment can be used to validate the microscopic cross sections contained in the ENDF version(s) employed by MCNP. Since fresh fuel principally consists of ^{235}U and ^{238}U, with a small amount of ^{234}U, the desired range of fuel enrichments between about 2.0 and 5.0 weight percent ^{235}U have been tested by a number of different critical experiment projects (CRWMS M&O 1998c; CRWMS M&O 1999a; BSC 2003b, Section 7).

It is equally important to validate the microscopic cross sections employed by MCNP for calculations that include credit for burnup of SNF. This would be a straightforward process if critical benchmark experiments were available that included the actinides of plutonium and uranium that are produced in SNF, as well as the fission products included in the Principal Isotope set. Unfortunately, such critical experiments are not generally available, so an alternative means of validation of the MCNP calculations for SNF must be found.

CRC benchmarks are a series of critical experiments performed on operational, commercial nuclear power reactors. Each startup of the reactor requires a verification of the fuel loading and setup of the reactor via a reactor physics experiment in which the reactor is brought to a critical condition at a very low power. Incorrect loading of the reactor fuel assemblies, due to either an incorrect placement of assemblies or use of improper assemblies, can be detected through comparison of actual control rod positions required to achieve criticality against the positions that were calculated with core physics codes. These startup critical experiments are recorded as "statepoints" and kept as part of the reactor records. Since only a portion of the SNF is replaced each time the reactor is restarted, the reactor statepoints are a direct measure of the macroscopic cross sections of SNF. Complications arise due to short-lived fission products such as isotopes of xenon, which have a substantial effect on reactor criticality, but because they are short-lived they will not be present to influence the preclosure and postclosure performance of the

repository. Careful selection of the statepoints used in the CRCs removes the detrimental effects of such isotopes. The CRCs are sometimes called "integral" experiments, in the sense that the effects of the isotopic concentrations and microscopic cross sections for many isotopes are mixed within the reactor fuel. The k_{eff} measurement performed by a reactor physics experiment is thus the composite of many isotopes.

6.1.1 CRC Data

The calculated k_{eff} for a set of 41 PWR statepoints using Principal Isotope results, extracted from *Summary Report of Commercial Reactor Critical Analyses Performed for the Disposal Criticality Analysis Methodology* (CRWMS M&O 1998c, p. 42), and a set of 16 BWR statepoints extracted from *Commercial Reactor Reactivity Analysis for Grand Gulf, Unit 1* (Saglam 2004, p. 8) are provided in Table 5. Note that all statepoints are for LWR reactors at zero power. Reactor conditions at these statepoints are isothermal, and the geometric configuration of the fuel and control rods or control blades are known. ^{135}Xe has decayed to essentially zero concentration for these statepoints. These CRC statepoints constitute the only available critical measurements for irradiated fuel. CRC data at full or partial power conditions are not appropriate due to the presence of ^{135}Xe and three-dimensional effects. Therefore, such data were not included.

Table 5. Tabulation of LWR CRC Reactivities

Fuel	Case Name	k_{eff}	σ	Case Name	k_{eff}	σ
PWR	Crystal River 2	1.00156	0.00043	Crystal River 23	1.00108	0.00045
	Crystal River 3	1.00867	0.00042	Crystal River 24	1.00331	0.00047
	Crystal River 4	1.00305	0.00044	Crystal River 25	1.01073	0.00048
	Crystal River 5	1.00267	0.00046	Crystal River 26	1.01154	0.00044
	Crystal River 6	1.00662	0.00044	Crystal River 27	1.01113	0.00048
	Crystal River 7	1.00686	0.00044	Crystal River 28	1.00055	0.00044
	Crystal River 8	0.99922	0.00045	Crystal River 29	1.01222	0.00048
	Crystal River 9	1.00481	0.00045	Crystal River 30	1.00534	0.00049
	Crystal River 10	1.01265	0.00043	Crystal River 31	1.01968	0.00046
	Crystal River 11	1.00096	0.00044	Crystal River 32	1.00108	0.00048
	Crystal River 12	1.0173	0.00044	Crystal River 33	1.01232	0.00053
	Crystal River 13	1.00423	0.00039	Three Mile Island 2	1.00048	0.00047
	Crystal River 14	1.00784	0.00048	Three Mile Island 3	1.00443	0.00046
	Crystal River 15	1.01418	0.00041	Sequoyah 2	1.00109	0.00046
	Crystal River 16	1.00008	0.00043	Sequoyah 3	1.00679	0.00047
	Crystal River 17	1.0075	0.00044	McGuire 2	0.99428	0.00043
	Crystal River 18	1.00819	0.00045	McGuire 3	1.00013	0.00045
	Crystal River 19	1.00824	0.00046	McGuire 4	0.99755	0.00049
	Crystal River 20	1.01973	0.00047	McGuire 5	1.00565	0.00043
	Crystal River 21	1.01584	0.00044	McGuire 6	1.00786	0.00047
	Crystal River 22	0.99788	0.00044			
BWR	Grand Gulf 5	1.0196	0.0001	Grand Gulf 15	1.0017	0.0001
	Grand Gulf 6	1.017	0.0001	Grand Gulf 16	1.0239	0.0001
	Grand Gulf 7	1.0172	0.0001	Grand Gulf 18	1.0166	0.0001
	Grand Gulf 10	1.0197	0.0001	Grand Gulf 19	1.0104	0.0001
	Grand Gulf 11	1.0228	0.0001	Grand Gulf 20	0.9878	0.0001
	Grand Gulf 12	1.0098	0.0001	Grand Gulf 21	1.0172	0.0001
	Grand Gulf 13	1.0086	0.0001	Grand Gulf 22	1.0195	0.0001
	Grand Gulf 14	1.0034	0.0001	Grand Gulf 23	1.0162	0.0001

NOTE: In the case names, the numbers denote which respective case from Summary Report of Commercial Reactor Critical Analyses Performed for the Disposal Criticality Analysis Methodology (CRWMS M&O 1998c, p. 42) or Commercial Reactor Reactivity Analysis for Grand Gulf, Unit 1 (Saglam 2004, p. 8). Sigma (σ) represents the standard deviation of k_{eff} about the average combined collision, absorption, and track-length estimate due to the Monte Carlo calculation statistics.

6.1.2 Calculation of CRC Bias and Uncertainty

The bias and uncertainty of the LWR CRC k_{eff} values were evaluated using the method described below, which is based upon the critical limit determination in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Section 3.5.3.2.8). The overall reactivity bias was quantified by calculating Δk_{eff} between the measured (always 1.0) and calculated k_{eff} for each CRC case. The standard deviation of the 57 LWR data points is calculated (Attachment IV, File "LWR CRC and RCA results tables.xls," Sheet "LWR CRC Results") as is the mean standard deviation of the MCNP calculations. A 95 percent confidence limit was used in calculating the standard deviations. Use of the following process for calculating the bias is based on the data set

having a normal distribution, which was tested using the Anderson-Darling test for normality as described in Attachment III (also Attachment IV, File "keff-normality test.mcd"). The bias and uncertainty is calculated as illustrated in Equation 3.

$$\text{bias and uncertainty} = \beta_{ave} - K_b\sqrt{\sigma_{\Delta k_{eff}}^{\ 2} + \sigma_{MCNP}^{\ 2}} \qquad \text{(Eq. 3)}$$

where

β_{ave} = the mean value of the Δk_{eff} values (i.e., bias) between the calculated CRC reactivity and the measured critical condition, where k_{eff} is 1.00

K_b = a multiplier from statistical tables for one-sided tolerance limits for normal distributions

$\sigma_{\Delta k_{eff}}$ = the nonbiased (distribution independent) standard deviation associated with the selected Δk_{eff} values as shown in Equation 4

σ_{MCNP} = the mean standard deviation of the MCNP calculation uncertainties, calculated as shown in Equation 5.

$$\sigma_{\Delta k_{eff}} = \sqrt{\frac{N\sum x^2 - (\sum x)^2}{N(N-1)}} \qquad \text{(Eq. 4)}$$

where

N = total number of values

x = Δk_{eff} values

$$\sigma_{MCNP} = \sqrt{\frac{1}{N}\sum \sigma_i^{\ 2}} \qquad \text{(Eq. 5)}$$

where

σ_i = the MCNP standard deviation for a CRC case

Bias and uncertainty values were calculated for the CRC data sets, as shown in Table 6.

Table 6. Bias and Uncertainty for CRC Data

	Bias (β_{ave})	$\sigma_{\Delta k_{eff}}$	σ_{MCNP}	**K_b[a]**	**Bias and Uncertainty**
LWR	0.0082[b]	0.0078[b]	0.0004[b]	2.034	-0.0077

NOTES: [a]Multiplier taken from Odeh and Owen (1980 Table 1.4.2) for a 95/95 tolerance limit.

[b]Attachment IV, File "LWR CRC and RCA results tables.xls," Sheet "LWR CRC Results."

The LWR CRCs show a bias of 0.0082, indicating an overprediction of k_{eff} for SNF of less than one percent. The standard deviation of the data set of 57 CRCs was 0.0078. Thus the sum of the bias and uncertainties at the 95 percent confidence level is -0.0077, or about 0.8 percent Δk_{eff}. The magnitude of this Δk_{eff} value, 0.0077, is the criterion that will be used in Section 8 to determine if the bounding isotopic parameter set is conservative. Thus, if the bounding parameter set produces an increase in k_{eff} greater than 0.0077, the set is conservative.

6.1.3 "Compensating Errors"

The isotopic concentrations used for the CRC calculations are obtained from SAS2H, while the microscopic cross sections are contained in ENDF, provided with the MCNP criticality code. A concern exists that concentration data for a given isotope and the microscopic cross section data could have "compensating errors" that yield accurate macroscopic cross section data that provide an accurate (i.e., agreement) k_{eff} for the CRC benchmark compared to the experimental value. This phenomenon could occur if adjustments were made to the microscopic cross sections to generate closer agreement between critical experiments, such as CRCs, and calculations. ENDF cross sections are used in this calculation without such adjustments for the CRCs, therefore these "compensating errors" do not occur.

6.1.4 Uncredited Margin

It is sometimes beneficial to know the magnitude of calculational margins that may not be credited for regulatory analysis purposes. The use of the Principal Isotope set introduces a margin relative to the actual conditions in spent fuel, since the isotopes that are not included in this isotope list are (primarily) fission product and actinide absorbers. These "additional" neutron absorbers possess chemical or radioactive decay characteristics that would discourage their use in a burnup credit analysis. The actual k_{eff} of a waste package is thus less than the value calculated using the Principal Isotope set. Although not included in this calculation which is based upon the Principal Isotope set, the magnitude of such an uncredited margin can be found by comparing the mean values of the LWR CRC critical experiments calculated using the Principal Isotope list against mean values using the "Best Estimate" list containing all of the Principal Isotope list plus all additional fission products for which isotopic and cross section data are available.

6.2 RADIOCHEMICAL ASSAYS

RCA data can provide direct confirmation of SAS2H isotopic concentrations. RCA data allows comparison of calculated concentrations of each isotope to a measured value, as well as comparison of k_{eff} values. The calculation utilizes 104 different PWR (74) and BWR (30) radiochemical assayed SNF samples. Note that the Limerick data were not used in the bias calculation, but are used in Section 6.3.3.

The irradiated fuel PWR samples evaluated span an initial enrichment range of 2.453 weight percent through 4.67 weight percent ^{235}U enrichment, and burnups from 6.92 GWd/MTU through 55.7 GWd/MTU. The BWR samples evaluated span an initial enrichment range of 2.53 weight percent through 3.95 weight percent ^{235}U enrichment, and burnups from 2.16 through 65.5 GWd/MTU. The sample parameters are given in Table 7.

The isotopes that were analyzed vary for each of the samples, and fission products were not measured for all samples. The total number of measurements for each isotope is provided in Table 8.

Table 7. LWR RCA Parameters

Reactor	Assembly Design	Number of Samples/Assemblies/ Rods	Sample Burnups (GWd/MTU)	Initial Enrichments (Wt% ^{235}U)
PWR				
Trino Vercelles	Westinghouse, Irregular[a]	14/3/6	12.042	3.897
			11.529-24.548	3.13
Yankee Rowe	Westinghouse, Irregular	8/1/3	15.95-35.97	3.4
Turkey Point	Westinghouse 15×15, 20 guide tubes	5/2/5	30.72-31.56	2.556
Mihama	Westinghouse 15×15, 20 guide tubes	9/3/NA[b]	6.92-8.3	3.208
			14.66-21.29	3.203
			29.5-34.32	3.210
H.B. Robinson	Westinghouse 15×15, 20 guide tubes, 12 BPRs[c]	4/1/1	16.02-31.66	2.561
Obrigheim	Siemens 14×14	6/5/special[d]	25.93-29.52	3.13
Calvert Cliffs	Combustion Engineering 14×14 BPRs present	9/3/3	27.35-44.34	3.038
			18.68-33.17	2.72
			31.40-46.46	2.453
Three Mile Island	B & W 15×15, 16 BPRs[c]	5/1/1	44.8-51.3	4.67
		6/1/1	44.8-55.7	4.67
		4/1/2	23.7-26.7	4.67
		4/1/3	22.8-29.9	4.67
BWR				
Cooper	GE 7×7, Gd @ 3.4 weight percent	6/1/2	17.84 - 33.94	2.93
Gundremmigen	Siemens 6×6	8/2/4	14.39-27.40	2.530
JPDR	PNC 6×6, No Gd	16/3/4	2.16 - 7.01	2.5966
Limerick[e]	GE 9×9, Gd @ 5.0 weight percent	8/1/3	37.0-65.5	3.6, 3.95

NOTES: [a] Non-standard PWR fuel arrays (e.g., contains cruciform fuel assemblies).
[b] NA = not available.
[c] BPR = Burnable Poison Rod.
[d] These samples were actual half fuel assemblies.
[e] Limerick data were not used in calculations of bias and uncertainty.

Source: PWR data: BSC 2002a, pp. 15-16; BWR data: BSC 2003a, Sections 5.2.1-5.2.3, Attachments I, II, and III; BSC 2003c, Table 5-4.

Table 8. Number of Samples for Each Isotope

Isotope[a, b, d]	# of Samples	Isotope	# of Samples	Isotope	# of Samples
^{234}U	66	^{145}Nd	47	^{155}Eu	20
^{235}U	104	^{146}Nd	36	^{155}Gd[c]	22
^{236}U	104	^{148}Nd	68	^{242}Cm	47
^{238}U	79	^{150}Nd	36	^{243}Cm	17
^{238}Pu	90	^{147}Pm[c]	3	^{244}Cm[e]	56
^{239}Pu	104	^{147}Sm[c]	22	^{241}Am	50
^{240}Pu	104	^{148}Sm[c]	3	^{242}Am[c]	6
^{241}Pu	104	^{149}Sm[c]	22	^{242m}Am	39
^{242}Pu	100	^{150}Sm[c]	22	^{243}Am[c]	34
^{237}Np	49	^{151}Sm[c]	22	^{232}U[c]	9
^{133}Cs[c]	3	^{151}Eu[c]	22	^{236}Pu[c]	3
^{134}Cs	31	^{152}Sm[c]	22	^{109}Ag[c]	11
^{135}Cs	9	^{153}Eu[c]	22	^{95}Mo[c]	11
^{137}Cs	52	^{154}Sm[c]	3	^{99}Tc	17
^{143}Nd	47	^{154}Eu	23	^{101}Ru[c]	11
^{144}Nd	28	^{154}Gd[c]	3	^{103}Rh[c]	11

NOTES: [a] Shaded isotopes represent the Principal Isotope set selected for burnup credit applications, which is a subset of all isotopes present in SNF. Note that no sample data was available for ^{233}U.

[b] Certain isotopes were omitted from the Three Mile Island sample MCNP calculations for having concentrations less than 0.0001 weight percent in either the measured or calculated composition. Among these were the isotopes ^{151}Eu and ^{242m}Am in the assembly NJ05YU MCNP calculations, and the isotopes ^{151}Eu, ^{242m}Am, ^{95}Mo, ^{99}Tc, ^{101}Ru, and ^{103}Rh in the NJ070G MCNP cases. In addition, the isotopes ^{146}Nd and ^{150}Nd were also omitted since the MCNP cross section libraries for these isotopes were not available, and their concentrations were very small (< 0.1 weight percent) (BSC 2002a, p 75).

[c] No measurements for BWR samples available.

[d] Limerick data not included in this table.

[e] Six samples were combined with ^{243}Cm in measurement.

Source: PWR data: BSC 2002a; BWR data: BSC 2003a.

6.2.1 RCA Data

The method used to determine the Δk_{eff} for RCAs compared to SAS2H calculations is illustrated in Figure 3. All k_{eff} calculations were performed in a waste package geometry corresponding to those illustrated in Attachment I and Attachment IV (BSC 2004a; BSC 2004b; BSC 2004c; BSC 2004d; file "att2.ZIP").

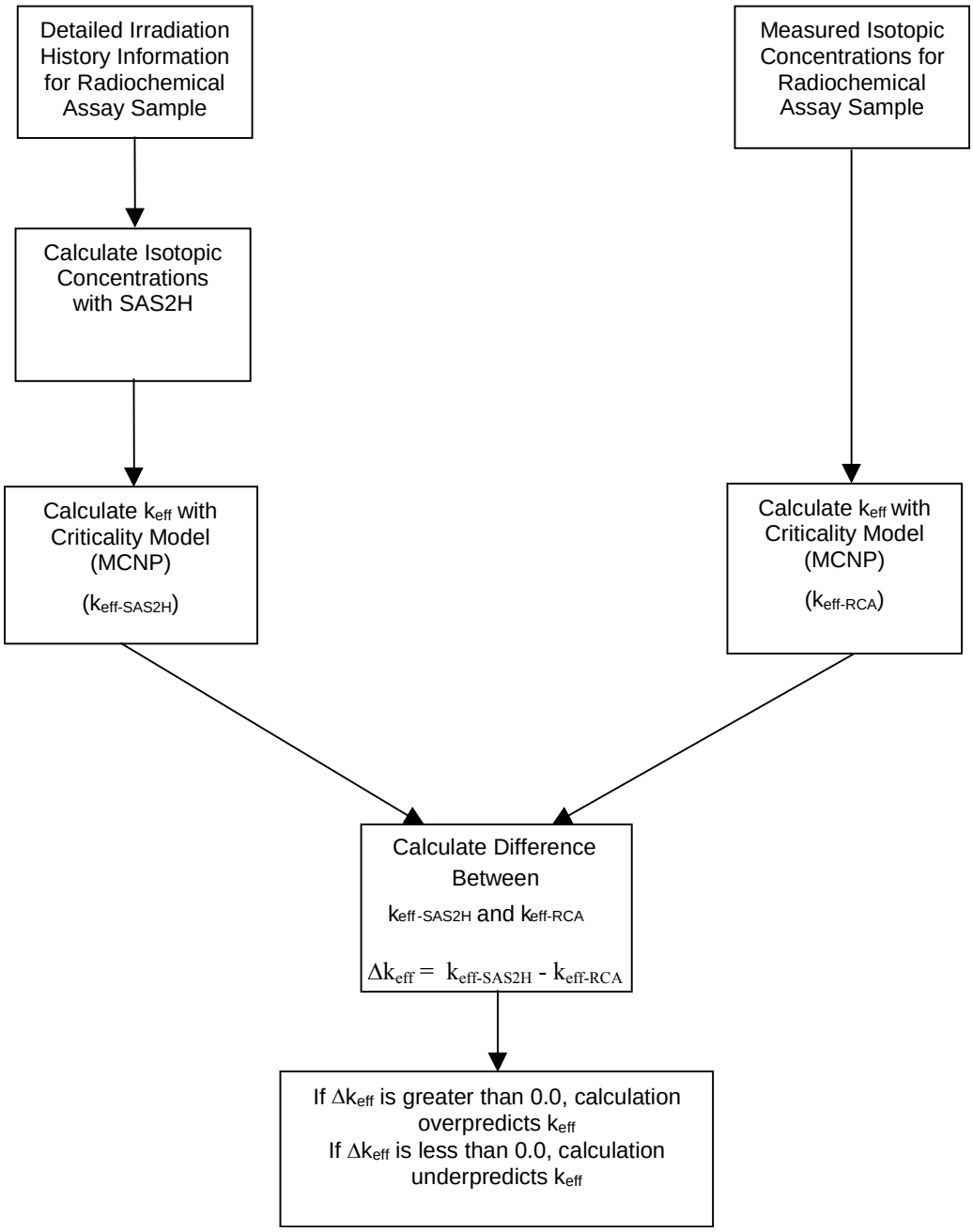


Figure 3. Isotopic Bias and Uncertainty Methodology Calculations

Each RCA data point provides measured isotopic data for a specific fuel rod sample location, and a SAS2H calculation is performed using the irradiation history data for that fuel rod sample location. The Δk_{eff} is the difference between the k_{eff} computed by MCNP using the measured isotopic data and the k_{eff} obtained by MCNP using the SAS2H calculated data. The isotopes used in the SAS2H calculation are limited to those isotopes available from the RCA measurement. The PWR reactivity data were obtained from *Calculation of Isotopic Bias and Uncertainty for PWR Spent Nuclear Fuel* (BSC 2002a, Section 6.2.1) and are presented in

Table 9. The BWR reactivity data were obtained from *Calculation of Isotopic Bias and Uncertainty for BWR SNF* (BSC 2003a, Attachment VI) and are included in Table 9.

