OCRWM	MODEL COVER SHEET	1. QA: QA Page 1 of 64

2. Type of Mathematical Model:

☒ Process Model ☐ Abstraction Model ☐ System Model

Describe Intended Use of Model:

Establish process to conservatively calculate isotopic concentrations for commercial spent nuclear fuel

3. Title:

Isotopic Model Report for Commercial SNF Burnup Credit

4. DI (including Rev. No. and Change No., if applicable):

MDL-DSU-NU-000001 REV 00 ICN 01

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ENCLOSURE 1

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4. Revision / Change Number:	5. Description of Revision/Change:
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00 / 01	Document modified to incorporate comments from DOE AP-6.28Q review. Changed lines are indicated by a black vertical line in the margin. Modifications were made in the following areas: Executive Summary, Sections 1, 4.2, 4.3, 4.4.2, 4.4.2, 5, 6, 6.1, 6.1.2, 6.2.1, 6.2.2, 6.4, 6.5, 7.1, 7.2, 7.4.3, 8, 9.1, 9.2, and 10.

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 methodology is the isotopic model. This model report documents the isotopic model and its validation. The validation uses current data for pressurized water reactor spent nuclear fuel and provides a validated model that may be updated as additional data becomes available.

The isotopic model is to be used for conservatively calculating isotopic concentrations for criticality calculations for commercial spent nuclear fuel waste forms. The isotopic model 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 model also provides the isotopic component of the critical limit, as required in *Disposal Criticality Analysis Methodology Topical Report*[1]. This isotopic model ensures that the Δk_{ISO} term of the critical limit equation may be set to zero, indicating that no additional isotopic term is needed to ensure conservatism.

This model 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 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."
>
> Open Item 11: "The DOE is required to develop an acceptable methodology for establishing bias and uncertainties for the isotopic depletion model."

This model report provides a description of the model and validation process, the intended use of the model, limitations of the model, and a discussion of how the isotopic model fits within the overall methodology from *Disposal Criticality Analysis Methodology Topical Report*[1]. This model report also provides a data example of the application.

Based on applicable pressurized water reactor experimental results from commercial reactor critical and radiochemical assays, this report concludes that the isotopic model is a valid tool for calculating the isotopic contents of spent nuclear fuel. This model report recommends that the isotopic model be implemented for pressurized water reactor spent nuclear fuel.

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[1] Yucca Mountain Site Characterization Project 2003. *Disposal Criticality Analysis Methodology Topical Report.* YMP/TR-004Q, Rev. 02D. Las Vegas, Nevada: Yucca Mountain Site Characterization Office. ACC: MOL.20030617.0322. TBV-5072

[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. ACC: MOL.20000919.0157.

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ACRONYMS

CRC	commercial reactor critical
ENDF	Evaluated Nuclear Data File
MTU	metric ton of uranium
PWR	pressurized water reactor
RCA	radiochemical assay
SNF	spent nuclear fuel

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1. PURPOSE

The scope of this model report is to document the isotopic model and its validation. The isotopic model will be used to conservatively calculate isotopic concentrations for commercial spent nuclear fuel waste forms. The isotopic model is a component of the methodology presented in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003). How the isotopic model fits in 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 spent nuclear fuel (SNF). A method was developed for confirming that bounding parameters for isotopic calculations are conservative. Results from calculations or analyses using this model will be used in generating waste form characteristics, which are used as input parameters in the criticality model for evaluating the criticality potential of the waste form configurations, and the geochemistry model for generating geochemical material performance characteristics.

The limitation of the isotopic model is that it is currently validated only for application to pressurized water reactor SNF.

The *Isotopic Model Report* addresses specific open items 7 and 11 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)

The isotopic model provides the Δk_{ISO} isotopic value required by *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Section 3.5.3.2.10). The method for confirming that the bounding parameters of the isotopic model 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 acceptance equation in *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Eq. 3-7).

Also, an issue of "compensating errors" between isotopic concentrations and the microscopic cross sections of an isotope has been addressed in Section 6.1.3.

This model activity follows the description in *Technical Work Plan for: Risk and Criticality Department* (BSC 2002a).