Table 9. Reactivity Data for RCAs

RCA Sample	RCA k_{eff}	RCA σ[a]	SAS2H k_{eff}	SAS2H σ	Δk_{eff}[b]
H.B. Robinson Samples					
S1	0.9000	0.0007	0.9037	0.0007	0.0037
S2	0.8428	0.0007	0.8538	0.0006	0.0110
S3	0.8418	0.0007	0.8336	0.0006	-0.0082
S4	0.8036	0.0007	0.8195	0.0006	0.0159
Calvert Cliffs Samples					
S1	0.7826	0.0007	0.7998	0.0006	0.0172
S2	0.7147	0.0005	0.7370	0.0005	0.0223
S3	0.6641	0.0006	0.7041	0.0006	0.0400
S4	0.8658	0.0006	0.8731	0.0007	0.0072
S5	0.8184	0.0005	0.8277	0.0007	0.0093
S6	0.7766	0.0006	0.8005	0.0006	0.0239
S7	0.7336	0.0006	0.7500	0.0005	0.0164
S8	0.7043	0.0006	0.7251	0.0006	0.0208
S9	0.6672	0.0006	0.7001	0.0004	0.0329
Obrigheim Samples					
S1	0.8551	0.0006	0.8699	0.0007	0.0148
S2	0.8463	0.0007	0.8660	0.0006	0.0197
S3	0.8440	0.0006	0.8604	0.0007	0.0164
S4	0.8420	0.0007	0.8584	0.0008	0.0164
S5	0.8392	0.0006	0.8542	0.0007	0.0150
S6	0.8363	0.0007	0.8526	0.0007	0.0163
Trino Vercelles Samples					
S1	0.9694	0.0004	0.9680	0.0004	-0.0014
S2	0.9115	0.0004	0.9140	0.0004	0.0025
S3	0.9053	0.0004	0.9099	0.0004	0.0046
S4	0.9257	0.0004	0.9263	0.0005	0.0006
S5	0.9211	0.0004	0.9213	0.0005	0.0002
S6	0.8914	0.0004	0.8954	0.0004	0.0040
S7	0.8757	0.0004	0.8844	0.0004	0.0087
S8	0.8761	0.0004	0.8802	0.0004	0.0041
S9	0.8816	0.0004	0.8840	0.0004	0.0024
S10	0.8750	0.0004	0.8795	0.0004	0.0045
S11	0.8820	0.0004	0.8839	0.0004	0.0019
S12	0.8749	0.0004	0.8794	0.0004	0.0045
S13	0.8832	0.0004	0.8835	0.0004	0.0003
S14	0.8766	0.0004	0.8799	0.0004	0.0033
Turkey Point Samples					
S1	0.8284	0.0006	0.8288	0.0006	0.0004
S2	0.8275	0.0007	0.8295	0.0006	0.0020
S3	0.8297	0.0007	0.8237	0.0007	-0.0060
S4	0.8286	0.0007	0.8258	0.0007	-0.0028
S5	0.8237	0.0006	0.8258	0.0006	0.0021

Table 9. Reactivity Data for RCAs (Continued)

RCA Sample	RCA k_{eff}	RCA σ[a]	SAS2H k_{eff}	SAS2H σ	Δk_{eff}[b]
Yankee Rowe Samples					
S1	0.7943	0.0004	0.7859	0.0004	-0.0084
S2	0.7667	0.0004	0.7461	0.0004	-0.0206
S3	0.7639	0.0004	0.7436	0.0004	-0.0203
S4	0.7848	0.0004	0.7712	0.0004	-0.0136
S5	0.7613	0.0004	0.7442	0.0004	-0.0171
S6	0.7584	0.0004	0.7430	0.0004	-0.0154
S7	0.7267	0.0004	0.7356	0.0004	0.0089
S8	0.7260	0.0004	0.7345	0.0004	0.0085
Mihama Samples					
S1	1.0129	0.0007	1.0070	0.0008	-0.0059
S2	1.0265	0.0007	1.0200	0.0008	-0.0065
S3	0.9747	0.0007	0.9584	0.0007	-0.0163
S4	0.9362	0.0007	0.9201	0.0007	-0.0161
S5	0.9766	0.0006	0.9647	0.0007	-0.0119
S6	0.8738	0.0007	0.8552	0.0007	-0.0186
S7	0.8666	0.0006	0.8416	0.0007	-0.0250
S8	0.8313	0.0007	0.8300	0.0007	-0.0013
S9	0.8399	0.0006	0.8383	0.0007	-0.0016
Three Mile Island Samples					
YU1	0.7466	0.0006	0.7917	0.0006	0.0451
YU2	0.7450	0.0006	0.7980	0.0006	0.0530
YU3	0.7557	0.0006	0.8027	0.0006	0.0470
YU4	0.7578	0.0006	0.7925	0.0007	0.0347
YU5	0.7738	0.0005	0.8320	0.0006	0.0582
YU6	0.7713	0.0006	0.8087	0.0006	0.0374
YU7	0.7346	0.0005	0.7702	0.0006	0.0356
YU8	0.7222	0.0006	0.7697	0.0006	0.0475
YU9	0.7260	0.0006	0.7787	0.0006	0.0527
YU10	0.7534	0.0006	0.7706	0.0005	0.0172
YU11	0.7514	0.0005	0.7945	0.0006	0.0431
S1	0.9717	0.0007	0.9896	0.0007	0.0179
S2	0.9407	0.0007	0.9702	0.0007	0.0295
S3	0.9622	0.0008	0.9922	0.0007	0.0300
S4	0.9847	0.0007	1.0020	0.0008	0.0173
S5	0.9732	0.0007	0.9891	0.0007	0.0159
S6	0.9964	0.0007	1.0082	0.0008	0.0118
S7	0.9879	0.0008	1.0093	0.0007	0.0214
S8	0.9720	0.0008	0.9903	0.0007	0.0183
Cooper Samples					
C1-Mo	0.74269	0.00057	0.74421	0.00056	0.00152
C2-Mo	0.62824	0.00052	0.64049	0.00050	0.01225
C3-Mo	0.60775	0.00060	0.61936	0.00058	0.01161
C4-Mo	0.76112	0.00063	0.75242	0.00060	-0.00870
C5-Mo	0.69403	0.00052	0.68134	0.00053	-0.01269
C6-Mo	0.64546	0.00058	0.63225	0.00057	-0.01321

Table 9. Reactivity Data for RCAs (Continued)

RCA Sample	RCA k_{eff}	RCA σ[a]	SAS2H k_{eff}	SAS2H σ	Δk_{eff}[b]
Gundremmingen Samples					
G1-Mo	0.54239	0.00055	0.53847	0.00050	-0.00392
G2-Mo	0.57673	0.00055	0.56828	0.00054	-0.00845
G3-Mo	0.61904	0.00052	0.59494	0.00061	-0.02410
G4-Mo	0.59490	0.00060	0.58321	0.00058	-0.01169
G5-Mo	0.56687	0.00054	0.56691	0.00057	0.00004
G6-Mo	0.60008	0.00056	0.59287	0.00062	-0.00721
G7-Mo	0.63762	0.00065	0.61921	0.00059	-0.01841
G8-Mo	0.59852	0.00060	0.60405	0.00052	0.00553
JPDR Samples					
J1-Mo	0.74199	0.00068	0.73809	0.00059	-0.00390
J2-Mo	0.73409	0.00066	0.73271	0.00067	-0.00138
J3-Mo	0.74063	0.00066	0.74143	0.00069	0.00080
J4-Mo	0.73466	0.00058	0.73224	0.00059	-0.00242
J5-Mo	0.71604	0.00060	0.71462	0.00062	-0.00142
J6-Mo	0.71045	0.00064	0.71648	0.00062	0.00603
J7-Mo	0.71615	0.00055	0.71490	0.00060	-0.00125
J8-Mo	0.71373	0.00060	0.71523	0.00059	0.00150
J9-Mo	0.74431	0.00073	0.74311	0.00070	-0.00120
J10-Mo	0.73430	0.00061	0.72975	0.00057	-0.00455
J11-Mo	0.72770	0.00067	0.72207	0.00063	-0.00563
J12-Mo	0.72280	0.00062	0.72047	0.00062	-0.00233
J13-Mo	0.72720	0.00059	0.72646	0.00060	-0.00074
J14-Mo	0.74480	0.00062	0.74277	0.00060	-0.00203
J15-Mo	0.72810	0.00060	0.72593	0.00065	-0.00217
J16-Mo	0.72280	0.00067	0.72248	0.00065	-0.00032

NOTES: [a] Sigma (σ) represents the standard deviation of k_{eff} about the average combined collision, absorption, and track-length estimate due to the Monte Carlo calculation statistics.

[b] $\Delta k_{eff} = k_{eff\text{-}SAS2H} - k_{eff\text{-}RCA}$.

Source: BSC 2002a, Section 6.2.1; BSC 2003a, Attachment VI.

6.2.2 Calculation of Bias and Uncertainty

The bias and uncertainty were evaluated using the method described below, which comes from the critical limit calculation in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Section 3.5.3.2.8). The overall isotopic bias was quantified by calculating Δk_{eff} between MCNP cases with the measured and calculated compositions for a given set of isotopics. The data set cannot be represented by a normal distribution at the 5 percent significance level since the value of the Anderson–Darling test for normality, described in Attachment III, exceeded the critical limit value. Note that the Limerick data were not used in the bias calculation, but are used in Section 6.3.3. Since this data set is not normally distributed, the Distribution-Free Tolerance Limit method is used (YMP 2003, Section 3.5.3.2.9).

The bias and uncertainty is calculated as illustrated in Equation 6.

$$\text{Bias and Uncertainty} = -0.0241 - \sigma_L \quad \text{(Eq. 6)}$$

where

-0.0241 is determined from the one-sided distribution free tolerance limit for 112 data points with 95 percent confidence, corresponding to an index value of 2 from Table A-31 of *Experimental Statistics* (Natrella 1963).

σ_L = the square root of the sum of the squares of the variances for the lower limit as calculated in Equation 7

$$\sigma_L = \sqrt{\sigma_{RCA}^2 + \sigma_{SAS2H}^2} \quad \text{(Eq. 7)}$$

where

σ_{RCA} = the standard deviation of the MCNP calculation using the RCA isotopics

σ_{SAS2H} = the standard deviation of the MCNP calculation using the SAS2H calculated isotopics

Bias and standard deviation values are presented in Table 10. Table 10 shows that on average, the calculated SAS2H isotopics result in MCNP overpredicting k_{eff} relative to values calculated with RCA measured isotopics.

Table 10. Isotopic Bias and Uncertainty Values for RCA Data

Isotope Set	Average Δk_{eff} (bias)	σ_L	Bias and Uncertainty
All Available Isotopes	0.0067	0.00080	-0.0249

This Δk_{eff} value of -0.0249 is the criterion that will be used in Section 8 to determine if the bounding isotopic parameter set is conservative. Thus, if the bounding parameter set produces an increase in k_{eff} greater than 0.0249, the set is conservative.

6.3 ADEQUACY OF ONE-DIMENSIONAL SAS2H

The objective of this section is to demonstrate that the use of the SAS2H point depletion code, ORIGEN-S (part of SCALE code), along with the one-dimensional transport code, XSDRNPM (part of SCALE code), provides an adequate representation of the PWR and older, simpler BWR assembly isotopics. This adequacy is demonstrated by a comparison of results from the SAS2H calculations with results from a transport code, CASMO-3 (referred to as GRCASMO-3), representing the assemblies in two (rectangular) dimensions.

6.3.1 Adequacy of SAS2H for PWR

Table 11 presents a summary of the results of a comparison (BSC 2002b) of the SAS2H code sequence to the GRCASMO-3 isotopic depletion code for the Calvert Cliffs 1 and Turkey Point 2 PWR assays. The measured isotopic concentrations obtained from RCAs discussed in Section 6.2.1 were used as the basis, or standard, for these comparisons.

Table 11. Percentage Difference Between Measured and Calculated Isotopic Inventories

Isotope	Calvert Cliffs Unit 1 SAS2H	Calvert Cliffs Unit 1 GRCASMO-3	Turkey Point Unit 2 SAS2H	Turkey Point Unit 2 GRCASMO-3
^{234}U	-0.6	-12.6	2.2	-10.0
^{235}U	-1.7	-4.3	-1.2	-1.2
^{236}U	2.9	-0.8	2.6	-0.4
^{238}U	-0.7	-0.6	-0.2	-0.02
^{237}Np	3.7	-0.8	[a]	[a]
^{238}Pu	-5.4	-12.2	-2.2	-1.1
^{239}Pu	-13.9	-4.3	4.3	-1.7
^{240}Pu	4.7	-2.1	1.6	-0.4
^{241}Pu	-2.2	-5.1	-0.8	-0.4
^{242}Pu	16.6	-9.0	2.3	-4.8
^{241}AM	-5.3	-9.9	[a]	[a]
^{143}Nd	1.8	0.3	[a]	[a]
^{145}Nd	-0.2	-2.7	[a]	[a]
^{149}SM	-35.5	-33.4	[a]	[a]
^{150}SM	0.0	-5.5	[a]	[a]
^{152}SM	14.9	0.6	[a]	[a]
^{153}EU	0.8	-0.2	[a]	[a]

NOTES: [a] Measurement not made for this isotope.

Percentage difference calculated as follows: $100 \times (C/M-1)$ where C represents calculated value, and M is measured value.

Source: BSC 2002b, p. 4-58.

Review of the comparison table shows good agreement for the better-known actinides of ^{235}U, ^{236}U, and ^{238}U. SAS2H more accurately predicts the ^{235}U contents, while GRCASMO-3 is better at predictions of ^{239}Pu. The prediction of ^{242}Pu is challenging for depletion codes due to the number of neutron captures required to produce this heavy isotope, but the actual quantity of ^{242}Pu in SNF is relatively small.

The code-to-code comparison may also be expressed in terms of the difference in k_∞ (infinite multiplication factor) caused by the difference in calculated isotopic concentrations. Table 12 illustrates this comparison and shows that only a small change in k_∞ results from substantial variations in isotopic composition of the fission products. This is because the fission products are strong thermal neutron absorbers, and the thermal neutron population in a fuel pellet is depressed due to the self-shielding effect. A variation in fission product absorbers thus does not

manifest as large a change in k_∞ because there is relatively little of the neutron population to affect.

Table 12. MCNP Calculated k_∞ for Measured and Predicted Isotopic Inventories

	k∞	Error	Difference in k∞ (measured - calculated isotopics)
Calvert Cliffs - measured	1.05628	0.00104	0
Calvert Cliffs - SAS2H	1.04204	0.00114	+0.01424
Calvert Cliffs - GRCASMO3	1.05718	0.00116	-0.00090
Turkey Point - measured	1.09378	0.00110	0
Turkey Point - SAS2H	1.09524	0.00114	-0.00146
Turkey Point - GRCASMO3	1.08924	0.00110	+0.00454

Source: BSC 2002b, p. 4-59.

Overall, the SAS2H-calculated isotopics produce k_∞ values that match measured values nearly as well as do the GRCASMO-3 calculated values.

These results demonstrate that the one-dimensional SAS2H performs as well as the two–dimensional GRCASMO-3 in calculating the isotopic inventory for commercial PWR SNF.

6.3.2 Adequacy of SAS2H for BWR

The GRCASMO-3 code was also used for a comparison of BWR calculations performed using SAS2H (BSC 2002b). The study investigated irradiation histories that had control blades both inserted and withdrawn for Grand Gulf and Quad Cities assemblies, respectively. The Grand Gulf analyses with blades inserted are presented in this document. Table 13 shows the reactivity comparison between SAS2H and GRCASMO-3 analyses as a function of axial position within the fuel assembly. Inspection of the table shows that the difference between the one–dimensional SAS2H code and two-dimensional GRCASMO-3 code averages -2.4 percent over the entire length of the fuel assembly. The difference is -3.1 percent at the most reactive position (node 9, at the upper end of the fuel assembly where the steam is drier). This level of agreement between the two codes for BWRs, combined with that for the PWR comparisons, (Section 6.3.1) indicates that the one dimensional code representation is adequate.

Table 13. Results of 1-D/2-D Comparisons Using GRCASMO3 and SAS2H

Node	EOL BU (10-node case)	GRCASMO3 (10-node-axial format)		SAS2H			
		k_{inf}	σ	k_{inf}	σ	Δk_{inf} [a]	% Δk_{inf} [b]
GG1 – Type G (controlled)							
1	7.50	0.7110	0.0003	0.7266	0.0004	0.0156	2.2%
2	35.02	0.9457	0.0005	0.9753	0.0004	0.0296	3.1%
3	42.39	0.8951	0.0005	0.9209	0.0004	0.0258	2.9%
4	43.87	0.9178	0.0005	0.9308	0.0005	0.0130	1.4%
5	44.43	0.9506	0.0005	0.9537	0.0005	0.0032	0.3%
6	42.62	0.9862	0.0005	0.9801	0.0005	-0.0061	-0.6%
7	38.93	1.0267	0.0005	1.0115	0.0005	-0.0153	-1.5%
8	34.15	1.0476	0.0005	0.9980	0.0005	-0.0495	-4.7%
9	27.89	1.0822	0.0005	1.0491	0.0005	-0.0330	-3.1%
10	9.42	0.7778	0.0004	0.7593	0.0004	-0.0185	-2.4%
						Mean	-0.24%

NOTES: [a] $\Delta k_{inf} = k_{SAS2H} - k_{GRCASMO3}$. The MCNP related standard deviation on all Δk_{inf} values was less than 0.0008.

[b] % $\Delta k_{inf} = 100\ \Delta k_{inf}/k_{GRCASMO3}$.

Source: BSC 2002b, Table 4-10.

6.3.3 Performance of SAS2H for Modern, Complex BWR SNF

GE has made substantial changes to the fuel design of BWR assemblies in order to improve the utilization of the more expensive, more highly enriched, fuel materials that are needed to attain the longer operational cycles desired in the 1990s and later. These changes include fuel enrichments over 4 weight percent ^{235}U in the inner zone of the assembly and the inclusion of substantial amounts of Gadolinia to provide adequate shutdown margin for the more highly enriched fuel. Gadolinium, in the form of Gd_2O_3, is added to a UO_2 fuel rod to reduce the reactivity of the fuel assembly during the early part of its operational life. The Gd is essentially burned out of the rods when the fuel has attained a 10 GWd/MTU burnup. Rods that contained Gd posses higher ^{235}U and ^{239}Pu concentrations than UO_2-only rods, at this point in the fuel assemblies operational history, due to the decrease in thermal neutron fluence in the Gd rods. The overall effect is to substantially alter the isotopic constituents of the Gd rods compared to UO_2-only rods and cause strong gradients in the flux between adjacent fuel rods of different types. Modern BWR assemblies may also contain part-length fuel rods that further complicate the isotopic behavior as the moderator density near these rods is different from the full-length rods.

A comparison of SAS2H isotopic calculations versus radiochemistry assays was performed for the modern GE-11 assembly (BSC 2003c). The results, shown in Table 14, indicate poor agreement for the ^{235}U and ^{239}Pu concentrations, with samples showing differences ranging from approximately –40 percent to +30 percent in ^{235}U concentration. Disagreement of this magnitude indicates a breakdown of the assumptions upon which SAS2H is based, that is, that the fuel assembly behaves in a homogenous fashion. Manipulation of the mathematical representation of the Path B portion of the SAS2H input is not sufficient to improve the agreement between

SAS2H calculations and measurements for the Limerick fuel, and the range of applicability for SAS2H for BWRs is thus limited to older, simpler fuel that behaves in a nearly homogenous fashion. Such complex fuel requires a two-dimensional code that can provide isotopics on an individual-rod basis.

Table 14. Assembly YJ1433 Sample Percent Differences

Sample	D8-3D2B	D8-4G3	D9-1D2	D9 2D2	D9 4D4	D9-4G1E1	H5-3A1C	H5-3A1G
Node	15	23	6	11	18	22	15	16
Isotope	(Calculated Concentration – Measured Concentration) × 100/Measured Concentration							
^{234}U	-7.42	1.29	-2.46	-4.58	-9.08	-7.70	-4.15	-4.18
^{235}U	-38.29	-24.06	25.07	8.82	-37.71	-28.20	-14.78	-13.97
^{236}U	-2.49	-0.48	1.92	2.65	2.09	2.60	-0.94	-0.87
^{238}Pu	1.43	-26.51	6.86	4.77	-15.10	-14.99	-8.79	-7.94
^{239}Pu	-11.15	-24.83	9.69	3.68	-21.40	-21.08	-13.45	-12.61
^{240}Pu	-4.36	-9.15	6.73	5.41	-2.40	-0.61	-4.82	-4.45
^{241}Pu	-8.47	-24.75	6.69	1.08	-22.65	-22.43	-10.29	-9.08
^{242}Pu	26.02	0.81	4.32	5.53	8.91	3.71	14.98	16.01
^{143}Nd	1.81	-1.76	17.36	12.49	-5.83	-2.60	2.67	3.34
^{145}Nd	11.07	5.39	6.10	5.92	5.20	5.05	6.22	5.97
^{146}Nd	13.67	3.25	4.98	5.48	6.52	5.14	4.42	5.05
^{148}Nd	11.06	2.56	4.45	4.56	4.14	3.32	4.09	4.23
^{150}Nd	12.60	0.85	7.05	6.68	5.48	3.69	4.77	5.26
^{134}Cs	6.17	-12.86	7.08	0.38	-1.25	1.99	-6.14	-5.27
^{137}Cs	9.75	1.61	9.55	6.62	9.30	11.13	4.24	4.60
^{151}Eu	10.62	-8.73	40.03	41.64	10.99	4.64	13.44	14.05
^{153}Eu	22.21	1.03	20.23	20.06	19.85	9.35	17.11	16.76
^{155}Eu	-16.92	-32.15	-14.57	-16.91	-18.27	-24.57	-20.45	-20.34
^{147}Sm	-3.55	3.42	1.86	-1.82	-1.71	-4.11	-1.72	-2.58
^{149}Sm	-8.41	-24.92	33.99	11.94	-14.44	-15.57	-8.47	-6.67
^{150}Sm	9.32	1.64	9.52	7.22	5.12	2.19	3.68	4.34
^{151}Sm	16.04	-5.42	41.50	37.36	7.96	4.97	12.84	15.72
^{152}Sm	46.44	35.72	33.68	38.76	48.12	38.11	46.94	47.24
^{155}Gd	-52.11	-67.61	-24.62	-26.59	-33.28	-33.56	-35.12	-30.99
^{241}Am	-10.07	-23.16	9.22	11.64	-22.54	-21.54	-7.02	-7.23
^{241m}Am	6.60	-19.25	48.26	55.83	-13.22	-15.18	7.19	6.32
^{243}Am	40.41	-3.71	22.30	30.55	13.12	9.33	27.68	26.81
^{237}Np	-3.74	-15.62	0.35	-2.91	-11.25	-13.96	-5.47	-5.46
^{95}Mo	3.72	-3.51	-1.04	3.47	6.37	2.97	3.81	3.58
^{99}Tc	8.87	0.17	6.35	12.66	8.18	17.11	13.64	17.20
^{101}Ru	11.07	0.23	1.11	5.44	7.09	2.97	6.51	3.13
^{103}Rh	-3.23	-10.73	1.78	1.88	-9.12	-8.15	-3.34	-7.10
^{109}Ag	13.10	-7.30	28.02	31.71	24.95	32.60	28.78	14.01
^{242}Cm	-4.01	-24.12	23.20	35.45	-15.68	-22.24	0.34	14.86
^{243}Cm	-14.65	-41.90	4.53	-1.57	-31.90	-32.31	-20.11	-22.32
^{244}Cm	27.45	-30.14	8.31	19.07	0.45	-7.46	3.40	3.16
^{245}Cm	-35.88	-69.04	-29.19	-27.70	-53.86	-54.28	-50.70	-49.38

Source: BSC 2003c, p. 32.

Table 15 presents a comparison of reactivities for the Limerick RCAs versus SAS2H calculations. The RCA reactivities are calculated using the measured isotopic composition, and the SAS2H reactivities are obtained by using the isotopic compositions calculated by SAS2H.

Table 15. MCNP Results for Limerick Spent Nuclear Fuel Samples

Sample #	Sample ID	RCA[a]			SAS2H[b]			Delta (SAS2H - RCA)[c]	
		k_{eff}	σ	AENCF	k_{eff}	σ	AENCF	Δk_{eff}	σ[d]
1	D8–3D2B	0.55913	0.00052	0.304	0.51709	0.00045	0.330	-0.04204	0.00069
2	D8–4G3	0.63515	0.00052	0.259	0.57645	0.00049	0.279	-0.05870	0.00071
3	D9–1D2	0.46612	0.00044	0.369	0.48665	0.00041	0.351	0.02053	0.00060
4	D9–2D2	0.50712	0.00047	0.339	0.51048	0.00043	0.335	0.00336	0.00064
5	D9–4D4	0.53262	0.00049	0.324	0.46549	0.00041	0.361	-0.06713	0.00064
6	D9–4G1E1	0.56781	0.00048	0.299	0.50364	0.00048	0.331	-0.06417	0.00068
7	H5–3A1C	0.58889	0.00047	0.290	0.5552	0.00042	0.305	-0.03369	0.00063
8	H5–3A1G	0.59134	0.00051	0.291	0.55936	0.00050	0.304	-0.03198	0.00071

NOTES: [a]Results based on measured compositions of spent nuclear fuel samples.

[b]Results based on SAS2H calculated compositions using reactor operating history information adjusted to yield the sample measured burnup.

[c]Values reported were calculated from MCNP reported values which lists results out to five significant digits, therefore computing delta values from table values will introduce some roundoff error.

[d]Delta σ value equals the square root of the sum of the squared σ values for RCAs and SAS2H.

Source: BSC 2003c, Table 6-2.

Inspection of Table 15 shows that the difference in reactivity between SAS2H and RCA isotopics for modern, complex BWR assemblies can be greater than six percent, substantially larger than the 2.4 percent mean difference for the older, simpler assemblies. The underprediction of reactivity due to the overprediction of ^{235}U depletion are greater than the typical administrative margin for preclosure criticality safety, so the range of applicability for the LWR Isotopic calculation is limited to older, simpler BWR assemblies that predate the GE-11 design.

A possible approach to allow the use of SAS2H for calculations for complex BWR SNF would be to use a two or three dimensional code to adjust the SAS2H Path B models, so that conservative results would be produced for modern, complex BWR assembly designs. This approach could also be effective for PWR fuel designs that are evolving which have fuel rods containing neutron absorbers.

6.4 SAS2H DEPLETION PARAMETERS

The objective of this section is to evaluate the effects of several important depletion parameters on SNF reactivity, to provide guidance for the selection of bounding parameters. This section evaluates how certain parameters affect isotopic production and decay during the calculated fuel depletion associated with PWR and BWR fuel assemblies. The scope of this calculation covers an initial enrichment range of 2.0 through 5.0 weight percent ^{235}U and a burnup range of 10 through 50 GWd/MTU. In many cases, the PWR and BWR assemblies behave in the same

fashion, so only the behavior of one assembly type is illustrated in the figures. Some parameters are specific to only PWRs or BWRs, and not both, and for such parameters the appropriate fuel type is described.

A set of PWR depletion parameters chosen based on typical reactor operating values was used for the sensitivity variations, as described in *PWR Depletion Parameter Sensitivity Evaluation* (BSC 2001). The PWR base case parameters are provided in Table 16. The moderator material specification contains soluble boron. An infinite lattice of fuel was used for all calculations, and results were normalized to the average value of k_∞ of each data series.

Table 16. SAS2H Sensitivity Study PWR Base Case Depletion Parameters

Parameter	Base Value
Fuel Temperature	1000 K
Boron Concentration	940.6 ppm
Specific Power	30 MW/MTU
Moderator Temperature	625 °F (602.6 K) @2200 psig
UO_2 Fuel Density[a]	10.121 g/cm^3

NOTE: [a] Calculated by dividing fuel mass by fuel volume where a uranium mass of 463.63 kg was used with a fuel height of 360.162 cm, and a pellet diameter of 0.9398 cm (Punatar 2001, pp. 2-5 and 3-1).

psig = pound per square inch guage

Source: BSC 2001, Table 2.

A set of BWR depletion parameters, chosen to represent typical reactor operating values, was used for the BWR sensitivity variations, as described in *BWR Depletion Parameter Sensitivity Evaluation* (Anderson 2003). The BWR base case parameters are provided in Table 17. The moderator material specification does not contain soluble boron, and the moderator density is an average of the density along the fuel length. Results were normalized to the nominal value of k_∞ of each data series.

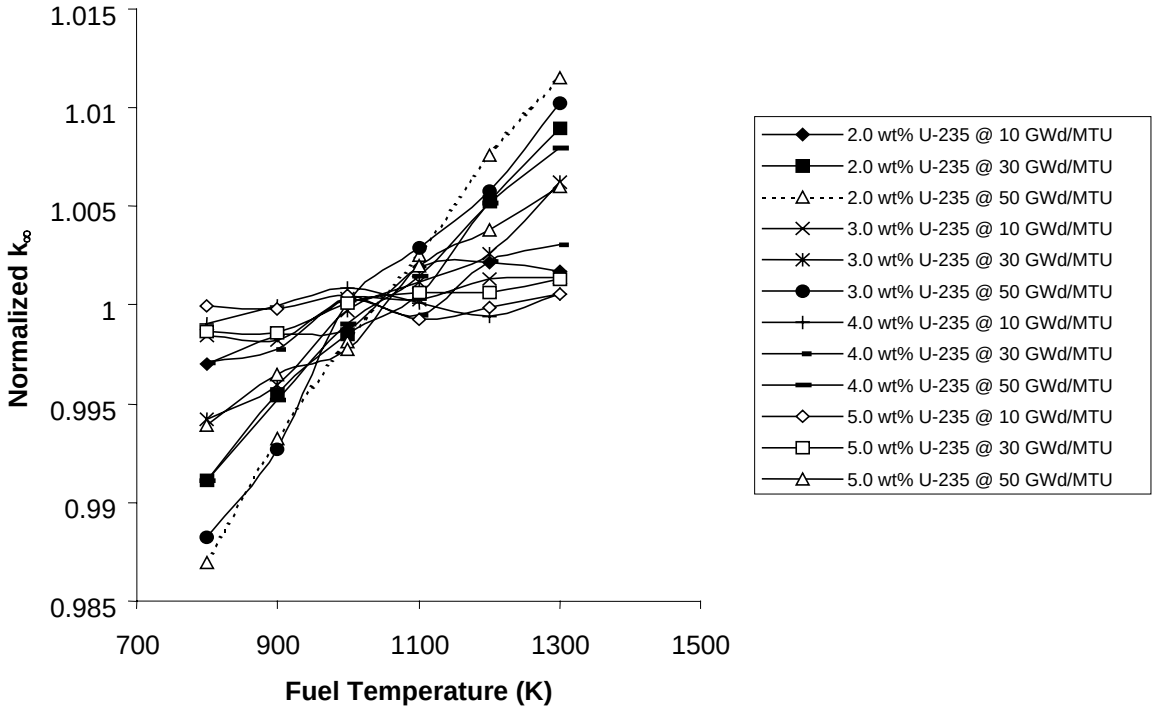
Table 17. SAS2H Sensitivity Study BWR Base Case Depletion Parameters

Parameter	Nominal Value	Source
Assembly type	8×8 BWR	(Anderson 2003, Section 5.1)
Fuel Temperature	1000 °F	(Anderson 2003, Section 6.1)
Moderator Density	0.43 g/cm^3	(Anderson 2003, Section 6.1)
Burnup	10-50 GWd/MTU	(Anderson 2003, Section 6.1)
Moderator Temperature	560.7 K	(Wimmer 2004, p. 17)
UO_2 Fuel Density	9.785 g/cm^3	(Anderson 2003, Section 6.1)
Gadolinia Rods	8 rods at 5.0 weight percent	(Anderson 2003, Section 6.1)
Control Blades	Fully Inserted or Withdrawn	(Anderson 2003, Section 6.1)

All results are presented for isotopics after a 5-year cooling time since this value is the required minimum cooling time of SNF stated in 10 CFR 961.11 (Appendix E).

6.4.1 Fuel Temperature Effects for PWRs and BWRs

The fuel temperature effects were evaluated in order to determine the sensitivity of Doppler broadening of primarily the ^{238}U resonance absorption cross section. Normalized k_∞ values are graphically illustrated in Figure 4. Values were normalized to the nominal k of each burnup/enrichment pair. PWR assemblies were evaluated, but the fuel temperature effects should be the same for BWRs because the ^{238}U resonance effects are the same.



Source: BSC 2001, p. 39.

Figure 4. Fuel Temperature Results

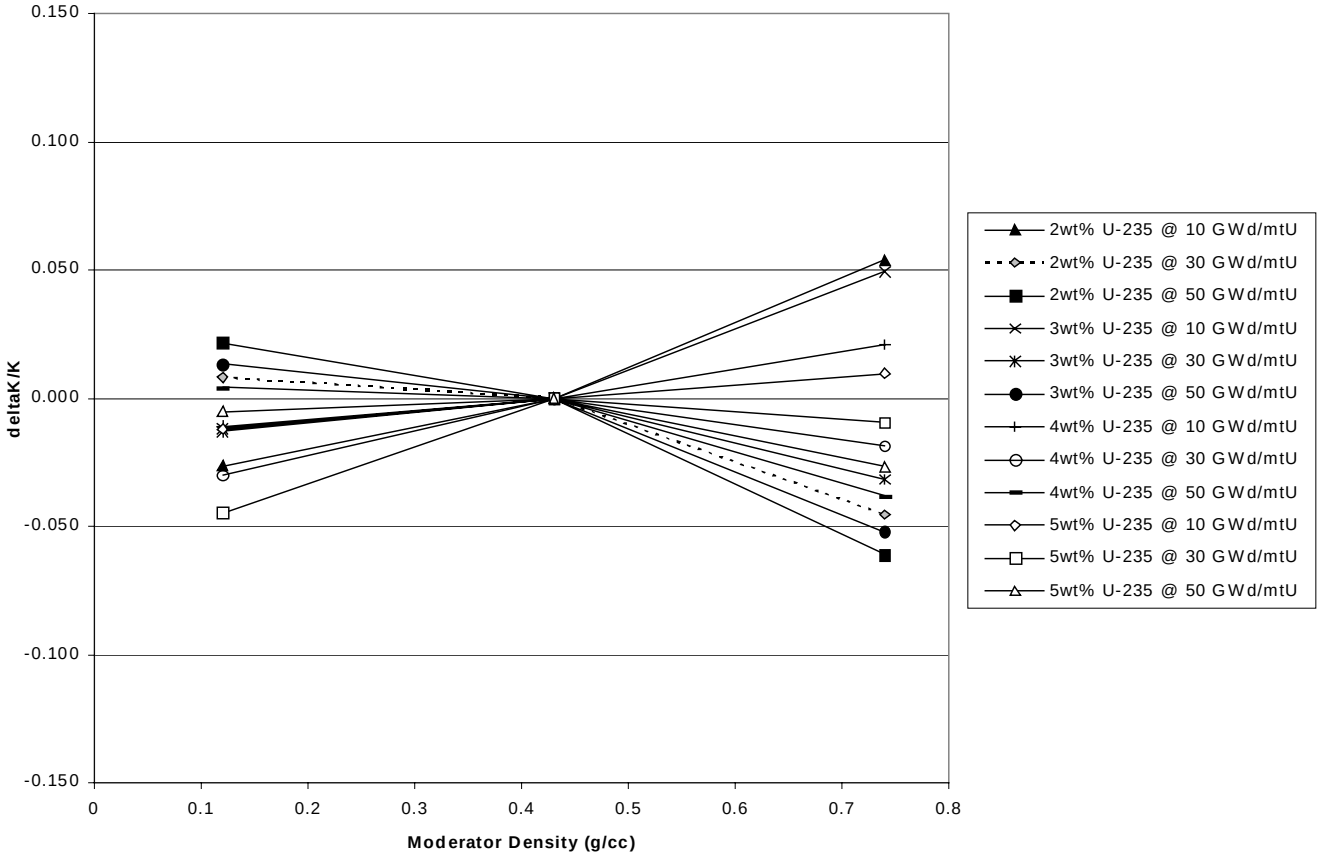
Inspection of the figure shows that the fuel pellet temperature may have a substantial effect upon the calculated reactivity of SNF. Higher fuel temperature results in a greater discharge reactivity.

6.4.2 Moderator Temperature and Density Effects

6.4.2.1 Moderator Density Effects for BWRs

The moderator density sensitivity effects were evaluated in order to determine the sensitivity of moderation primarily affecting the neutron energy spectrum. This set of cases was performed in order to independently evaluate the spectral effects from moderator density changes.

Normalized k_∞ values are graphically illustrated in Figure 5. Values were normalized to the nominal k_∞ of each burnup/enrichment pair.



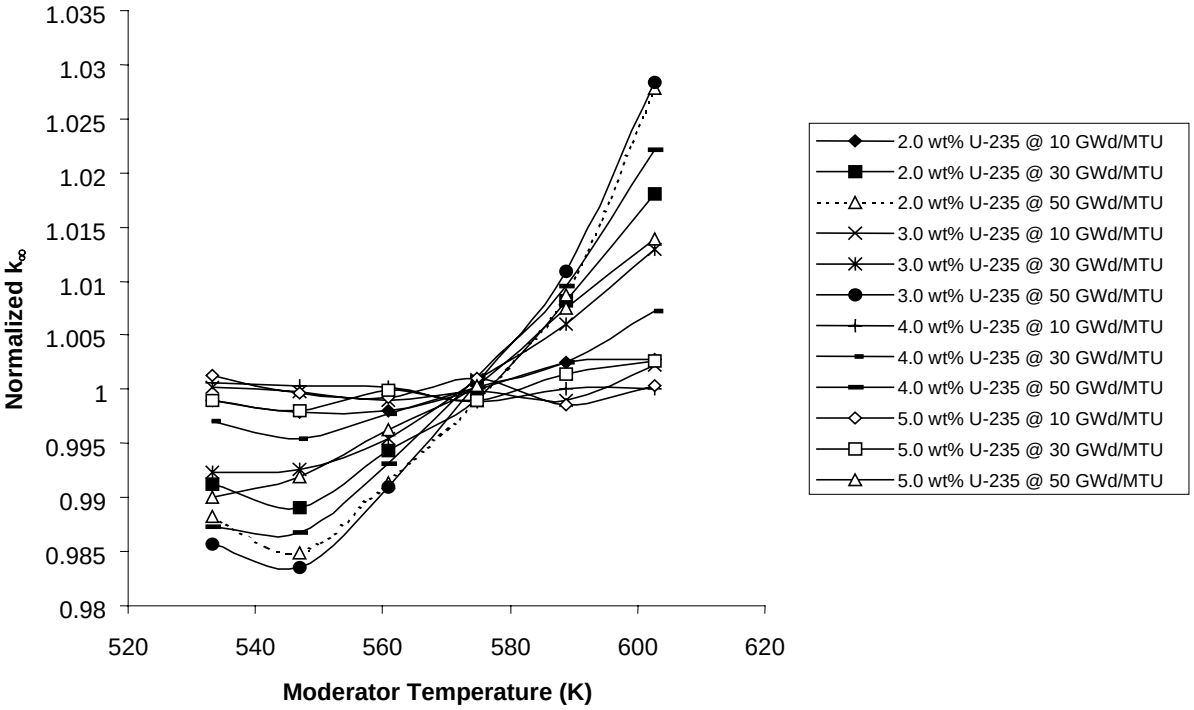
Source: Anderson 2003, p. 17, Figure 3.

Figure 5. BWR Moderator Density Effects with No Soluble Boron

Inspection of the figure shows that the moderator density may have a substantial effect upon the calculated reactivity of SNF. Lower moderator density generally results in greater discharge reactivity.

6.4.2.2 Nominal Borated Moderator for PWRs

The moderator temperature sensitivity effects were evaluated in order to determine the sensitivity of moderation primarily affecting the neutron energy spectrum. This case was performed with nominal borated moderator present in order to evaluate the spectral effects from moderator density changes. Normalized k_∞ values are graphically illustrated in Figure 6. Values were normalized to the average k_∞ of each burnup/enrichment pair.



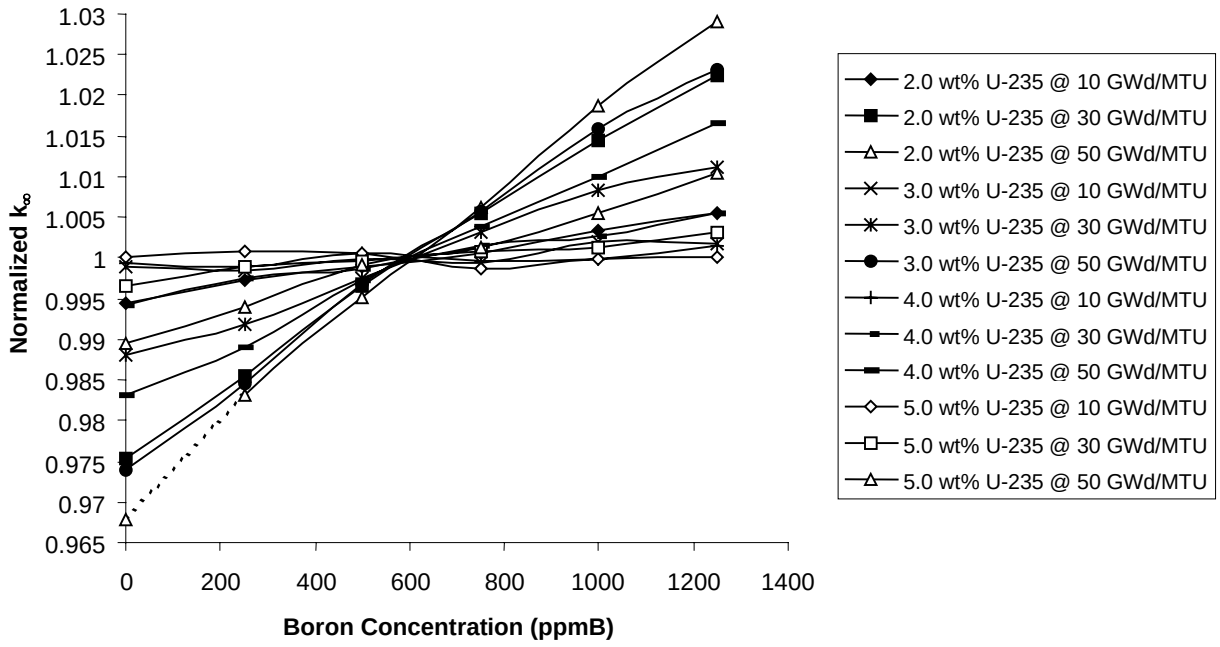
Source: BSC 2001, p. 44.

Figure 6. Moderator Temperature Effects

Inspection of the figure shows that the borated water moderator temperature may have a substantial effect upon the calculated reactivity of SNF.

6.4.3 Borated Moderator Concentration Effects for PWRs

The boron concentration sensitivity effects were evaluated in order to determine the sensitivity of the boron concentration primarily affecting the neutron energy spectrum. Normalized k_∞ values are graphically illustrated in Figure 7. Values were normalized to the average k_∞ of each burnup/enrichment pair.



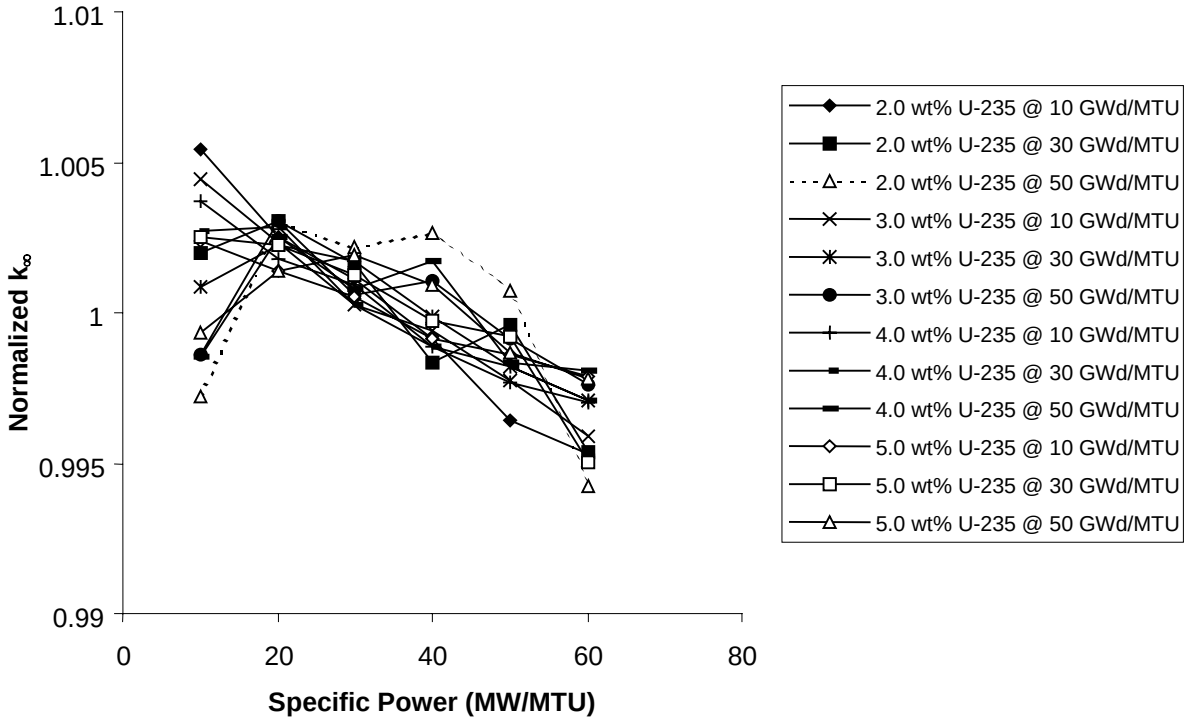
Source: BSC 2001, p. 46.

Figure 7. Boron Concentration Effects

Inspection of the figure shows that the boron concentration of the water moderator may have a substantial effect upon the calculated reactivity of SNF. Higher dissolved boron concentrations result in a greater reactivity.

6.4.4 Specific Power Effects for PWRs and BWRs

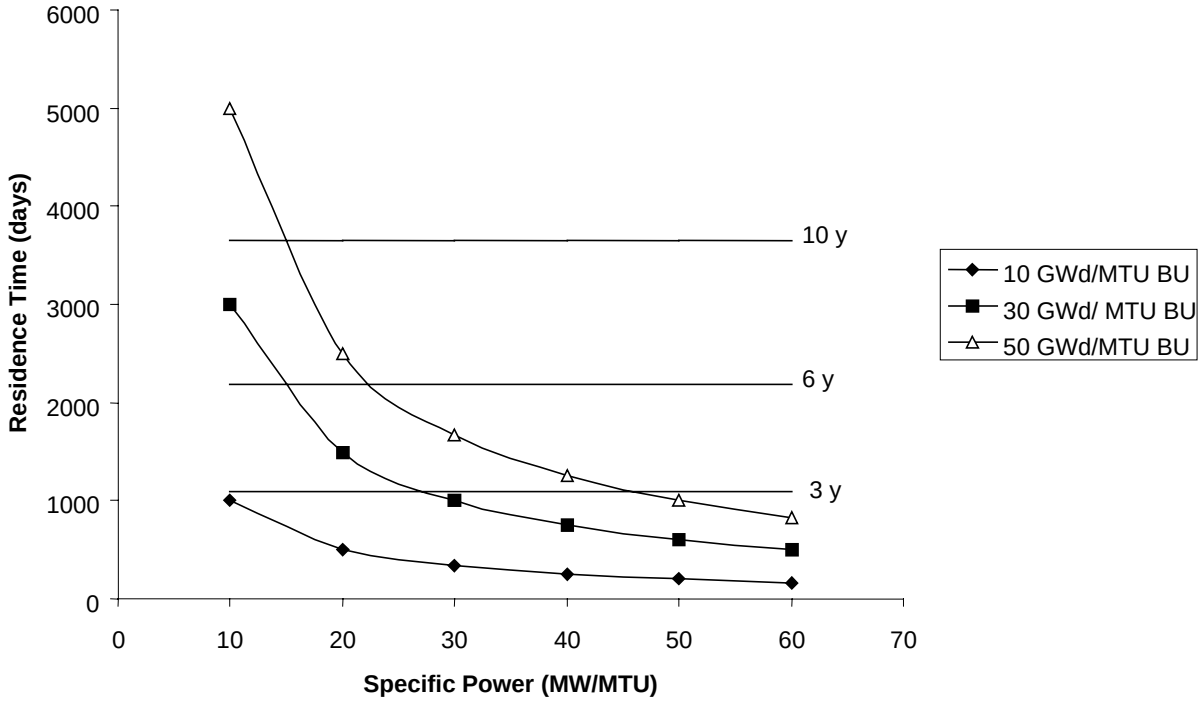
The specific power depletion parameter is being evaluated in order to determine the sensitivity of the irradiation time on the production and decay of isotopes as the fuel is being irradiated. Normalized k_∞ values are graphically illustrated in Figure 8. Values were normalized to the average k_∞ of each burnup/enrichment pair. PWR fuel assemblies were evaluated but the specific power effects should be the same for PWR and BWR because the production and decay of isotopes are the same.



Source: BSC 2001, p. 49.

Figure 8. Specific Power Effects

The results show that specific power has a weak effect upon reactivity. Lower specific power values (down to about 20 MW/MTU) result in a greater reactivity. Specific power values below 20 MW/MTU are not economical because the power plant could not produce its rated power. A specific power of 30 MW/MTU allows a PWR fuel assembly to achieve a desired target burnup of 30 GWd/MTU in about three years, which is a typical cycle length for earlier fuel cycles, as shown in Figure 9. BWR specific powers are typically less due to the effect of boiling in the fuel assembly, thus specific powers as low as 20 MW/MTU may appear. Thus, lower specific power values are chosen for the bounding depletion parameter. Specific power effects are the same for PWR SNF and BWR SNF, since the specific power is related to the time needed to produce energy from low-enriched uranium, and the build-up and decay of radionuclides is the same for both reactor types.



Source: BSC 2001, p. 49.

Figure 9. Time Required to Achieve Target Burnup versus Specific Power

6.4.5 Homogenized Spacer Grid Effects for PWRs and BWRs

The homogenization of spacer grid material effects were evaluated in order to determine their effects on neutron energy spectrum. The intermediate spacer grids were homogenized in the moderator composition based on the volume fraction of spacer grids in the moderator from *Summary Report of Commercial Reactor Criticality Data for Crystal River Unit 3* (Punatar 2001, p. 2-6). Inconel spacer grids were used for the base case depletions. These results demonstrate the effects of homogenized spacer grids mixed throughout the moderator versus no spacer grids. The results of the sensitivity cases are presented in Table 18. PWR fuel assemblies were evaluated but the effect of spacers on PWRs and BWRs is probably the same since the spacers are quite similar in the two fuel types.

The tabulated k_∞ differences indicate that the spacer grids have an effect upon the calculated reactivity of SNF. If the spacer grids are included in the geometric description of the fuel assembly, they must be included for both nominal and bounding calculations. If not, then the spacer grids must be omitted from both nominal and bounding calculations.

Table 18. Homogenized Spacer k_∞ Sensitivity Results with 5-Year Cooling Time

Wt% ^{235}U	Burnup/ Homogenized Spacer?	10 GWd/MTU	σ[a]	30 GWd/MTU	σ	50 GWd/MTU	σ
2.0	Yes	1.13878	0.00075	0.92962	0.00073	0.83151	0.00069
	No	1.14198	0.00067	0.94715	0.0008	0.85286	0.00071
	Δk_∞ (yes-no)	-0.0032		-0.0175		-0.0214	
3.0	Yes	1.26046	0.00082	1.04617	0.00081	0.89194	0.00069
	No	1.26185	0.0009	1.05551	0.00084	0.91088	0.00076
	Δk_∞ (yes-no)	-0.0014		-0.0093		-0.0189	
4.0	Yes	1.33795	0.00085	1.14542	0.00083	0.97507	0.00082
	No	1.33943	0.00086	1.15016	0.00079	0.99163	0.00083
	Δk_∞ (yes-no)	-0.0015		-0.0047		-0.0166	
5.0	Yes	1.39132	0.00078	1.22081	0.00085	1.05888	0.00082
	No	1.39217	0.00079	1.22598	0.00088	1.07206	0.00082
	Δk_∞ (yes-no)	-0.0009		-0.0052		-0.0132	

NOTE: [a]Sigma (σ) represents the standard deviation of k_∞ about the average combined collision, absorption, and track-length estimate due to the Monte Carlo calculation statistics.

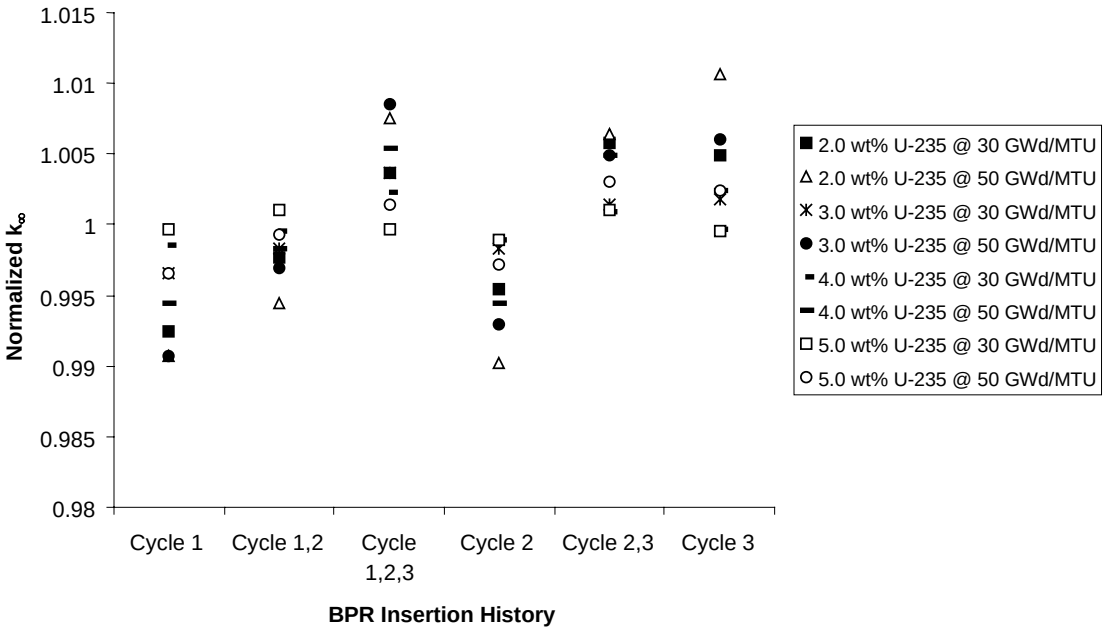
Source: BSC 2001, p. 50.

6.4.6 Burnable Poison Rod Assembly Insertion Effects for PWRs

The burnable poison rod insertion history depletion parameter is being evaluated in order to determine the sensitivity of the depletion calculation to the spectral hardening and shifting with time caused by burnable poison rod insertion and subsequent depletion. In order to determine the effects of the changes in spectrum over time, sets of cases where the burnable poison rod insertion history was varied were performed. Normalized k_∞ values are graphically illustrated in Figure 10. Values were normalized to the average k_∞ of each burnup/enrichment pair.

Figure 10 shows that the effect of burnable poison rods is maximized if the rods are present in cycles one through three of operation. The effect is less if the burnable poison rod is present for only two cycles (cycles 1 and 2 or cycles 2 and 3). The effect is minimized if the burnable poison rod is only present for one cycle (cycle 1 or cycle 2). Insertion of the rod for only the third cycle has a strong effect because plutonium creation and burning is greatest during the final cycle.

The isotopic calculation process may be used for PWR fuel with or without burnable poison rods. In either case, the test for conservatism of the bounding parameters is the same.



Source: BSC 2001, p. 53.

Figure 10. Burnable Poison Rod Insertion History Effects

6.4.7 Depletion Time Step Results for PWRs and BWRs

The depletion time step lengths were varied in order to determine the effects that flux weighted cross section library updating frequency has on the generation of SNF isotopics. In order to determine the effects of the changes in spectrum over time, sets of cases where the cross section library update frequency was varied, were performed and the reactivity was calculated. The reactivity results are presented in Table 19.

Generally, a depletion time step length has a small effect on system reactivity, especially at lower burnups. Therefore, a time step length of less than 80 days provides adequate cross section update frequency for SAS2H runs. PWR assemblies were evaluated but the effects should be the same for PWRs and BWRs because the time dependence of isotopic precursors is the same.

Table 19. Depletion Time Step k_∞ Sensitivity Results

Burnup (GWd/ MTU)	Time Step Length (days)	2.0 Wt% ^{235}U		3.0 Wt% ^{235}U		4.0 Wt% ^{235}U		5.0 Wt% ^{235}U	
		k_∞	σ[a]	k_∞	σ	k_∞	σ	k_∞	σ
10	37.037	1.15116	0.00068	1.26439	0.00079	1.33662	0.00078	1.39196	0.0008
	55.556	1.15075	0.00076	1.26473	0.00072	1.33855	0.0007	1.39145	0.00082
	83.333	1.15162	0.00079	1.26647	0.00073	1.33877	0.00081	1.39189	0.00078
	111.111	1.14928	0.00075	1.26528	0.0007	1.3399	0.00075	1.39113	0.00079
	166.667	1.14888	0.00079	1.26394	0.00077	1.34043	0.00081	1.3927	0.0008
	333.333	1.14924	0.00071	1.26421	0.00078	1.33957	0.00077	1.39039	0.00078
30	40	0.97275	0.00075	1.07252	0.00081	1.15912	0.00079	1.22704	0.00076
	76.923	0.97174	0.0009	1.07231	0.00076	1.15977	0.00089	1.22908	0.00085
	111.111	0.96795	0.00083	1.06943	0.0008	1.15717	0.00084	1.22827	0.00091
	166.667	0.96901	0.00076	1.07035	0.00072	1.15812	0.00097	1.22831	0.00078
	333.333	0.96618	0.00076	1.07165	0.00087	1.15848	0.00087	1.22811	0.00093
	500	0.96506	0.00074	1.06833	0.00079	1.16004	0.00092	1.22982	0.00081
50	39.683	0.88146	0.00074	0.93587	0.00081	1.00869	0.00079	1.08318	0.00096
	79.365	0.8825	0.00078	0.93876	0.00085	1.00882	0.00078	1.07881	0.00081
	151.515	0.8788	0.00063	0.93313	0.00069	1.00557	0.00084	1.07927	0.00089
	208.333	0.87706	0.00082	0.93288	0.00071	1.00737	0.00089	1.08037	0.00087
	333.333	0.87464	0.00077	0.93546	0.00078	1.009	0.00086	1.08031	0.00085
	555.556	0.87087	0.0008	0.93309	0.00066	1.00859	0.00087	1.08308	0.00079

NOTE: [a]Sigma (σ) represents the standard deviation of k_{eff} about the average combined collision, absorption, and track-length estimate due to the Monte Carlo calculation statistics.

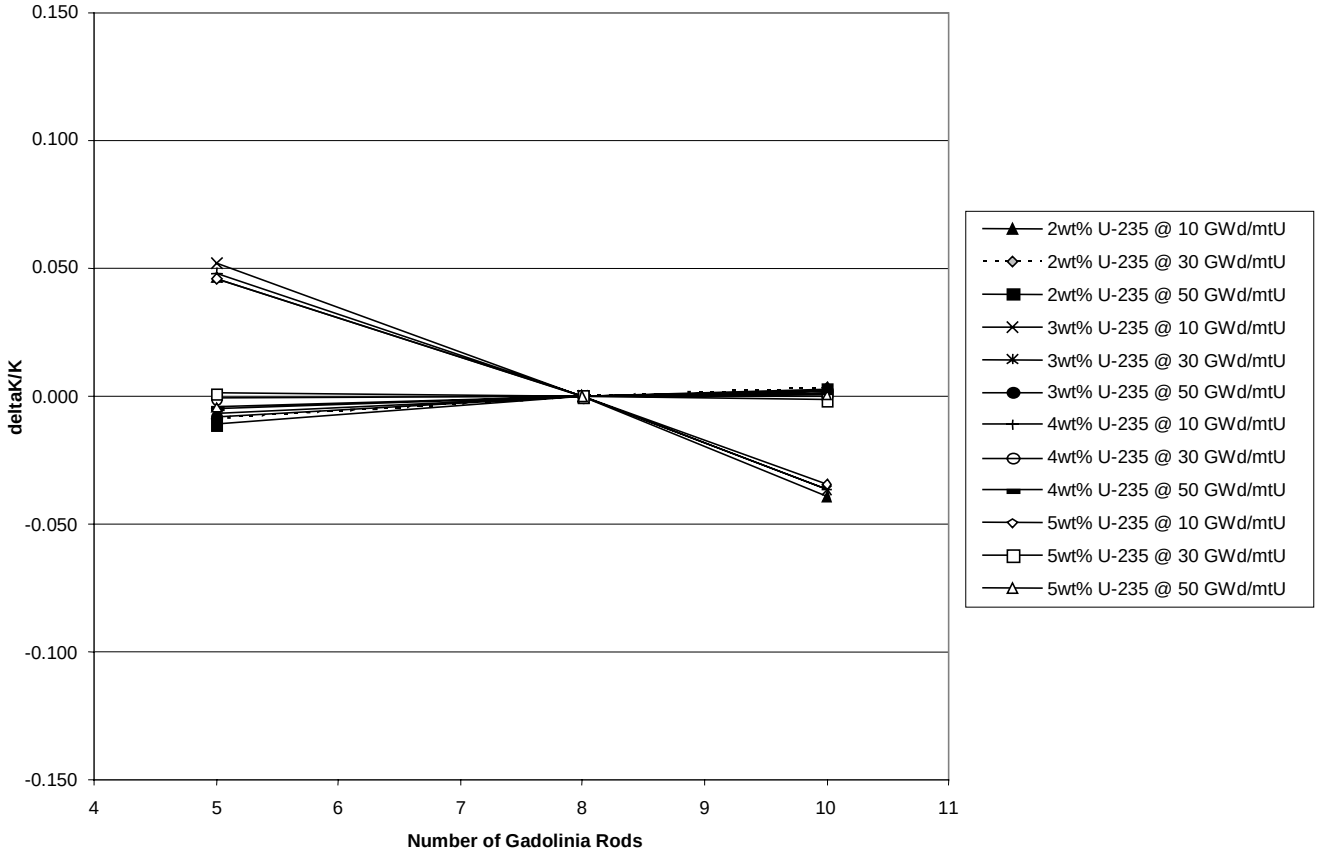
Source: BSC 2001, p. 54.

6.4.8 Gadolinium Effects for BWRs

BWR fuel assemblies may have gadolinium in the form of Gd_2O_3 (gadolinia) added to some UO_2 fuel rods to control excess reactivity of fresh fuel assemblies. The quantity of natural gadolinium present in the assembly is determined by the gadolinia weight percentage in the fuel rod and the number of fuel rods that contain gadolinia.

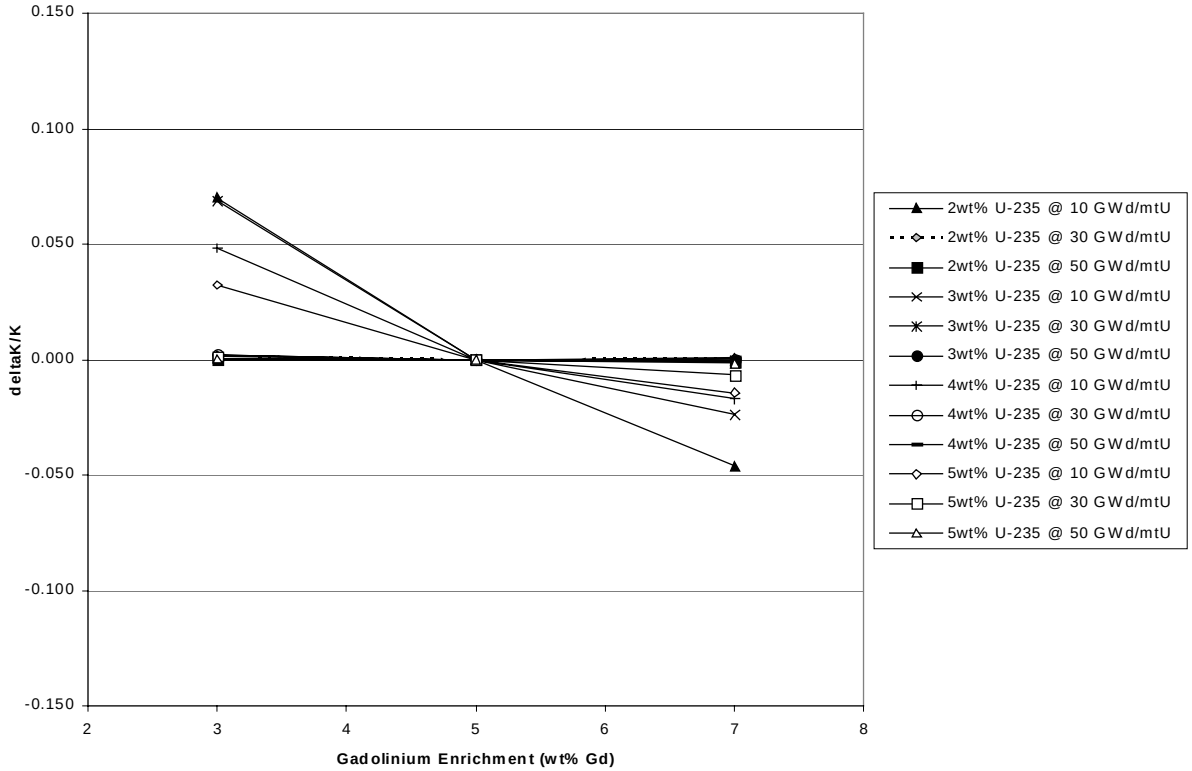
The effect of the number of gadolinia rods is shown in Figure 11. As more rods contain Gd, the reactivity of the discharged BWR assembly increases. The effect of the concentration of gadolinia in the rod is shown in Figure 12. As the concentration of Gd increases, the reactivity of the discharged BWR assembly increases. Normalized k values are graphically illustrated in these two figures. Values were normalized to the nominal k of each burnup/enrichment pair.

Thus the maximum reactivity is achieved when the maximum number of gadolinium rods with the greatest gadolinium content are used.



Source: Anderson 2003, p. 31.

Figure 11. Sensitivity to Number of Gadolinia Rods



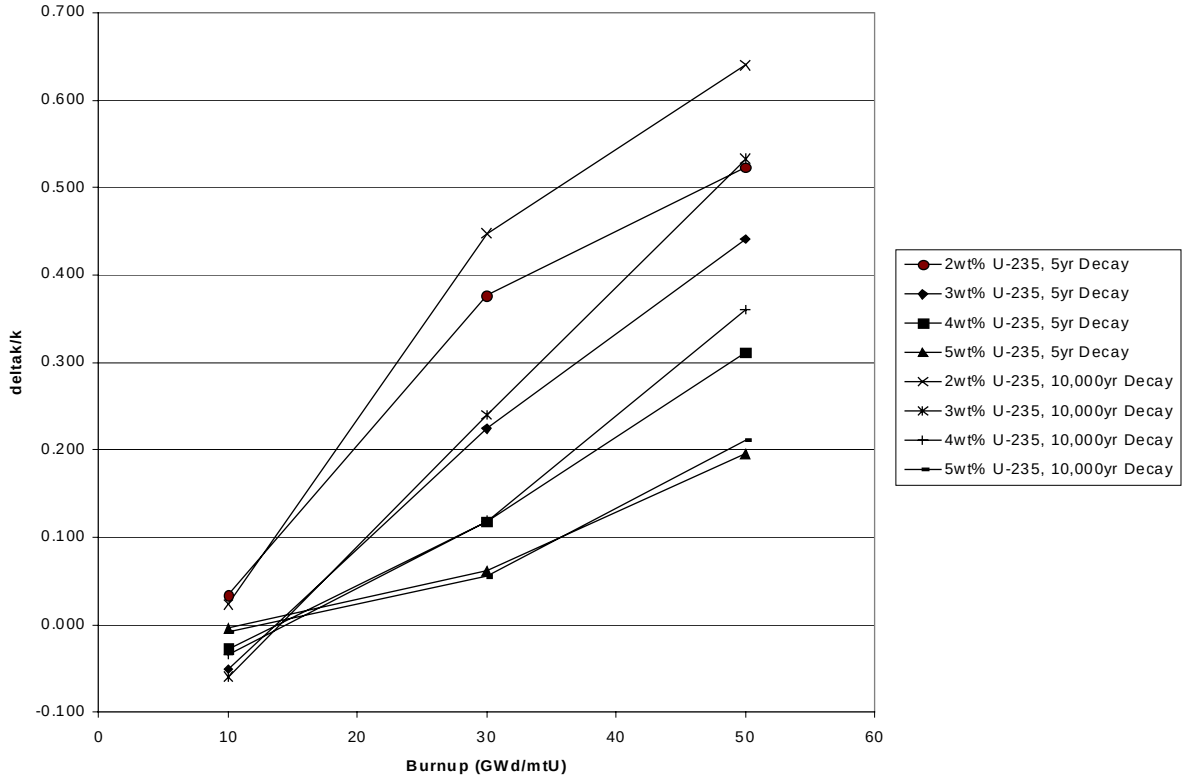
Source: Anderson 2003, p. 24.

Figure 12. Sensitivity to Gadolinium Content

6.4.9 Control Blade History Effect for BWRs

The effect of BWR control blade history is illustrated in Figure 13. Inspection of the figure shows that insertion of the control blades leads to a higher discharge reactivity for a BWR assembly. Normalized k values are graphically illustrated in Figure 13. The Δ k/k is equal to $(k_{in} - k_{out})/k_{out}$ where *in* means control blades inserted and *out* means control blades out.

Also, note that the ranges of delta-k/k of Figures 11 (number of gadolinia rods) and 12 (concentration of gadolinia) are -0.05 to +0.05 while the range of Figure 13 is –0.05 to +0.65. The effect of control blade insertion is thus very strong relative to the number and content of gadolinia rods. This allows the gadolinia rods to be omitted from the representation of the bounding BWR assembly, substituting an insertion of control blades for 15 GWd/MTU of burnup versus the typical burnout of gadolinium in gadolinia rods at 7-8 GWd/MTU. The control blade insertion is placed at the end of the irradiation history of the bounding assembly to maximize production of ^{239}Pu immediately prior to discharge of the fuel assembly.



Source: Anderson 2003, p. 34.

Figure 13. Control Blade History Effect

6.5 BOUNDING PARAMETERS

The isotopic calculation methodology must be capable of predicting conservative reactivities for a variety of LWR spent fuel assemblies without recourse to detailed knowledge of the fuel and reactor characteristics. This can be accomplished by selecting bounding depletion parameters for SAS2H to use in determining Principal Isotope burnup credit loading curves for LWR waste packages.

PWR SAS2H depletion parameters were chosen to illustrate the isotopic calculation process test for conservatism. BWR SAS2H bounding depletion parameters were obtained from Wimmer 2004, pp. 16 and 17, which also provides the isotopic concentrations for the bounding cases, i.e., SAS2H was not run for the BWR bounding cases. The bounding parameters are as follows:

- Fuel temperature, 1200 K–PWR and BWR
- Moderator temperature, 625°F (602.6 K)–PWR and 560.7 K-BWR
- Moderator density, 0.6516 g/cm^3–PWR and 0.30 g/cm^3 BWR
- Boron concentration, 950 parts per million boron by mass, constant (no boron letdown curve)–PWR (No dissolved boron for BWR)
- Specific power, 30 MW/MTU–PWR and 22.38 MW/MTU BWR

- Irradiation timestep, 80 days (or less)–PWR and BWR
- No spacer grids represented–PWR and BWR
- Control blades inserted final 15 GWd/MTU, No Gd rods–BWR

Bounding parameters may be chosen for PWRs with burnable poison rods, and a separate set of bounding parameters may also be chosen for PWRs without burnable poison rods. PWR fuel without burnable poison rods was analyzed.

6.6 BIAS AND UNCERTAINTY OF THE FISSION AND RADIOACTIVITY PROCESSES

The isotopic concentrations calculated by the SAS2H code sequence depend upon the nuclear data libraries that represent the physical processes of fission and radioactive decay. The number and type of isotopes created by the fission process are generally termed the fission yield curve, and define the isotopic concentrations generated by the fission process. Many of the isotopes produced by fission are radioactive, and decay at measured rates to produce other isotopes ("buildup"). Measurements of the physical parameters are generally considered accurate enough that it is not necessary to be concerned about any bias and uncertainty in the measurements. The very long time periods of the post-closure period could allow very small uncertainties for ten or twenty years to grow to significant proportions. Thus, the magnitude of the bias and uncertainty of isotopic concentrations over long time periods must be evaluated.

A study (Hermann et al. 1998) was performed at Oak Ridge National Laboratory to re-evaluate the nuclear data libraries used by SAS2H using newer data from the Evaluated Nuclear Data File (ENDF-B/VI) and the Evaluated Nuclear Structure Data File (ENSDF). 404 radionuclides were unchanged and 1126 were modified due to ENDF-B/VI data, with a further two modifications due to an update of ENDF-B/VI (Hermann et al. 1998, Table 3). Also, 139 radioisotopes were changed based upon the ENSDF data. One stable, non-radioactive isotope was changed and 21 radioisotopes were added. These changes were incorporated into the SCALE code package and are now used in all isotopic calculations.

Hermann et al. (1998, Appendix A) also evaluated the bias and uncertainty of the radioactive half-lives of the isotopes. These uncertainties were used by a statistical sampling methodology (CRWMS M&O 1999b) to evaluate the reactivity effect for the principal isotope data set for time periods up to 200,000 years. The reactivity effect ranged from -0.0000064 at 10 years to a maximum of 0.0000078 at 200,000 years (CRWMS M&O 1999b, Table 6-1). The magnitude of the reactivity effects of radioactive half-lives, 10^{-5}, is one hundred times smaller than the statistical uncertainty of typical calculations, 10^{-3}. Thus the effect of bias and uncertainty of radioactive half-lives is negligible.

In summary, the use of the updated data libraries for SCALE, does not contain a significant bias and uncertainty and no correction factor is required for the critical limit calculation.

7. CALCULATION INPUT PARAMETERS

This section presents a systematic approach for determining the conservatism of the bounding parameter calculational method used to determine the isotopic concentrations of SNF for any burnup. The means to determine the range of burnup for which the bounding parameters are conservative is to calculate the reactivity for a nominal fuel assembly with nominal LWR SAS2H depletion parameters and calculate the reactivity of an equivalent fuel assembly with the bounding SAS2H depletion parameters. The calculated reactivity with the bounding parameters should be conservative (i.e., larger than the calculated reactivity for the nominal parameters). Further, the difference between these reactivities should be larger than the sum of the bias and uncertainty determined for the LWR CRCs (-0.0077 from Table 6). Note that these calculations are performed using only the Principal Isotope data set. Alternatively, the RCA sum of the bias and uncertainty for the PWR RCAs (-0.0249, from Table 10) could be used, or both could be applied simultaneously.

The bounding parameters are only applicable to commercial LWR SNF.

A listing of corroborating or supporting data or information used to determine the burnup range for which the bounding parameters are conservative, along with their sources, is provided in Table 20.

Table 20. Supporting Information and Sources for Conservatism of Bounding Parameters

Description	Source
Representative assembly characteristics	(Punatar 2001), (DOE 1992), (Larsen et al. 1976)
Equation for fresh fuel compositions	(Bowman et al. 1995)
Material composition for Zircaloy-4	(ASTM B 811-97 2000)
Density for Zircaloy-4	(ASM International 1990)
Atomic mass values	(Audi and Wapstra 1995)
General reference to MCNP code manual	(Briesmeister 1997)
Material composition for Alloy 22 (UNS N06022)	(DTN: MO0003RIB00071.000)
Material composition for SA-240 S31600	(ASM International 1987, p. 931), (ASME 2001, Section II, SA-240)
Material composition for Neutronit A978	(Kugler 1991), (Kugler 1996)
Material composition for Al 6061	(ASM International 1990)
Density of Al 6061 and Stainless Steels 304 and 316	(ASTM G 1-90 1999), (ASME 2001)
Material composition for Grade 70 Carbon Steel Type A516	(ASTM A 516/A 516M-90 1991), (ASME 2001)
Material composition for Stainless Steel Type 304	(ASTM A 240/A 240M-03b 2003)
Material composition for Inconel 718	(Lynch 1989)
General reference to principal isotopes	(YMP 2003)
General reference to SCALE manual	(CRWMS M&O 2000a)

7.1 NOMINAL DEPLETION PARAMETER SELECTION

The PWR nominal depletion parameters were selected by reviewing the assemblies of Crystal River Unit 3. Values selected as nominal were chosen based on information presented in *Summary Report of Commercial Reactor Criticality Data for Crystal River Unit 3* (Punatar 2001). Assemblies reviewed are B & W 15×15 fuel assemblies for which the operating temperatures, boron letdown curve, irradiation power levels, and exposure times are known.

The BWR nominal depletion parameters were selected based upon information presented in Wimmer (2004) and GE 7×7 dimensions were obtained from Larsen et al. (1976) and DOE (1992).

The depletion parameters for PWRs and BWRs were as follows:

- Fuel temperature, 861.3 K–PWR and 1000K–BWR
- Fuel cladding temperature, 640 K–PWR and 588.6 K–BWR
- Moderator temperature, 579.8 K–PWR and 560.7 K–BWR
- Moderator density, 0.7556 g/cm^3–PWR and 0.430 g/cm^3–BWR
- Specific power, 43.029 MW/MTU–PWR and variable (see Table 2)–BWR
- Moderator boron concentration values for PWR are presented in Table 21 and were interpolated from the nominal values specified in Section 4. There is no dissolved boron for BWRs.
- PWR UO_2 fuel density of 10.121 g/cm^3 calculated by dividing fuel mass by fuel volume where a uranium mass of 463.63 kgU was used with a fuel height of 360.162 cm, and a pellet diameter of 0.9398 cm (Punatar 2001, pp. 2-5 and 3-1). BWR UO_2 fuel density of 10.741 g/cm^3 was used with a fuel height of 365.76 cm, and a pellet diameter of 1.267 cm and clad thickness of 35.5 mils (DOE 1992, Page 2A-15). The BWR fuel density was obtained from Wimmer (2004, p. 18, Table 5) and the same density was used in conservative and nominal calculations to insure a direct comparison of the bounding depletion parameters.
- BWR zircaloy-4 channel based upon a 120 mil thickness and outer dimension of 5.438 (DOE 1992, pp. 2.8-10 and Larsen et al. 1976 pp. A-2). Note that the fuel assembly/channel pitch is 6.000 inches (Larsen et al. 1976 pp. A-3, Table 3).
- BWR Control Blade data are homogenized over the volume outside the channels (Wimmer 2004, Section 5.1, p. 14).

Table 21. Nominal Boron Letdown Data

10 GWd/MTU			20 GWd/MTU			30 GWd/MTU			40 GWd/MTU		
Step Length (EFPD)[a]	Conc. (ppmB)[b]	BFRAC[c]	Step Length (EFPD)	Conc. (ppmB)	BFRAC	Step Length (EFPD)	Conc. (ppmB)	BFRAC	Step Length (EFPD)	Conc. (ppmB)	BFRAC
16.8	962.1053	1.0000	33.6	910.918	1.0000	50.4	915.9672	1.0000	67.2	921.0164	1.0000
16.8	915.9672	0.9520	33.6	931.1148	1.0222	50.4	903.3	0.9862	67.2	872.2394	0.9470
16.8	926.0656	0.9625	33.6	894.9	0.9824	50.4	822.0078	0.8974	67.2	738.2884	0.8016
16.8	923.5349	0.9599	33.6	838.7517	0.9208	50.4	721.5445	0.7877	67.2	608.1684	0.6603
17.775	902.8125	0.9384	35.55	769.8327	0.8451	53.325	662.4054	0.7232	71.1	518.6474	0.5631
17.775	885.0375	0.9199	35.55	696.2434	0.7643	53.325	560.5768	0.6120	71.1	256.1082	0.2781
7.275	861.1018	0.8950	14.55	634.6203	0.6967	21.825	435.5344	0.4755	29.1	237.5449	0.2579
13.875	840.0224	0.8731	27.75	619.1737	0.6797	41.625	335.625	0.3664	55.5	688.9265	0.7480
13.875	812.3651	0.8444	27.75	708.9949	0.7783	41.625	281.7162	0.3076	55.5	527.5075	0.5727
13.875	784.7078	0.8156	27.75	564.2079	0.6194	26.775	231.1362	0.2523	55.5	353.475	0.3838
14.04175	756.8843	0.7867	28.0835	437.2034	0.4800	56.9753	686.106	0.7491	56.167	880.3779	0.9559
14.04175	728.8947	0.7576	28.0835	348.3596	0.3824	42.12525	547.2231	0.5974	56.167	694.6803	0.7543
14.04175	699.0531	0.7266	28.0835	265.235	0.2912	42.12525	419.408	0.4579	56.167	536.647	0.5827
10.1875	667.4783	0.6938	20.375	286.4277	0.3144	20.1742	328.4785	0.3586	40.75	382.5951	0.4154
10.1875	643.4066	0.6687	20.375	273.214	0.2999	40.9208	898.5897	0.9810	40.75	267.1631	0.2901
9.125	621.7595	0.6462	11.7995	230.0942	0.2526	27.375	805.3961	0.8793	36.5	234.6383	0.2548
9.125	655.9768	0.6818	24.7005	793.0185	0.8706	27.375	702.7882	0.7673	36.5	128.1642	0.1392

NOTES: [a] effective full-power days.
[b] parts per million boron by mass.
[c] BFRAC represents SAS2H input parameter value.

7.1.1 SAS2H Computation Description

The SAS2H control sequence accesses five calculation modules of the SCALE code system for performing fuel depletion and decay calculations. The five modules include BONAMI, NITAWL-II, XSDRNPM, COUPLE, and ORIGEN-S. Each of the modules has a specific purpose in the sequence to perform the fuel depletion and decay calculations. The following provides a brief description of what each module does with a more detailed description being provided in *Users Manual for SCALE-4.4A* (CRWMS M&O 2000a).

BONAMI applies the Bondarenko method of resonance self-shielding to nuclides for which Bondarenko data is available.

NITAWL-II performs Nordheim resonance self-shielding corrections for nuclides that have resonance parameter data available.

XSDRNPM performs a one-dimensional neutron transport calculation on a specified geometry to facilitate production of cell-weighted cross sections for fuel depletion calculations.

COUPLE updates all cross section constants included on an ORIGEN-S working nuclear data library with data from the cell-weighted cross section library obtained from the XSDRNPM calculation. Additionally, the weighting spectrum produced by XSDRNPM is applied to update

all nuclides in the ORIGEN-S working library that were not included in the XSDRNPM calculation.

ORIGEN-S performs point depletion, buildup, and decay calculations for the specified assembly irradiation history. Additionally, it can be run as a stand-alone case to provide isotopic concentrations at various decay times.

The SAS2H control module uses ORIGEN-S to perform a point depletion calculation for the fuel assembly section described in the SAS2H input file. The ORIGEN-S module uses cell-weighted cross sections based on one-dimensional transport calculations performed by XSDRNPM. One-dimensional transport calculations are performed on two representations, Path A and Path B, to calculate energy dependent spatial neutron flux distributions necessary to perform cross section cell-weighting calculations.

7.2 BOUNDING DEPLETION PARAMETER SELECTION

A set of depletion parameters based on bounding reactor operation values was used for generating SNF isotopes. The bounding parameters were provided previously (Section 6.5), and the depletion time steps and power per fuel node are provided in Table 22 for each of the burnups evaluated. Values are provided for both PWRs and BWRs in the table (note that different unit masses are used).

Table 22. Bounding SAS2H Base Case Depletion Time Steps

Burnup (GWd/MTU)	Power (MW) (PWR Node/BWR Assembly)	Time Step (days) (P/B)
10	0.77244/NA	66.667/NA
20	0.77244/ 4.79125	74.074/50
30	0.77244/ 4.79125	55.556/50
40	0.77244/ 4.79125	74.074/50
50	NA/ 4.79125	NA/50

NOTE: PWR Values were derived based on a node height of 20.0025 cm.

Source (BWR): Wimmer 2004, Section 5.1.1.7, p. 18.

7.3 SAS2H MATERIAL SPECIFICATIONS

The material specification section defines the UO_2 fresh fuel composition for the SAS2H calculation. The UO_2 fresh fuel composition is characterized by the fuel density, fuel temperature, and weight percentages of ^{234}U, ^{235}U, ^{236}U, and ^{238}U. The fresh fuel compositions for each ^{235}U enrichment used in this evaluation are specified in Table 23 and were calculated using Equation 8 (Bowman et al. 1995, p. 20) for each isotope based on the ^{235}U weight percent. The material specification for Inconel 718 is specified in Table 24.

Table 23. SAS2H Fresh Fuel Compositions

Enrichment (Wt% ^{235}U)	Wt% ^{234}U	Wt% ^{235}U	Wt% ^{236}U	Wt% ^{238}U
2.0	0.0164	2.0000	0.0092	97.9744
3.0	0.0254	3.0000	0.0138	96.9608
4.0	0.0347	4.0000	0.0184	95.9469
5.0	0.0442	5.0000	0.0230	94.9328

$$U^{234}\ wt\% = (0.007731) * (U^{235}\ wt\%)^{1.0837}$$

$$U^{236}\ wt\% = (0.0046) * (U^{235}\ wt\%) \qquad \text{(Eq. 8)}$$

$$U^{238}\ wt\% = 100 - U^{234}\ wt\% - U^{235}\ wt\% - U^{236}\ wt\%$$

Table 24. SAS2H Inconel 718 Material Composition

Element	Composition ID[a]	Wt%	Element	Composition ID	Wt%
C	6012	0.040	Ni	28000	52.5
Si	14000	0.180	Ti	22000	0.90
S	16000	0.008	Al	13027	0.50
Cr	24000	19.0	Nb	41093	5.13
Mn	25055	0.18	Mo	42000	3.05
Fe	26000	18.5	Density[b] = 8.19 g/cm^3		

NOTES: [a] ID = identifier.
[b] Converted from a reference value of 0.296 lb/in^3.

Source: Lynch 1989, p. 496.

The PWR fuel rod cladding material composition was given a base temperature of 640 K. The fuel rod cladding was made up of Zircaloy-4. The Zircaloy-4 cladding specifications used in the SAS2H input are presented in Table 25. The Zircaloy-2 cladding of BWR fuel is represented as Zircaloy-4 in the SAS2H calculations since the compositions differ only by the addition of a small quantity of nickel to Zircaloy-2 (Larsen 1976 pp. A-8) and differences of several hundredths of a percent for the Zr, Fe, and Sn components. A BWR fuel rod cladding temperature of 588.6 K was used.

Table 25. SAS2H Zircaloy-4 Material Composition

Element	Composition ID[a]	Wt%
Cr	24000	0.10
Fe	26000	0.21
O	8016	0.125
Sn	50000	1.45
Zr	40000	98.115
Density[b] = 6.56 g/cm^3		

NOTES: [a] ID = identifier.
[b] ASM International 1990, p. 666, Table 6.

Source: ASTM B 811-97 2000, p. 2, Table 2.

7.4 MCNP REPRESENTATION

The MCNP representation for a 21 PWR waste package was developed from the configuration shown in Attachment I. The waste package is treated as containing B & W 15×15 fuel assemblies in a fully flooded condition and at room temperature. Similarly, the MCNP representation for a 44 BWR waste package, was developed from the configuration drawings (BSC 2004a; BSC 2004b; BSC 2004c; BSC 2004d), Attachment IV (file "att2.ZIP"). Calculations for the BWR system were performed with the waste package containing GE 7×7 fuel assemblies in a fully flooded condition and at room temperature.

7.4.1 MCNP Computation Description

MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport, including the capability to calculate eigenvalues for critical systems. The code treats an arbitrary three-dimensional configuration of materials in geometric cells bounded by first- and second-degree surfaces and fourth-degree elliptical tori (Briesmeister 1997, p. ix). The Monte Carlo method is used to duplicate a statistical process theoretically. The individual probabilistic events that comprise a process are simulated sequentially. The probability distributions governing these events are statistically sampled to describe the total phenomenon (Briesmeister 1997, p. 1-3).

In order to quantify the overall effect that the differences between the calculated and measured isotopic concentrations have on system reactivity, MCNP calculations were performed to calculate the neutron multiplication factor (k) that results from using the different sets of isotopics and provide a comparison in terms of Δk. The results represent the average combined collision, absorption, and track-length estimator from the MCNP calculations. The standard deviation (σ) represents the standard deviation of k about the average combined collision, absorption, and track-length estimate due to the Monte Carlo calculation statistics.

7.4.2 Waste Package MCNP Material Descriptions

When performing reactivity effects evaluations, changes in reactivity based on a k_∞ or k_{eff} basis should yield about the same fractional Δk. Selected sets of sensitivity cases were evaluated in waste package MCNP representations. The single corrosion resistant material waste package follows the same description as that shown in the design variants included as Attachment I and file "att2.ZIP", Attachment IV (CD). These waste packages are only used to provide a representative geometric arrangement of SNF for the MCNP calculations. The outer barrier was represented as SB-575 N06022 (as described in Table 26). The inner barrier was represented as SA-240 S31600, which is nuclear-grade Stainless Steel Type 316 with tightened control on carbon and nitrogen content (ASM International 1987, p. 931; ASME 2001, Section II, SA-240, Table 1), as described in Table 27. The fuel basket plates were represented as Neutronit A978 with 1.62 weight percent boron as described in Table 28. The thermal shunts were represented as aluminum 6061 (as described in Table 29), and the basket side and corner guides were represented as Grade 70 Carbon Steel Type A516 (as described in Table 30). The waste package was represented in a fully flooded condition with an effectively infinite water reflector surrounding the waste package. The water composition is pure H_2O at 1.0 g/cm^3 density. The basket stiffeners were represented as water since they are not solid over the length of the basket and representing them as water is conservative for criticality calculations.

The chromium, nickel, and iron elemental weight percents obtained from the references were expanded into their constituent natural isotopic weight percents for use in MCNP. This expansion was performed by (1) calculating a natural weight fraction of each isotope in the elemental state and (2) multiplying the elemental weight percent in the material of interest by the natural weight fraction of the isotope in the elemental state to obtain the weight percent of the isotope in the material of interest. This is described mathematically in Equations 9 and 10. The atomic mass values and atom percent of natural element values for these calculations are from work by Audi and Wapstra (1995).

$$\begin{pmatrix} \textit{Weight Fraction} \\ \textit{of Isotope}_i \textit{ in the} \\ \textit{Natural Element} \end{pmatrix} = \frac{(\textit{Atomic Mass of Isotope}_i)(\textit{Atom Percent of Isotope}_i \textit{ in Natural Element})}{\sum_{i=1}^{I} (\textit{Atomic Mass of Isotope}_i)(\textit{Atom Percent of Isotope}_i \textit{ in Natural Element})} \quad \text{(Eq. 9)}$$

where

I is the total number of isotopes in the natural element

$$\begin{pmatrix} \textit{Weight Percent} \\ \textit{of Isotope}_i \textit{ in} \\ \textit{Material Composition} \end{pmatrix} = \begin{pmatrix} \textit{Weight Fraction} \\ \textit{of Isotope}_i \textit{ in the} \\ \textit{Natural Element} \end{pmatrix} \begin{pmatrix} \textit{Reference Weight Percent of} \\ \textit{Element in Material Composition} \end{pmatrix} \quad \text{(Eq. 10)}$$

Table 26. Alloy 22 (UNS N06022) Material Composition

Element/ Isotope	ZAID[a]	Wt%	Element/ Isotope	ZAID	Wt%
C-nat	6000.50c	0.0150	^{59}Co	27059.50c	2.5000
^{55}Mn	25055.50c	0.5000	^{182}W	74182.55c	0.7877
Si-nat	14000.50c	0.0800	^{183}W	74183.55c	0.4278
^{50}Cr	24050.60c	0.8879	^{184}W	74184.55c	0.9209
^{52}Cr	24052.60c	17.7863	^{186}W	74186.55c	0.8636
^{53}Cr	24053.60c	2.0554	V-nat	23000.50c	0.3500
^{54}Cr	24054.60c	0.5202	^{54}Fe	26054.60c	0.2260
^{58}Ni	28058.60c	36.8024	^{56}Fe	26056.60c	3.6759
^{60}Ni	28060.60c	14.6621	^{57}Fe	26057.60c	0.0865
^{61}Ni	28061.60c	0.6481	^{58}Fe	26058.60c	0.0116
^{62}Ni	28062.60c	2.0975	^{32}S	16032.50c	0.0200
^{64}Ni	28064.60c	0.5547	^{31}P	15031.50c	0.0200
Mo-nat	42000.50c	13.5000	Density = 8.69 g/cm^3		

NOTE: [a] ZAID = MCNP material identifier.

Source: DTN: MO0003RIB00071.000.

Table 27. Material Specifications for SA-240 S31600

Element/Isotope	ZAID[a]	Wt%	Element/Isotope	ZAID	Wt%
C-nat[b]	6000.50c	0.0200	^{54}Fe	26054.60c	3.6911
^{14}N[b]	7014.50c	0.0800	^{56}Fe	26056.60c	60.0322
Si-nat	14000.50c	1.0000	^{57}Fe	26057.60c	1.4119
^{31}P	15031.50c	0.0450	^{58}Fe	26058.60c	0.1897
^{32}S	16032.50c	0.0300	^{58}Ni	28058.60c	8.0641
^{50}Cr	24050.60c	0.7103	^{60}Ni	28060.60c	3.2127
^{52}Cr	24052.60c	14.2291	^{61}Ni	28061.60c	0.1420
^{53}Cr	24053.60c	1.6443	^{62}Ni	28062.60c	0.4596
^{54}Cr	24054.60c	0.4162	^{64}Ni	28064.60c	0.1216
^{55}Mn	25055.50c	2.0000	Mo-nat	42000.50c	2.5000
Density[c] = 7.98 g/cm^3					

NOTES: [a] ZAID = MCNP material identifier

[b] Carbon and nitrogen specifications are from ASM International 1987 and remaining material compositions are from ASME 2001

[c] Density is for stainless steel 316 from ASTM G 1-90 1999.

Source: ASM International 1987, p. 931; ASME 2001, Section II, SA-240, Table 1; ASTM G 1-90 1999, p. 7, Table X1.

Table 28. Material Specifications for Neutronit A978 with 1.62 Weight Percent Boron

Element/Isotope	ZAID[a]	Wt%	Element/Isotope	ZAID	Wt%
^{10}B	5010.50c	0.2986	^{57}Fe	26057.60c	1.3928
^{11}B	5011.56c	1.3214	^{58}Fe	26058.60c	0.1872
C-nat	6000.50c	0.0400	^{59}Co	27059.50c	0.2000
^{50}Cr	24050.60c	0.7730	^{58}Ni	28058.60c	8.7361
^{52}Cr	24052.60c	15.4846	^{60}Ni	28060.60c	3.4805
^{53}Cr	24053.60c	1.7894	^{61}Ni	28061.60c	0.1539
^{54}Cr	24054.60c	0.4529	^{62}Ni	28062.60c	0.4979
^{54}Fe	26054.60c	3.6411	^{64}Ni	28064.60c	0.1317
^{56}Fe	26056.60c	59.2189	Mo-nat	42000.50c	2.2000
Density = 7.76 g/cm^3					

NOTE: [a] ZAID = MCNP material identifier.

Source: Kugler 1996, p. 14; Kugler 1991, p. 15, for Mo content.

Table 29. Material Specifications for Al 6061

Element/Isotope	ZAID[a]	Wt%	Element/Isotope	ZAID	Wt%
Si-nat	14000.50c	0.6000	Mg-nat	12000.50c	1.0000
^{54}Fe	26054.60c	0.0396	^{50}Cr	24050.60c	0.0081
^{56}Fe	26056.60c	0.6433	^{52}Cr	24052.60c	0.1632
^{57}Fe	26057.60c	0.0151	^{53}Cr	24053.60c	0.0189
^{58}Fe	26058.60c	0.0020	^{54}Cr	24054.60c	0.0048
^{63}Cu	29063.60c	0.1884	Ti-nat	22000.50c	0.1500
^{65}Cu	29065.60c	0.0866	^{27}Al[b]	13027.50c	96.9300
^{55}Mn	25055.50c	0.1500	Density[c] = 2.7065 g/cm^3		

NOTES: [a] ZAID = MCNP material identifier.

[b] Zn cross-section data unavailable; therefore, it was substituted as ^{27}Al.

[c] ASTM G 1-90 (1999, p. 7, Table X1) indicates 2.7 g/cm^3; ASME (2001, Section II, Table NF-2) indicates a converted value from 0.098 lb/in^3 of 2.713 g/cm^3; therefore the midpoint was used.

Source: ASM International 1990, p. 102.

Table 30. Grade 70 Carbon Steel Type A516 Composition

Element/Isotope	ZAID[a]	Wt%	Element/Isotope	ZAID	Wt%
C-nat	6000.50c	0.2700	^{54}Fe	26054.60c	5.5558
^{55}Mn	25055.50c	1.0450	^{56}Fe	26056.60c	90.3584
^{31}P	15031.50c	0.0350	^{57}Fe	26057.60c	2.1252
^{32}S	16032.50c	0.0350	^{58}Fe	26058.60c	0.2856
Si-nat	14000.50c	0.2900	Density = 7.850 g/cm^3		

NOTE: [a] ZAID = MCNP material identifier.

Source: ASTM A 516/A 516M-90 1991, p. 2, Table 1; density from ASME 2001, Sec II, Part A, SA-20, Section 14.1.

7.4.3 MCNP Fuel Assembly Material Descriptions

The fuel assembly materials listed in this section refer to the upper and lower end-fitting materials. The primary material components in the upper and lower end-fitting regions are Stainless Steel Type 304, Inconel, and moderator. Both the upper and lower end-fitting regions are represented with material compositions that represent the homogenization of all of the components in the regions. Table 31 presents the material composition of Stainless Steel Type 304. Table 32 presents the material composition of Zircaloy-4. Table 33 presents the material composition of Inconel 718. Equations 14 and 15 were used for determining the end–fitting material volume fractions. Table 34 presents the component material volume fractions for the upper and lower end-fitting regions for the B & W 15×15 assembly design. Table 35 presents the upper and lower end-fitting homogenized material compositions for the B & W 15×15 assembly design. These homogenized material compositions are made of various base components such as Stainless Steel Type 304, Inconel, Zircaloy-4, and moderator that are present in certain volume fractions. The homogenization of the base components into single homogenized material compositions is performed using Equations 11 through 15.

$$Homogenized\ Material\ Density = \sum_{m}^{M} \left[(\rho)_m \left(Volume\ Fraction\ in\ Homogenized\ Material \right)_m \right] \quad \text{(Eq. 11)}$$

where

m = a single component material of the homogenized material
M = total number of component materials in the homogenized material
ρ = the mass density of the component material

$$\begin{pmatrix} Mass\ Fraction\ of\ Component \\ Material\ in\ Homogenized\ Material \end{pmatrix} = \left[\frac{(\rho)_m \left(Volume\ Fraction\ in\ Homogenized\ Material \right)_m}{Homogenized\ Material\ Density} \right] \quad \text{(Eq. 12)}$$

$$\begin{pmatrix} Weight\ Percent\ of \\ Component\ Material \\ Constituent\ in \\ Homogenized\ Material \end{pmatrix} = \begin{pmatrix} Mass\ Fraction\ of \\ Component\ Material\ in \\ Homogenized\ Material \end{pmatrix} \begin{pmatrix} Weight\ Percent\ of\ Component \\ Material\ Constituent \\ in\ Component\ Material \end{pmatrix} \quad \text{(Eq. 13)}$$

$$\begin{pmatrix} End-Fitting\ Material \\ Volume \end{pmatrix} = \sum \frac{mass_i}{density_i} \quad \text{(Eq. 14)}$$

where

i represents a common material such as Stainless Steel Type 304

$$(Volume\ Fraction)_i = \frac{\begin{pmatrix} End-Fitting\ Material \\ Volume \end{pmatrix}_i}{\begin{pmatrix} Total\ End-Fitting \\ Volume \end{pmatrix}} \quad \text{(Eq. 15)}$$

where

i represents a common material such as Stainless Steel Type 304

Table 31. Stainless Steel Type 304 Material Composition

Element/Isotope	ZAID[a]	Wt%	Element/Isotope	ZAID	Wt%
C-nat[b]	6000.50c	0.0300	^{54}Fe	26054.60c	3.8448
^{14}N	7014.50c	0.1000	^{56}Fe	26056.60c	62.5318
Si-nat[b]	14000.50c	0.7500	^{57}Fe	26057.60c	1.4707
^{31}P	15031.50c	0.0450	^{58}Fe	26058.60c	0.1977
^{32}S	16032.50c	0.0300	^{58}Ni	28058.60c	6.7201
^{50}Cr	24050.60c	0.7939	^{60}Ni	28060.60c	2.6773
^{52}Cr	24052.60c	15.9031	^{61}Ni	28061.60c	0.1183
^{53}Cr	24053.60c	1.8378	^{62}Ni	28062.60c	0.3830
^{54}Cr	24054.60c	0.4652	^{64}Ni	28064.60c	0.1013
^{55}Mn	25055.50c	2.0000	Density[c] = 7.94 g/cm^3		

NOTES: [a] ZAID = MCNP material identifier.
[b] C-nat and Si-nat weight percents correspond to that of Stainless Steel Type 304L.
[c] From ASTM G 1-90 (1999, p. 7, Table X1).

Source: ASTM A 240/A 240M-03b 2003, p. 2, Table 1.

Table 32. Zircaloy-4 Material Composition

Element/Isotope	ZAID[a]	Wt%	Element/Isotope	ZAID	Wt%
^{50}Cr	24050.60c	0.0042	^{57}Fe	26057.60c	0.0045
^{52}Cr	24052.60c	0.0837	^{58}Fe	26058.60c	0.0006
^{53}Cr	24053.60c	0.0097	^{16}O	8016.50c	0.1250
^{54}Cr	24054.60c	0.0024	Zr-nat	40000.60c	98.1150
^{54}Fe	26054.60c	0.0119	Sn-nat	50000.35c	1.4500
^{56}Fe	26056.60c	0.1930	Density[b] = 6.56 g/cm^3		

NOTES: [a] ZAID = MCNP material identifier.
[b] From ASM International (1990, p. 666, Table 6).

Source: ASTM B 811-97 2000, p. 2, Table 2.

Table 33. Inconel 718 Material Composition

Element/Isotope	ZAID[a]	Wt%	Element/Isotope	ZAID	Wt%
C-nat	6000.50c	0.0400	^{58}Fe	26058.60c	0.0537
Si-nat	14000.50c	0.1800	^{58}Ni	28058.60c	35.2846
^{32}S	16032.50c	0.0080	^{60}Ni	28060.60c	14.0574
^{50}Cr	24050.60c	0.7940	^{61}Ni	28061.60c	0.6214
^{52}Cr	24052.60c	15.9050	^{62}Ni	28062.60c	2.0110
^{53}Cr	24053.60c	1.8380	^{64}Ni	28064.60c	0.5319
^{54}Cr	24054.60c	0.4652	Ti-nat	22000.50c	0.9001
^{55}Mn	25055.50c	0.1800	^{27}Al	13027.50c	0.5001
^{54}Fe	26054.60c	1.0454	^{93}Nb[b]	41093.50c	5.1306
^{56}Fe	26056.60c	17.0031	Mo-nat	42000.50c	3.0504
^{57}Fe	26057.60c	0.3999	Density = 8.19 g/cm^3		

NOTES: [a] ZAID = MCNP material identifier.
[b] Reference identifies this material as “columbium,” which is actually the element niobium.

Source: Lynch 1989, p. 496.

Table 34. End-Fitting Component Material Volume Fractions for B & W 15×15 Assembly

Assembly Design	Stainless Steel Type 304	Inconel	Zircaloy-4	Moderator
Upper End-Fitting	0.2756	0.0441	0.0081	0.6722
Lower End-Fitting	0.1656	0.0306	0.0125	0.7913

Source: Punatar 2001, Section 2.

Table 35. End-Fitting Homogenized Material Compositions for B & W 15×15 Assembly

Element/ Isotope	ZAID[a]	Upper End-Fitting Wt%	Lower End-Fitting Wt%
C-nat	6000.50c	0.0245	0.0203
^{14}N	7014.50c	0.0668	0.0539
Si-nat	14000.50c	0.5210	0.4229
^{31}P	15031.50c	0.0301	0.0243
^{32}S	16032.50c	0.0209	0.0170
^{50}Cr	24050.60c	0.6181	0.5098
^{52}Cr	24052.60c	12.3822	10.2114
^{53}Cr	24053.60c	1.4309	1.1800
^{54}Cr	24054.60c	0.3622	0.2987
^{55}Mn	25055.50c	1.3563	1.0968
^{54}Fe	26054.60c	2.6847	2.1808
^{56}Fe	26056.60c	43.6633	35.4677
^{57}Fe	26057.60c	1.0269	0.8342
^{58}Fe	26058.60c	0.1380	0.1121
^{58}Ni	28058.60c	8.3820	7.2490
^{60}Ni	28060.60c	3.3394	2.8880
^{61}Ni	28061.60c	0.1476	0.1277
^{62}Ni	28062.60c	0.4777	0.4132
^{64}Ni	28064.60c	0.1263	0.1093
^{1}H	1001.50c	2.2972	3.6312
^{16}O	8016.50c	18.2314	28.8196
^{27}Al	13027.50c	0.0552	0.0514
Ti-nat	22000.50c	0.0993	0.0925
^{93}Nb	41093.50c	0.5659	0.5272
Mo-nat	42000.50c	0.3364	0.3135
Zr-nat	40000.60c	1.5920	3.2990
Sn-nat	50000.35c	0.0235	0.0488
Density (g/cm^3)		3.2748	2.4388

NOTE: [a] ZAID = MCNP material identifier.

7.4.4 PWR Fuel Material

For each of the various depletion parameter cases the irradiated fuel was represented as having a unique material composition. An active fuel height of 360.172 cm (Punatar 2001, p. 2-5) was used in the MCNP calculations for PWRs. The SNF isotopes used in the MCNP cases correspond to those of the Principal Isotope set (YMP 2003, p. 3-34), and come from the SAS2H calculations. Each depleted fuel composition is contained on the compact disc in Attachment IV.

The fuel rod components include the fuel rod cladding, the upper and lower fuel rod plenums (including end-caps), and the fuel. The fuel rod cladding was represented as Zircaloy-4 in this analysis (Table 32). The upper and lower fuel rod plenum regions were represented as containing Stainless Steel Type 304 springs. Table 36 contains the upper and lower fuel rod plenum volume fractions, and Table 37 contains the homogenized material compositions for the

upper and lower fuel rod plenum regions. The spacer grids were omitted from the MCNP calculations since they have a negligible effect on fuel assembly reactivity calculations.

Table 36. Fuel Rod Plenum Material Volume Fractions

Assembly Design	Plenum Location	Type 304 Stainless Steel	Gas (treated as void)	Zircaloy-4
B & W 15×15	Upper	0.0811	0.7793	0.1396
	Lower	0.1569	0.5973	0.2458

NOTE: Volume fractions are renormalized to exclude the cladding, which is represented explicitly in the input.

Source: Punatar 2001, Section 2.

Table 37. Fuel Rod Plenum Homogenized Material Compositions for B & W 15×15 Assembly

Element/Isotope	ZAID[a]	Weight Percent of Element/Isotope in Material Composition	
		Upper Fuel Rod Plenum	Lower Fuel Rod Plenum
C-nat	6000.50c	0.0124	0.0131
^{14}N	7014.50c	0.0413	0.0436
Si-nat	14000.50c	0.3096	0.3270
^{31}P	15031.50c	0.0186	0.0196
^{32}S	16032.50c	0.0124	0.0131
^{50}Cr	24050.60c	0.3302	0.3485
^{52}Cr	24052.60c	6.6148	6.9806
^{53}Cr	24053.60c	0.7644	0.8067
^{54}Cr	24054.60c	0.1935	0.2042
^{55}Mn	25055.50c	0.8257	0.8720
^{54}Fe	26054.60c	1.5943	1.6829
^{56}Fe	26056.60c	25.9299	27.3712
^{57}Fe	26057.60c	0.6099	0.6438
^{58}Fe	26058.60c	0.0820	0.0865
^{58}Ni	28058.60c	2.7744	2.9298
^{60}Ni	28060.60c	1.1053	1.1672
^{61}Ni	28061.60c	0.0489	0.0516
^{62}Ni	28062.60c	0.1581	0.1670
^{64}Ni	28064.60c	0.0418	0.0442
^{16}O	8016.50c	0.0734	0.0705
Zr-nat	40000.60c	57.6077	55.3392
Sn-nat	50000.35c	0.8514	0.8178
Density (g/cm^3)		1.5597	2.8583

NOTE: [a] ZAID = MCNP material identifier.

Several calculations are performed in order to make the proper conversions from the SAS2H/ORIGEN-S output files to values that are to be put into MCNP input files. The SAS2H program creates files with decayed fuel isotopic concentrations at different decay times specified in the ORIGEN-S portion of the SAS2H input.

Up to 29 Principal Isotopes are extracted from the SAS2H outputs and then combined with the initial oxygen mass and renormalized in terms of weight percents. The data are in units of moles, so in order to convert these into a mass value, the moles for each of the Principal Isotopes is multiplied of by its corresponding atomic mass to convert to units of grams. These values are summed and added to the oxygen mass, which is calculated using Equations 16 through 18. In Equations 16 and 17 the atomic mass values (*A*) come from work by Audi and Wapstra (1995).

$$\frac{U\ Mass}{mol\ UO_2} = \begin{bmatrix} (A)(U^{234}\,wt\%) + (A)(U^{235}\,wt\%) + \\ (A)(U^{236}\,wt\%) + (A)(U^{238}\,wt\%) \end{bmatrix} (0.01) \qquad \text{(Eq. 16)}$$

where the weight percentages of the uranium isotopes (U^{234}, U^{236}, and U^{238}) in uranium for a given initial enrichment were calculated using Equation 8.

$$\frac{O\ Mass}{mol\ UO_2} = (2)(A\ for\ oxygen) \qquad \text{(Eq. 17)}$$

$$O\ Mass\ in\ UO_2 = \left(\frac{O\ Mass \,/\, mol\ UO_2}{U\ Mass \,/\, mol\ UO_2} \right) (U\ Mass\ in\ UO_2) \qquad \text{(Eq. 18)}$$

where the *U Mass in UO_2* is the fresh fuel uranium mass

The weight percent values for each isotope listed in the MCNP input files were calculated using Equation 19.

$$wt\%_i = \frac{M_i W_i}{\sum_i^N M_i W_i + MassO_{node}} \qquad \text{(Eq. 19)}$$

where

i is the individual isotope
M_i is the number of moles of the particular isotope
W_i is the atomic mass of the individual isotope
Mass O_{node} is the mass of oxygen in the node from Equation 17
N is equal to the number of Principal Isotopes in the SNF composition

The density for the node is calculated by taking the total mass of the 29 Principal Isotopes plus the oxygen mass and dividing it by the fuel volume. The fuel volume per node used in this calculation was 2885.72 cm^3 calculated in Equation 20.

$$V = \frac{\pi}{4} D^2 N_p H \qquad \text{(Eq. 20)}$$

where

D = Fuel pellet diameter in cm (0.9398)
N_p = The number of fuel pins present in the assembly (208)
H = the node height in cm (rounded to 20.00 cm)

The nodal fuel isotopic compositions are listed in the input files in terms of ZAIDs, weight percents, and density (g/cm^3). Each nodal fuel composition is identified by node, initial enrichment, and burnup in the material specification section of the input files described in Attachment II and listed in Attachment IV (compact disc).

7.4.5 BWR Fuel Material

For each of the various depletion parameter cases, the irradiated fuel was represented as having a unique material composition. An active fuel height of 365.76 cm was used in the MCNP calculations for BWRs. The SNF isotopes used in the MCNP cases correspond to those of the Principal Isotope set (YMP 2003, p. 3-34), and come from the SAS2H calculations using Equations 16-19. Each depleted fuel composition is contained on the compact disc in Attachment IV.

The constituent parts of the BWR upper and lower tie plates were homogenized into upper and lower tie plate regions using Equations 11-15. Table 38 contains the homogenized material compositions for the upper and lower tie plates. A detailed description of the tie plate components and the calculation of the homogenized material compositions is contained in the file "BWR tie_plates.xls" (Attachment IV). Note that this spreadsheet also contains the material composition of Zircaloy-2.

Table 38. Tie Plate Homogenized Material Compositions for GE 7×7 Assembly

Element/ Isotope	ZAID[a]	Upper Tie Plate Wt%	Lower Tie Plate Wt%
^{1}H	1001.50c	4.6404	0.0203
C-nat	6000.50c	0.0167	0.0539
^{14}N	7014.50c	0.0209	0.4229
^{16}O	8016.50c	36.8761	0.0243
Si-nat	14000.50c	0.1567	0.0170
^{31}P	15031.50c	0.0094	0.5098
S-nat	16000.60c	0.0063	10.2114
^{50}Cr	24050.60c	0.1675	1.1800
^{52}Cr	24052.60c	3.3546	0.2987
^{53}Cr	24053.60c	0.3877	1.0968
^{54}Cr	24054.60c	0.0981	2.1808
^{55}Mn	25055.50c	0.4179	35.4677
^{54}Fe	26054.60c	0.8152	0.8342
^{56}Fe	26056.60c	13.2579	0.1121
^{57}Fe	26057.60c	0.3118	7.2490
^{58}Fe	26058.60c	0.0419	2.8880
^{58}Ni	28058.60c	1.3073	0.1277
^{60}Ni	28060.60c	0.5208	0.4132
^{61}Ni	28061.60c	0.023	0.1093
^{62}Ni	28062.60c	0.0745	3.6312
^{64}Ni	28064.60c	0.0197	28.8196
Zr	40000.60c	36.9275	0.0514
Sn	50000.35c	0.5457	0.0925
Density (g/cm^3)		2.0063	2.3765

NOTE: [a] ZAID = MCNP material identifier.

8. RESULTS AND CONCLUSIONS

The results of PWR k_{eff} calculations using bounding versus nominal isotopic parameters is shown in Table 39. The data points were chosen to represent enrichment and burnup values that would be likely for PWR SNF, with a five-year cool time. The calculated Δk_{eff} values are shown in Table 39 and plotted in Figure 14. As expected, all k_{eff} values calculated with the bounding isotopic depletion parameters exceed the equivalent calculations using the nominal parameters. These calculations used the Principal Isotope data set and represented PWR SNF inserted into a 21 PWR waste package.

Table 39. PWR Δk_{eff} versus Burnup for Different Enrichments

Burnup (GWd/MTU)	PWR Initial Enrichment (Weight Percent ^{235}U)					
	3.0	σ[a]	4.0	σ	5.0	σ
10	0.00676	0.00079	0.00421	0.00082	0.00365	0.00091
20	0.02096	0.00078	0.01246	0.00083	0.00604	0.00081
30	0.03577	0.00075	0.02327	0.00072	0.01349	0.00079
40	0.05480	0.00064	0.04012	0.00072	0.02712	0.00084

NOTE: [a] Sigma (σ) represents the standard deviation of k_{eff} about the average combined collision, absorption, and track-length estimate due to the Monte Carlo calculation statistics.

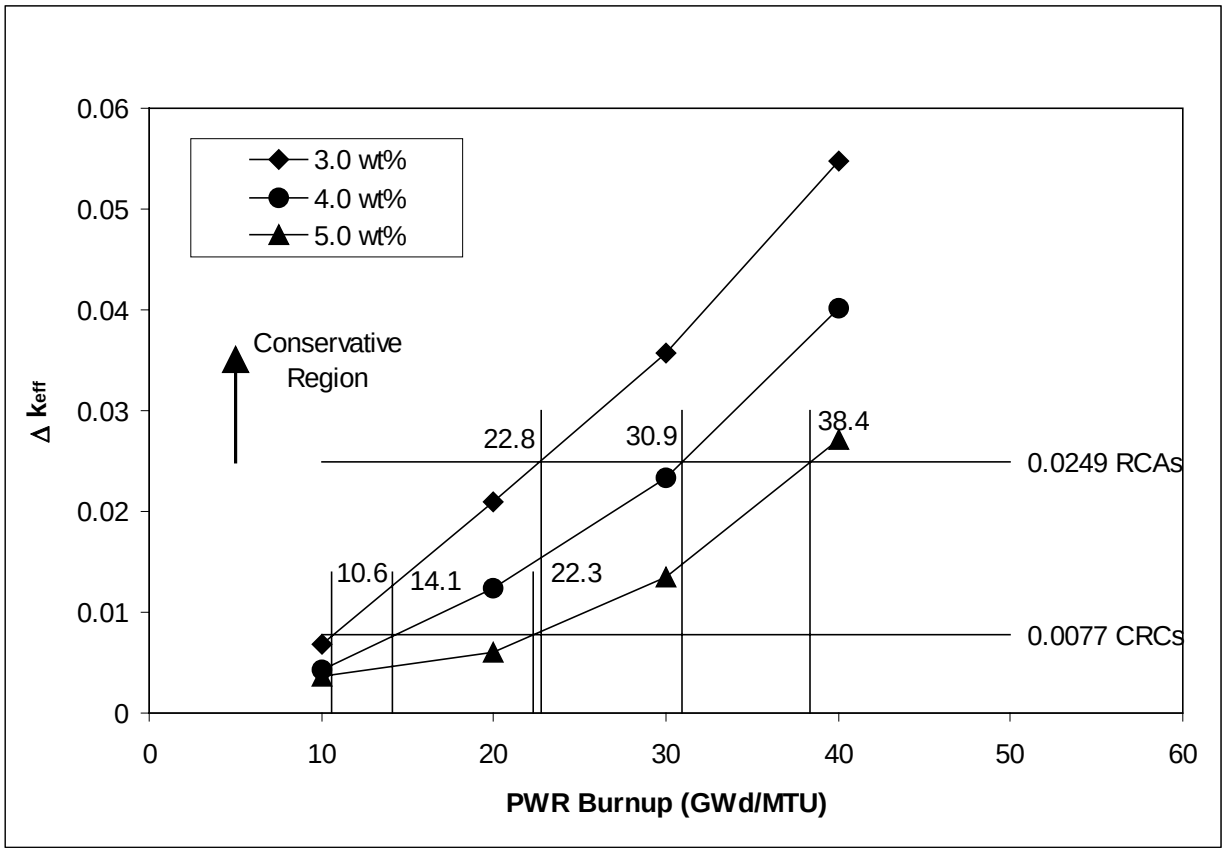


Figure 14. PWR Δk_{eff} Values for Bounding versus Nominal Parameters

Figure 14 shows the bias plus uncertainty for the CRCs as a horizontal line at 0.0077 (from Table 6) and the lower limit and uncertainty from the RCAs at 0.0249 (from Table 10). Inspection of the figure indicates that the bounding depletion parameter set is conservative, using the CRCs, for a 3.0 weight percent enriched fuel assembly if the burnup exceeds 10.6 GWd/MTU, for a 4.0 weight percent enriched fuel assembly if the burnup exceeds 14.1 GWd/MTU, and for a 5.0 weight percent enriched fuel assembly if the burnup exceeds 22.3 GWd/MTU. The conservative cutoff values using the RCA lower limit and uncertainty are at 22.8 GWd/MTU for the 3.0 weight percent enriched fuel, 30.9 GWd/MTU for the 4.0 weight

percent enriched fuel, and 38.4 for the 5.0 weight percent enriched fuel. If the burnup of a fuel assembly is lower than these cut-off values, then the calculated k_{eff} may not be conservative. This will not cause difficulties for the disposal of typical spent fuel assemblies since the threshold for conservative calculations is only about half of the burnup capability, and economics provide utilities incentive to achieve the maximum burnup before discharging an assembly. Underburned fuel assemblies, such as those discharged prematurely from a reactor due to assembly failure, might not possess sufficient burnup to satisfy the waste package loading curve, and could be handled under a fresh fuel assumption. The figure also shows that the use of the RCA dataset would cover a smaller portion of the PWR SNF, principally because of the poorer statistics of this dataset. The calculations of Figure 14 should be performed at five-year and 10,000-year cool times to ensure that differences in the range of applicability are determined.

A similar set of calculations was performed for BWR SNF. The BWR results are similar to the PWR results; however, the BWR k_{eff} values are much lower than the PWR values because of the more effective neutron absorption within the 44-BWR basket. The results for BWR SNF are provided in Table 40 and plotted in Figure 15.

Table 40. BWR Δk_{eff} versus Burnup for Different Enrichments

Burnup (GWd/MTU)	BWR Initial Enrichment (Weight Percent ^{235}U)					
	3.0	σ[a]	4.0	σ	5.0	σ
20	0.06791	0.005	0.03735	0.0005	0.01534	0.0005
30	0.09910	0.0005	0.06410	0.0005	0.03756	0.0005
40	0.14290	0.0005	0.10309	0.0005	0.06901	0.0005
50	0.16910	0.0005	0.13377	0.0005	0.08701	0.0005

NOTE: [a] Sigma (σ) represents the standard deviation of k_{eff} about the average combined collision, absorption, and track-length estimate due to the Monte Carlo calculation statistics.

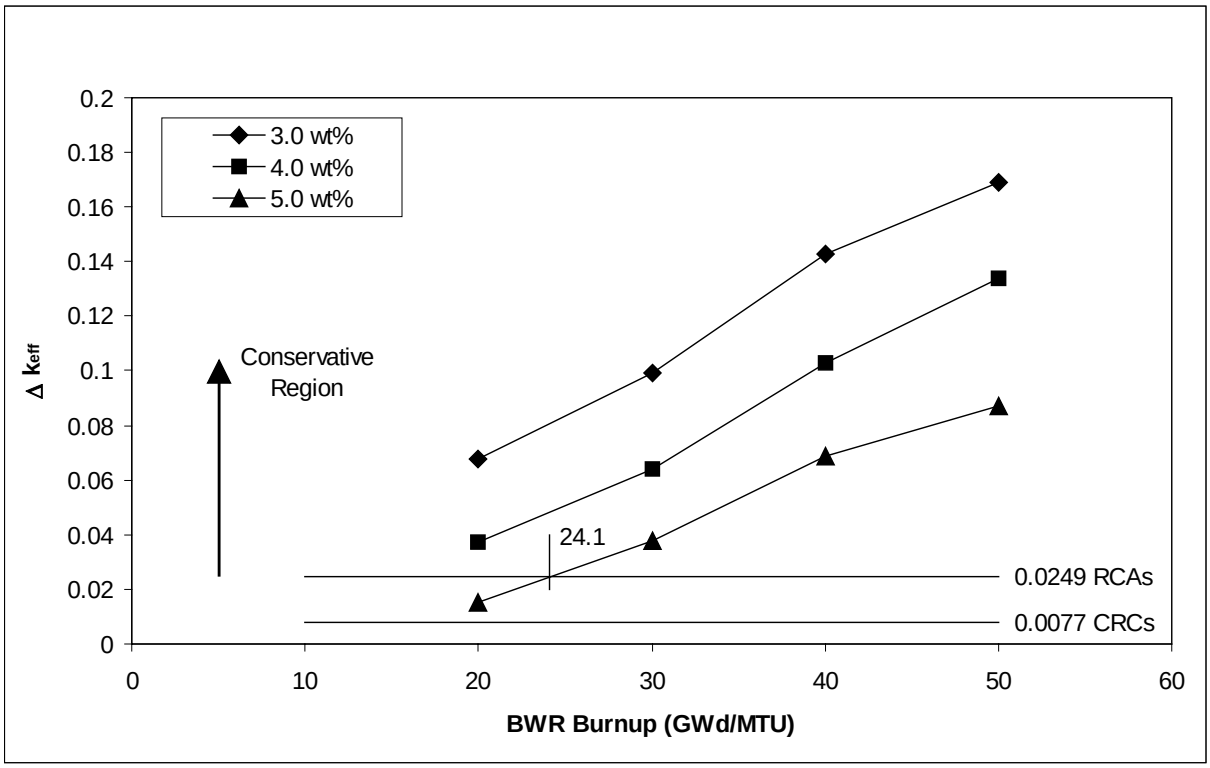


Figure 15. BWR Δk_{eff} Values for Bounding versus Nominal Parameters

Inspection of Figure 15 indicates that the bounding depletion parameter set is conservative, using the CRCs, for a 3.0, 4.0, or 5.0 weight percent enriched fuel assembly if the burnup exceeds 20.0 GWd/MTU. The conservative cutoff values using the RCA lower limit and uncertainty are at 20.0 GWd/MTU for the 3.0 weight percent enriched fuel; at 20.0 GWd/MTU for the 4.0 weight percent enriched fuel; and 24.1 GWd/MTU for the 5.0 weight percent enriched fuel. As for PWR SNF, calculations such as these for a five-year cool time should be repeated at 10,000 years to ensure that the calculations are always conservative.

This report documented the isotopic calculation process and the demonstration of conservatism for the bounding depletion parameters. This report used current data for light water reactor spent nuclear fuel. The isotopic calculation process was discussed in Section 6, and illustrates how to conservatively calculate isotopic concentrations for commercial SNF waste forms over a long time period.

The use of bounding depletion parameters produces isotopic concentrations that will ensure the calculation of conservative reactivities for typical commercial PWR and BWR SNF with initial enrichments between 3.0 and 5.0 weight percent ^{235}U. A set of bounding isotopic depletion parameters was selected that produce conservative criticality results. The magnitude of the conservatism due to the bounding parameters must be greater than the magnitude of the bias plus uncertainty values shown in Figures 14 and 15. The isotopic calculation might not produce conservative reactivities for underburned spent fuel assemblies that were discharged prematurely from the reactor, but these assemblies could be handled using a fresh fuel assumption. Currently, this calculation is only applicable to commercial PWR and BWR SNF. The isotopic calculation

process causes the Δk_{ISO} isotopic value required by *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Section 3.5.3.2.5) to be greater than or equal to zero, then set to zero, because the bounding depletion parameters produce conservative results over the range of applicability.

Three open items from Reamer (2000) were addressed in this document. They were open items 7, 11, and 15, as listed in Section 1 of this report. Open item 7 is addressed in Section 6.3 by a comparison against a two-dimensional code that results in comparable results to the one-dimensional SAS2H. Open item 11 is addressed by the discussion of how to calculate biases and uncertainties in terms of Δk_{eff} (Sections 6.1 and 6.2), a study of half-life and branching fraction uncertainties (Section 6.6), and testing a set of isotopics generated under bounding operating parameters to determine where conservative isotopics are assured (Section 8, Figures 14 and 15). Input for open item 15 is addressed by providing the Δk_{ISO} isotopic bias value required by the *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Section 3.5.3.2.5, Equation 3-1). The bounding depletion parameters cause the isotopic bias to be greater than or equal to zero, which is then set to zero, for any burnup that exceeds the minima established by Figures 14 and 15.

The bounding parameters shown to be conservative in this report can be used in the development of waste package loading curves and in the criticality FEPs screening analyses (BSC 2004e, Section 4).

The results of these calculations are reasonable compared to the inputs. The results are suitable for the intended uses of the open items, loading curves, and criticality FEPs.

9. INPUTS AND REFERENCES

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BSC 2003a. *Calculation of Isotopic Bias and Uncertainty for BWR SNF.* CAL–DSU–NU–000003 REV 00A. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20031030.0007.

BSC 2003b. *Criticality Model Report.* MDL-EBS-NU-000003 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20031013.0002.

BSC 2003c. *Limerick Unit 1 Radiochemical Assay Comparisons to SAS2H Calculations.* CAL–DSU-NU-000002 REV 00A. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20030825.0001.

BSC 2004a. *Design and Engineering, 44 BWR C & E Fuel Plates.* 000-MW0-DSU0-01901-000-00A. Las Vegas, Nevada: Bechtel SAIC Company. ACC: ENG.20040309.0004.

BSC 2004b. *Design and Engineering, 44 BWR Corner Guide.* 000-MW0-DSU0-01601-000-00A. Las Vegas, Nevada: Bechtel SAIC Company. ACC: ENG.20040303.0052.

BSC 2004c. *Design and Engineering, 44-BWR Waste Package Configuration.* 000-MW0-DSU0-00501-000-00B. Las Vegas, Nevada: Bechtel SAIC Company. ACC: ENG.20040213.0005.

BSC 2004d. *Design and Engineering, 44-BWR Waste Package Configuration.* 000–MW0-DSU0-00503-000-00B. Las Vegas, Nevada: Bechtel SAIC Company. ACC: ENG.20040213.0006.

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CRWMS M&O 1998b. *Software Qualification Report for MCNP Version 4B2, A General Monte Carlo N–Particle Transport Code.* CSCI: 30033 V4B2LV. DI: 30033-2003, Rev. 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980622.0637.

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9.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

10 CFR 961. Energy: Standard Contract for Disposal of Spent Nuclear Fuel and/or High-Level Radioactive Waste. Readily available.

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ASTM A 516/A 516M-90. 1991. *Standard Specification for Pressure Vessel Plates, Carbon Steel, for Moderate-and Lower-Temperature Service.* West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: 240032.

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LP-SI.11Q-BSC, Rev. 0, ICN 0. *Software Management.* Washington, D.C.: U.S Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20040225.0007.

9.3 SOURCE DATA, LISTED BY DATA TRACKING NUMBER

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9.4 SOFTWARE CODES

MCNP. 4B2LV. HP. 30033 V4B2LV.

SCALE. V4.4A. HP. 10129-4.4A-00.

10. ATTACHMENTS

The description of the attachments is provided in Table 41.

Table 41. Attachment Listing

Attachment	No. of Pages	Description
I	4	21-PWR Absorber Plate Waste Package Design. (44-BWR Absorber Plate waste package design provided in Attachment IV.)
II	4	Description of SAS2H Input Files, SAS2H Outputs, MCNP Inputs, MCNP Outputs, and 44-BWR Drawings (BSC 2004d) Contained in Attachment IV
III	8	Anderson-Darling Test for Normality
IV	N/A	Compact Disk containing information listed in Attachment II

ATTACHMENT I

21-PWR Absorber Plate Waste Package Design

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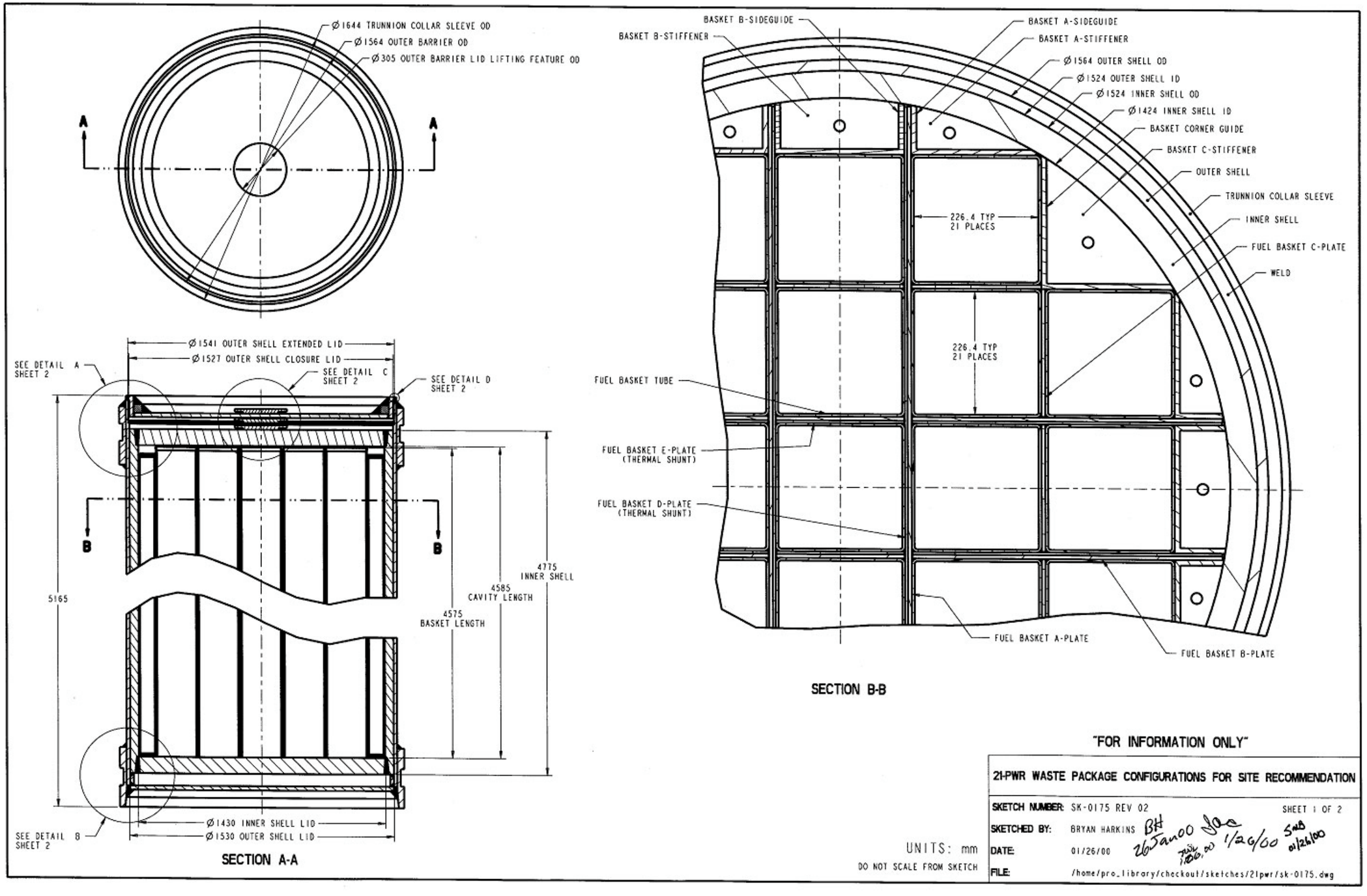
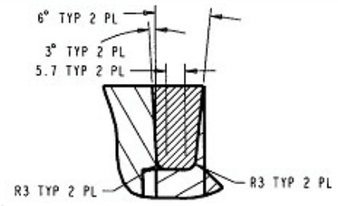
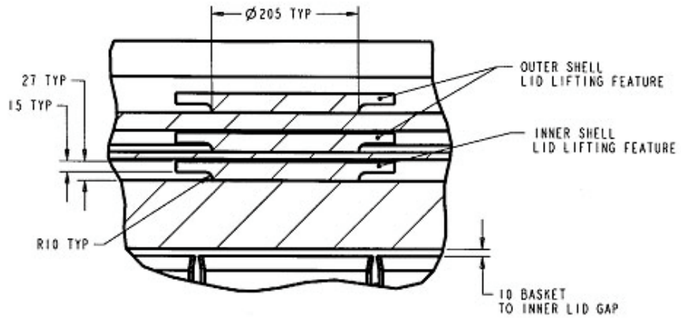
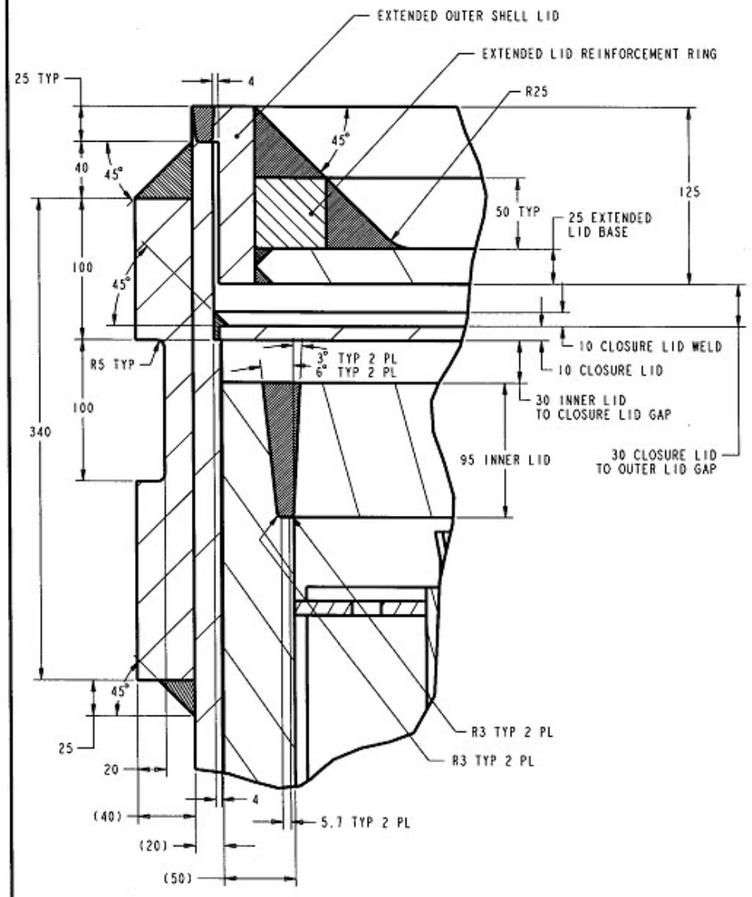

Ø1644 TRUNNION COLLAR SLEEVE OD
Ø1564 OUTER BARRIER OD
Ø305 OUTER BARRIER LID LIFTING FEATURE OD
A
A
Ø1541 OUTER SHELL EXTENDED LID
Ø1527 OUTER SHELL CLOSURE LID
SEE DETAIL A SHEET 2
SEE DETAIL C SHEET 2
SEE DETAIL D SHEET 2
B
B
5165
4775 INNER SHELL
4585 CAVITY LENGTH
4575 BASKET LENGTH
SEE DETAIL B SHEET 2
Ø1430 INNER SHELL LID
Ø1530 OUTER SHELL LID
SECTION A-A
BASKET B-SIDEGUIDE
BASKET B-STIFFENER
BASKET A-SIDEGUIDE
BASKET A-STIFFENER
Ø1564 OUTER SHELL OD
Ø1524 OUTER SHELL ID
Ø1524 INNER SHELL OD
Ø1424 INNER SHELL ID
BASKET CORNER GUIDE
BASKET C-STIFFENER
OUTER SHELL
TRUNNION COLLAR SLEEVE
INNER SHELL
FUEL BASKET C-PLATE
WELD
226.4 TYP 21 PLACES
226.4 TYP 21 PLACES
FUEL BASKET TUBE
FUEL BASKET E-PLATE (THERMAL SHUNT)
FUEL BASKET D-PLATE (THERMAL SHUNT)
FUEL BASKET A-PLATE
FUEL BASKET B-PLATE
SECTION B-B
"FOR INFORMATION ONLY"
21-PWR WASTE PACKAGE CONFIGURATIONS FOR SITE RECOMMENDATION
SKETCH NUMBER: SK-0175 REV 02
SHEET 1 OF 2
SKETCHED BY: BRYAN HARKINS
DATE: 01/26/00
FILE: /home/pro_library/checkout/sketches/21pwr/sk-0175.dwg
UNITS: mm
DO NOT SCALE FROM SKETCH



DETAIL D



DETAIL C

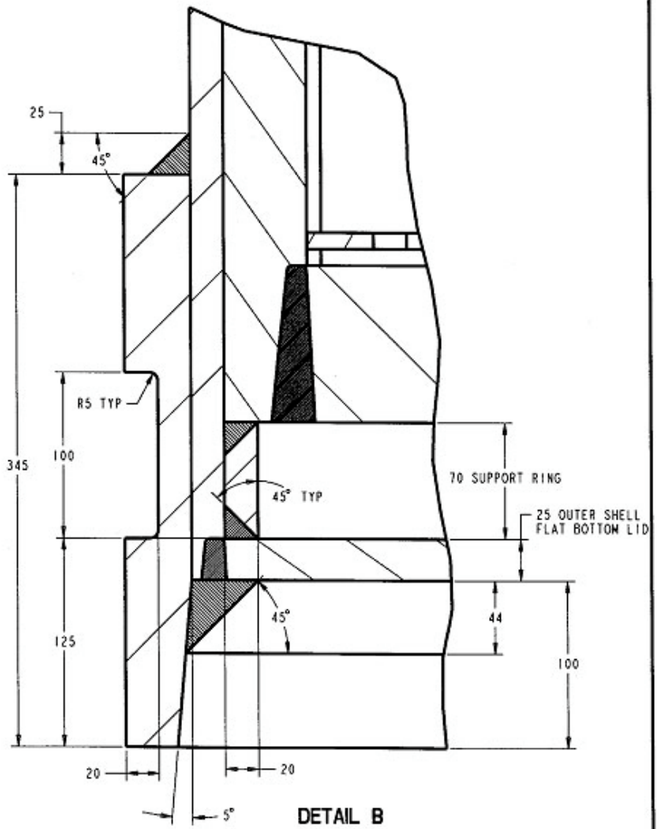


DETAIL A

21-PWR WASTE PACKAGE ASSEMBLY WITH STAINLESS STEEL/BORON PLATES

21-PWR CONTROL ROD WASTE PACKAGE ASSEMBLY WITH CARBON STEEL PLATES

COMPONENT NAME	MATERIAL	THICKNESS	MASS (KG)	QTY ROD
BASKET A-SIDEGUIDE	SA-516 K02700	10	27	32
BASKET A-STIFFENER	SA-516 K02700	10	0.72	64
BASKET B-SIDEGUIDE	SA-516 K02700	10	36	16
BASKET B-STIFFENER	SA-516 K02700	10	1.5	32
BASKET C-STIFFENER	SA-516 K02700	10	2.3	32
BASKET CORNERGUIDE	SA-516 K02700	10	42	16
FUEL BASKET A-PLATE	NEUTRONIT A 978	7	85	8
	#SA-516 K02700	#7	#86	#8
FUEL BASKET B-PLATE	NEUTRONIT A 978	7	85	8
	#SA-516 K02700	#7	#86	#8
FUEL BASKET C-PLATE	NEUTRONIT A 978	7	44	16
	#SA-516 K02700	#7	#45	#16
FUEL BASKET D-PLATE	SB-209 A96061 T4	5	21	8
FUEL BASKET E-PLATE	SB-209 A96061 T4	5	21	8
FUEL BASKET TUBE	SA-516 K02700	5	164	21
INNER SHELL	SA-240 S31600	50	8709	1
INNER SHELL LID	SA-240 S31600	95	1200	2
INNER LID LIFTING FEATURE	SA-240 S31600	27	12	1
OUTER SHELL	SB-575 N06022	20	4193	1
EXTENDED OUTER SHELL LID	SB-575 N06022	25	132	1
EXTENDED OUTER SHELL LID BASE	SB-575 N06022	25	366	1
OUTER LID LIFTING FEATURE	SB-575 N06022	27	13	2
EXTENDED LID REINFORCEMENT RING	SB-575 N06022	50	97	1
OUTER SHELL FLAT CLOSURE LID	SB-575 N06022	10	159	1
OUTER SHELL FLAT BOTTOM LID	SB-575 N0-6022	25	396	1
UPPER TRUNNION COLLAR SLEEVE	SB-575 N06022	40	507	1
LOWER TRUNNION COLLAR SLEEVE	SB-575 N06022	40	497	1
INNER SHELL SUPPORT RING	SB-575 N06022	20	41	1
TOTAL ALLOY 22 WELDS	SFA-5.14 N06022	-	249	**
TOTAL 316 WELDS	SFA-5.9 S31680	-	128	**
WASTE PACKAGE ASSEMBLY	-	-	26035	1
	-	-	#26059	#1
PWR FUEL ASSEMBLY	-	-	773.4*	21
WP ASSEMBLY WITH SNF	-	-	42277	1
	-	-	#42301	#1



DETAIL B

* CRWMS M&O 1997. WASTE CONTAINER CAVITY SIZE DETERMINATION. BBAA00000-01717-0200-00026 REV 00. LAS VEGAS, NV: CRWMS M&O. ACC: MOL.19980106.0061

** REFER TO SK-0191 REV 00 "21-PWR WASTE PACKAGE WELD CONFIGURATION"

02 SMB 01/27/00

SK-0175 REV ~~01~~ | SHEET 2 OF 2

ATTACHMENT II

Description of SAS2H Input Files, SAS2H Outputs, MCNP Inputs, MCNP Outputs, and 44-BWR Drawings Contained in Attachment IV

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ATTACHMENT II: Description of SAS2H Input Files, SAS2H Outputs, MCNP Inputs, MCNP Outputs, and 44-BWR Drawings Contained in Attachment IV

This attachment contains a listing and description of the zip files contained on Attachment IV (read-only CD) of this report. The CD was written using ROXIO Easy CD Creator 5 Basic installed on CRWMS M&O tag number 152395 central processing unit, and can be viewed on most standard CD-ROM drives. The zip archive was created using WINZIP 8.1. The file attributes on the CD are as follows:

Archive Filename	File Size (bytes)	File Date	File Time
Att.zip	5,465,600	09/04/2003	12:55p
Att1.zip	4,690,681	05/13/2004	02:23p
att2.ZIP	593,522	05/12/2004	10:08a
BWR tie_plates.xls	38,912	07/21/2004	02:55p
keff-normality test.mcd	43,601	07/22/2004	10:37a
LWR Bounding MCNP Results and Comparison.xls	46,080	06/04/2004	04:21a
LWR CRC and RCA results tables.xls	55,296	06/04/2004	04:21a

The file "Att.zip" contains the PWR data files, and the file "Att1.zip" contains the BWR data files. There are 168 total files (not including folders) contained in the PWR directory structure, and 108 files in the BWR directory structure.

The file "att2.ZIP" contains four drawings (BSC 2004a; BSC 2004b; BSC 2004c; BSC 2004d) of the 44-BWR waste package design variant in ".pdf" format in four files that provide the geometric details necessary to create the MCNP input file.

The Excel file "BWR tie_plates.xls" contains the detailed description and composition calculation of the BWR upper and lower tie plates for the MCNP calculations.

The Mathcad® file "keff-normality test.mcd" contains the calculations for the k_{eff} normality tests listed in Attachment III.

The Excel file "LWR Bounding MCNP Results and Comparison.xls" contains the data and calculations for Figures 14 and 15.

The Excel file "LWR CRC and RCA results tables.xls" contains the data and calculations for Sections 6.1 and 6.2.

The file "Att.zip" (PWR data files), and the file "Att1.zip" (BWR data files), have similar file structures. Upon extraction of these files from the zip file, the file naming system corresponds as follows for the SAS2H cases of Att.zip and Att1.zip:

- *N01.inp* files are the SAS2H input files.
- *N01.msgs* files contain the standard run-time messages associated with the SAS2H calculations (these are generated by SAS2H).
- *ft72f001.N01* files are ASCII files generated by SAS2H, which were retained, that contain the isotopic concentrations as a function of time (the actual SAS2H output file contains a large amount of information that is not needed for this calculation, therefore it is discarded, but the temporary files SAS2H creates are retained).
- *Ft72-case*_PI_MCNP.N01* files contain the extracted isotope concentrations corresponding to the end of the cooling time specified in the input. The '*' indicates the discharge isotopics based on the number of time steps in the input.
- *N01.log* contains an echo of the input and pertinent information extracted from the SAS2H output file to indicate that the case ran successfully.

The following extracted directory structure corresponds as follows:

/*iso_mod*/: the first level will be iso_mod.

//: the second level is designated *nominal* or *conservative,* where the *nominal* subdirectory contains SAS2H and MCNP files which used the nominal depletion parameters, and the *conservative* subdirectory contains files which used the bounding depletion parameters. The file Att1.zip does not require or contain *conservative* SAS2H files since the isotopics were taken from Wimmer (2004); *conservative* MCNP files are provided.

//*X.XatYY*/: this is a third level subdirectory where the X.X represents the initial ^{235}U enrichment in terms of weight percent ^{235}U and YY represents the burnup in terms of GWd/MTU.

//*MCNP*/: this is a third level subdirectory which contains the MCNP input and output files which, for PWRs, uses an axxyy.z naming system where the a is ether an *n* (nominal case) or a *c* (bounding case); xx represents the initial enrichment (e.g., 30 is 3.0 weight percent ^{235}U initial enrichment); yy represents the burnup in GWd/MTU (e.g., 40 is 40 GWd/MTU); and z is either an *i* or an *O* standing for input or output file, respectively. For BWRs, the file names use a axyy.z naming system where the a is ether an *n* (nominal case) or a *c* (bounding case); x represents the initial enrichment (e.g., 3 is 3.0 weight percent ^{235}U initial enrichment); yy represents the burnup in GWd/MTU (e.g., 40 is 40 GWd/MTU); and z is either an *i* or an *io* standing for input or output file, respectively.

ATTACHMENT III

Anderson-Darling Test for Normality

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ATTACHMENT III: Anderson-Darling Test for Normality

Tests for Normality

The following provides the CRC keff data from (Table 5). There are a total of 57 data points that are tested to verify if the data is normally distributed. To test the data for normality, the Anderson Darling test at the 5 percent significance level is used (D'Agostino and Stephens, 1986 Table 4.7, p. 123).

keff data from (CRCs)

$k1_{eff} :=$

	1
1	1.00156
2	1.00867
3	1.00305
4	1.00267
5	1.00662
6	1.00686
7	0.99922
8	1.00481
9	1.01265
10	1.00096
11	1.0173
12	1.00423
13	1.00784
14	1.01418
15	1.00008
16	1.0075
17	1.00819
18	1.00824
19	1.01973
20	1.01584
21	0.99788
22	1.00108
23	1.00331
24	1.01073
25	1.01154
26	1.01113
27	1.00055
28	1.01222
29	1.00534

$k2_{eff} :=$

	1
1	1.01968
2	1.00108
3	1.01232
4	1.00048
5	1.00443
6	1.00109
7	1.00679
8	0.99428
9	1.00013
10	0.99755
11	1.00565
12	1.00786
13	1.0196
14	1.017
15	1.0172
16	1.0197
17	1.0228
18	1.0098
19	1.0086
20	1.0034
21	1.0017
22	1.0239
23	1.0166
24	1.0104
25	0.9878
26	1.0172
27	1.0195
28	1.0162

$n := 57$ number of data points

$j := 1..29$ $m := 1..28$

$k3_{eff_j} := k1_{eff_j}$

$k4_{eff_m} := k2_{eff_m}$

$k_{eff} := \text{stack}\left(k3_{eff}, k4_{eff}\right)$

$$\mu_{keff} := \frac{1}{n} \cdot \sum_{i=1}^{n} k_{eff_i} \qquad \mu_{keff} = 1.00819$$ mean keff

$$\sigma_{keff} := \sqrt{\frac{1}{n-1} \cdot \sum_{i=1}^{n} \left(k_{eff_i} - \mu_{keff}\right)^2} \qquad \sigma_{keff} = 0.00776$$ keff standard deviation

Set up data for plotting and performing an Anderson-Darling Test.

$i := 1 .. n$

$$CDF_i := \frac{i - 0.3}{n + 0.4} \qquad k := sort\left(k_{eff}\right)$$

$$p_{keff}(x) := pnorm\left(x, \mu_{keff}, \sigma_{keff}\right)$$

Anderson-Darling Test is used to check for goodness-of-fit of the data to the normal distribution.

$w_i := pnorm\left(k_i, \mu_{keff}, \sigma_{keff}\right)$ w is the standard normal cdf of the fitted data.

$$A2 := -n - \left(\frac{1}{n}\right) \cdot \sum_{i=1}^{n} (2 \cdot i - 1) \cdot \left(\ln\left(w_i\right) + \ln\left(1 - w_{n-i+1}\right)\right)$$ A2 is the test equation for the Anderson-Darling test.

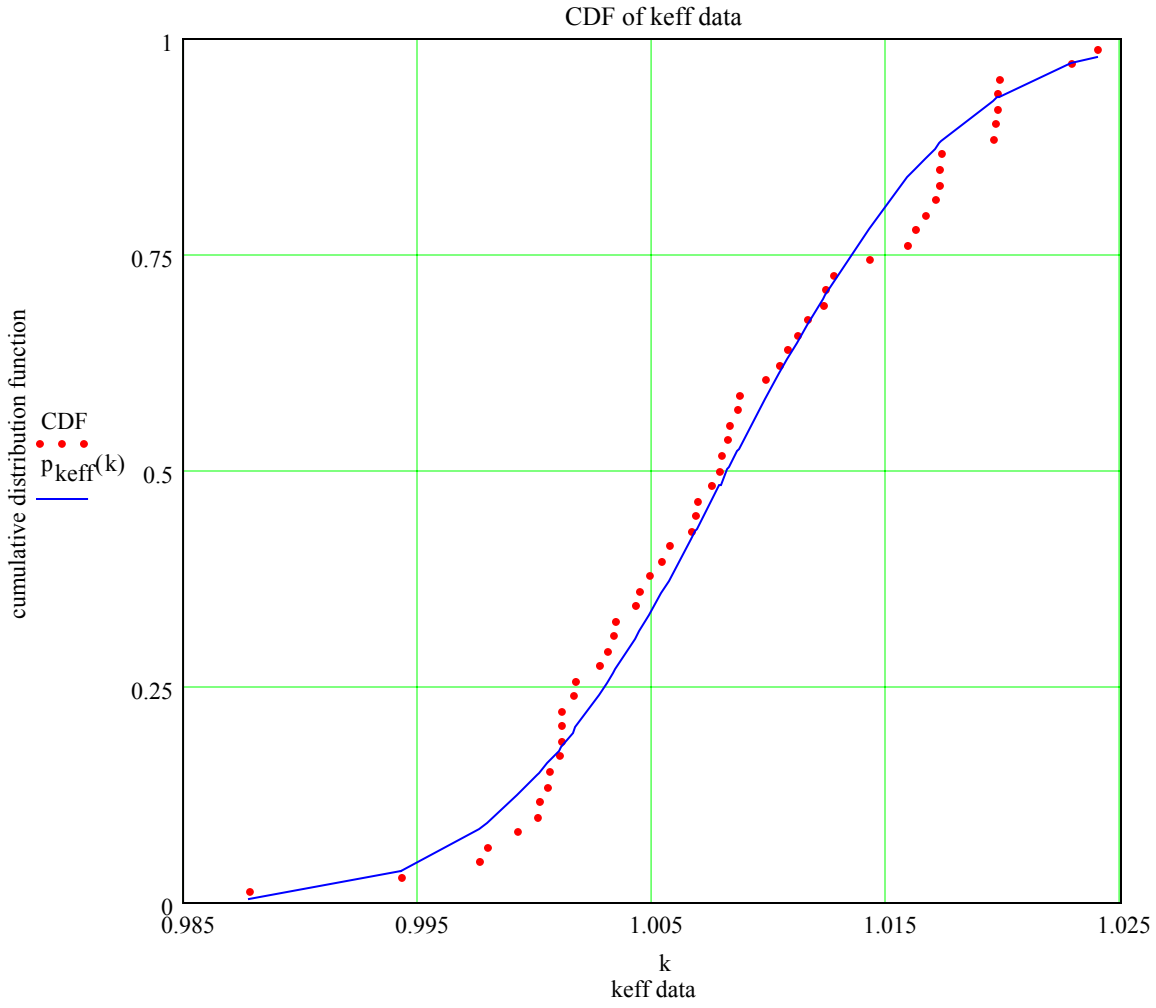
$A2 = 0.51101$

$$A2m := A2 \cdot \left(1 + \frac{0.75}{n} + \frac{2.25}{n^2}\right)$$ A2m is used to adjust the test limit due to the small amount of data points.

$A2m = 0.51809$

Anderson-Darling test for 5 percent significance requires the test value to be less than critical limit based on a small amount of data points and a significant level of 0.05. Anderson-Darling critical limit at the 0.05 significance level is 0.752

A2m < A-Dcrit; therefore, the normal distribution can be used to represent the data.


CDF of keff data
cumulative distribution function
CDF
$p_{keff}(k)$
1
0.75
0.5
0.25
0
0.985
0.995
1.005
1.015
1.025
k
keff data

The Δkeff data (calculated minus measured) for RCAs from Table 9 are tested for normality using the Anderson Darling Test (D'Agostino and Stephens, 1986 Table 4.7, p. 123).

Δkeff data (RCAs)

$\Delta k_{eff1} :=$

	1
1	0.00412227
2	0.0130995
3	-0.00976433
4	0.0198865
5	0.01858666
6	0.02809463
7	0.05933095
8	0.00833882
9	0.01135142
10	0.03084154
11	0.02237036
12	0.02951951
13	0.04937124
14	0.01734063
15	0.02532874
16	0.02035515
17	0.01671021
18	0.01712044
19	0.02349891
20	0.00103132
21	0.00354524
22	0.00506662
23	0.00060525
24	0.00142203
25	0.00438838
26	0.01073427
27	0.00434396
28	0.00359896
29	0.00558787
30	0.00173558

$\Delta k_{eff2} :=$

	1
1	0.00625558
2	-0.00035095
3	0.00487309
4	0.00026534
5	0.00347327
6	-0.0034783
7	-0.00305559
8	-0.01842102
9	-0.01055057
10	-0.02685675
11	-0.02662582
12	-0.01740549
13	-0.02247442
14	-0.02027927
15	0.01233056
16	0.01176373
17	-0.0038099
18	-0.00697934
19	-0.01591327
20	-0.01331596
21	-0.01182123
22	-0.01923143
23	-0.02597508
24	-0.00162439
25	-0.00332755
26	0.05596062
27	0.06750739
28	0.06073996
29	0.04333645
30	0.07466646

$\Delta k_{eff3} :=$

	1
1	0.04682395
2	0.04717904
3	0.06351614
4	0.07560005
5	0.0178536
6	0.0548018
7	0.01646112
8	0.03235751
9	0.03117026
10	0.01576827
11	0.01651195
12	0.01516507
13	0.01853633
14	0.01794261
15	-0.00446
16	-0.00111
17	0.00038
18	-0.00246
19	-0.00353
20	0.00502
21	-0.00335
22	-0.00051
23	-0.00387
24	-0.00627
25	-0.00766
26	-0.00635
27	-0.00423
28	-0.00288
29	-0.00507
30	-0.00015

$j := 1..30$

$\Delta k_{eff5_j} := \Delta k_{eff1_j}$ $\Delta k_{eff6_j} := \Delta k_{eff2_j}$ $\Delta k_{eff7_j} := \Delta k_{eff3_j}$

$\Delta k_{eff4} :=$

	1
1	-0.00319
2	-0.00297
3	-0.02147
4	-0.00719
5	0.00086
6	-0.00519
7	-0.01665
8	0.00771
9	0.0015
10	0.00811
11	0.00489
12	-0.00881
13	-0.01547
14	-0.01865
15	-0.04204
16	-0.0587
17	0.02053
18	0.00336
19	-0.06713
20	-0.06417
21	-0.03369
22	-0.03198

$m := 1 .. 22$

$\Delta k_{eff8_m} := \Delta k_{eff4_m}$

$\Delta k_{eff} := stack(\Delta k_{eff5}, \Delta k_{eff6}, \Delta k_{eff7}, \Delta k_{eff8})$

$n_{\Delta k} := length(\Delta k_{eff})$

$n_{\Delta k} = 112$ number of data points

$i := 1 .. n_{\Delta k}$

$\mu_{\Delta keff} := \frac{1}{n_{\Delta k}} \cdot \sum_{i=1}^{n_{\Delta k}} \Delta k_{eff_i}$ $\mu_{\Delta keff} = 0.00545$ Δkeff mean

$\sigma_{\Delta keff} := \sqrt{\frac{1}{n_{\Delta k} - 1} \cdot \sum_{i=1}^{n_{\Delta k}} \left(\Delta k_{eff_i} - \mu_{\Delta keff}\right)^2}$ $\sigma_{\Delta keff} = 0.02569$ Δkeff standard deviation

Set up data for plotting and performing an Anderson-Darling Test.

$$CDF_i := \frac{i - 0.3}{n_{\Delta k} + 0.4} \qquad \Delta k := sort\left(\Delta k_{eff}\right)$$

$$p_{\Delta keff}(x) := pnorm\left(x, \mu_{\Delta keff}, \sigma_{\Delta keff}\right)$$

Anderson-Darling Test is used to check for goodness-of-fit of the data to the normal distribution.

$w_i := pnorm\left(\Delta k_i, \mu_{\Delta keff}, \sigma_{\Delta keff}\right)$ w is the standard normal cdf of the data.

$$A2 := -n_{\Delta k} - \left(\frac{1}{n_{\Delta k}}\right) \cdot \sum_{i=1}^{n_{\Delta k}} (2 \cdot i - 1) \cdot \left(\ln\left(w_i\right) + \ln\left(1 - w_{n_{\Delta k} - i + 1}\right)\right)$$

A2 is the test equation for the Anderson-Darling test.

$A2 = 2.2793$

$$A2m := A2 \cdot \left(1 + \frac{0.75}{n_{\Delta k}} + \frac{2.25}{n_{\Delta k}^{\,2}}\right)$$

A2m is used to adjust the test limit due to the small amount of data points.

$A2m = 2.29497$

Anderson-Darling test for 5 percent significance requires the test value to be less than critical limit based on a small amount of data points and a significant level of 0.05. Anderson-Darling critical limit at the 0.05 significance level is 0.752

A2m > A-Dcrit; therefore, the normal distribution should not be used to represent the data.