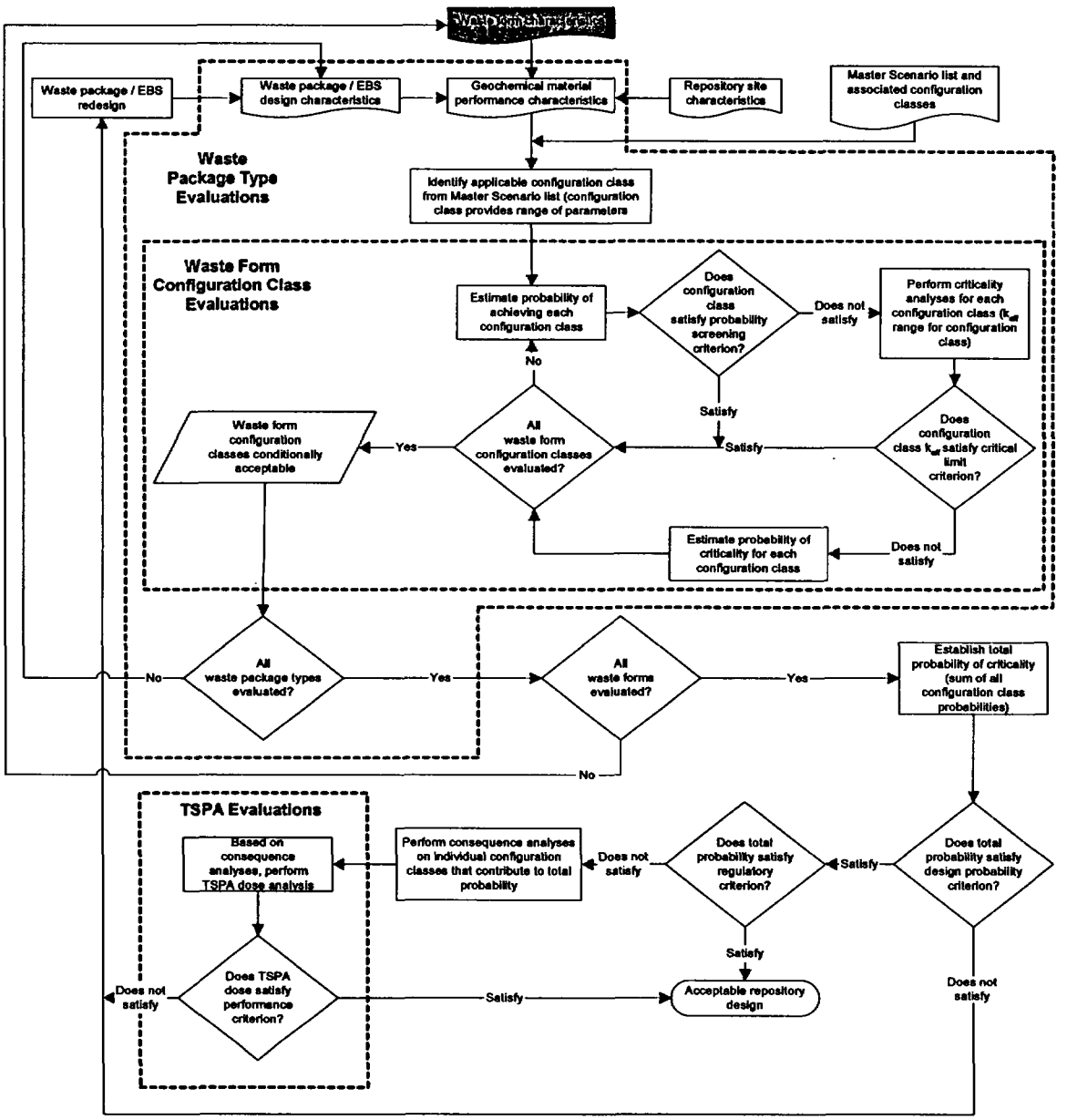


Figure 1. Disposal Criticality Analysis Methodology

2. QUALITY ASSURANCE

Development of this model report and the supporting modeling activities have been determined to be subject to the Yucca Mountain Project's quality assurance program in *Technical Work Plan for: Risk and Criticality Department* (BSC 2002a, Section 8). Approved quality assurance procedures identified in the technical work plan (BSC 2002a, Section 4) have been used to conduct and document the activities described in this model report. The technical work plan also identifies the methods used to control the electronic management of data (BSC 2002a, Section 8) during the modeling and documentation activities.

This model report concerns engineered barriers that are included in *Q-List* (YMP 2001) as "Quality Level - 1" items important to waste isolation. The report contributes to the analysis and modeling data used to support performance assessment; however, the conclusions do not directly impact engineered features important to safety, as defined in AP-2.22Q, *Classification Analyses and Maintenance of the Q-List.*

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
- Version/Revision Number: Version 4.4A
- Status/Operating System: Qualified/HP-UX B.10.20
- Software Tracking Number: 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. The SAS2H code sequence of SCALE that was used is (1) appropriate for the application of commercial 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 SNF compositions. The software specifications are as follows:

- Program Name: MCNP
- Version/Revision Number: Version 4B2LV
- Status/Operating System: Qualified/HP-UX B.10.20
- Computer Software Configuration Item 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. The MCNP software used was (1) appropriate for the application of multiplication factor calculations, (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 1998a) and *MCNP-A General Monte Carlo N-Particle Transport Code* (Briesmeister 1997), and (3) obtained from Software Configuration Management in accordance with appropriate procedures.

4. INPUTS

4.1 DATA AND PARAMETERS

No direct input was used in the development of this model. Input sources for the demonstration of the model are listed in Section 4.4.

4.2 CRITERIA

This report complies with the Yucca Mountain Project's Quality Assurance program as stated in *Technical Work Plan for: Risk and Criticality Department* (BSC 2002a, Section 3), is in accordance with Bechtel SAIC Company, LLC management directives, and is in compliance with the Bechtel SAIC Company, LLC program, Planning and Control processes.

The applicable requirement(s) come from *Project Requirements Document* (Canori and Leitner 2003), and is as follows:

"The methodology defined in the *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003) shall be used to demonstrate acceptable criticality control for canisters and the waste packages in which they are disposed." (Canori and Leitner 2003, PRD-013/T-016).

Applicable open items from "Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0" (Reamer 2000, Section 4) addressed by this work include numbers 7 and 11, 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."
>
> Open Item 11 – "The DOE is required to develop an acceptable methodology for establishing bias and uncertainties for the isotopic depletion model."

4.3 CODES AND STANDARDS

The following codes and standards are used for the bases of this report:

- *1998 ASME Boiler and Pressure Vessel Code* (ASME 1998)
- *1995 ASME Boiler and Pressure Vessel Code* (ASME 1995)
- *Standard Specification for Heat-Resisting Chromium and Chromium-Nickel Stainless Steel Plate, Sheet, and Strip for Pressure Vessels* (ASTM A 240/A 240M-94b, 1994)

- *Standard Specification for Wrought Zirconium Alloy Seamless Tubes for Nuclear Reactor Fuel Cladding* (ASTM B 811-90, 1991)
- *Standard Practice for Preparing, Cleaning, and Evaluating Corrosion Test Specimens* (ASTM G 1-90, 1999).

4.4 INPUT PARAMETERS

The following data tracking numbers were used for representing material properties:

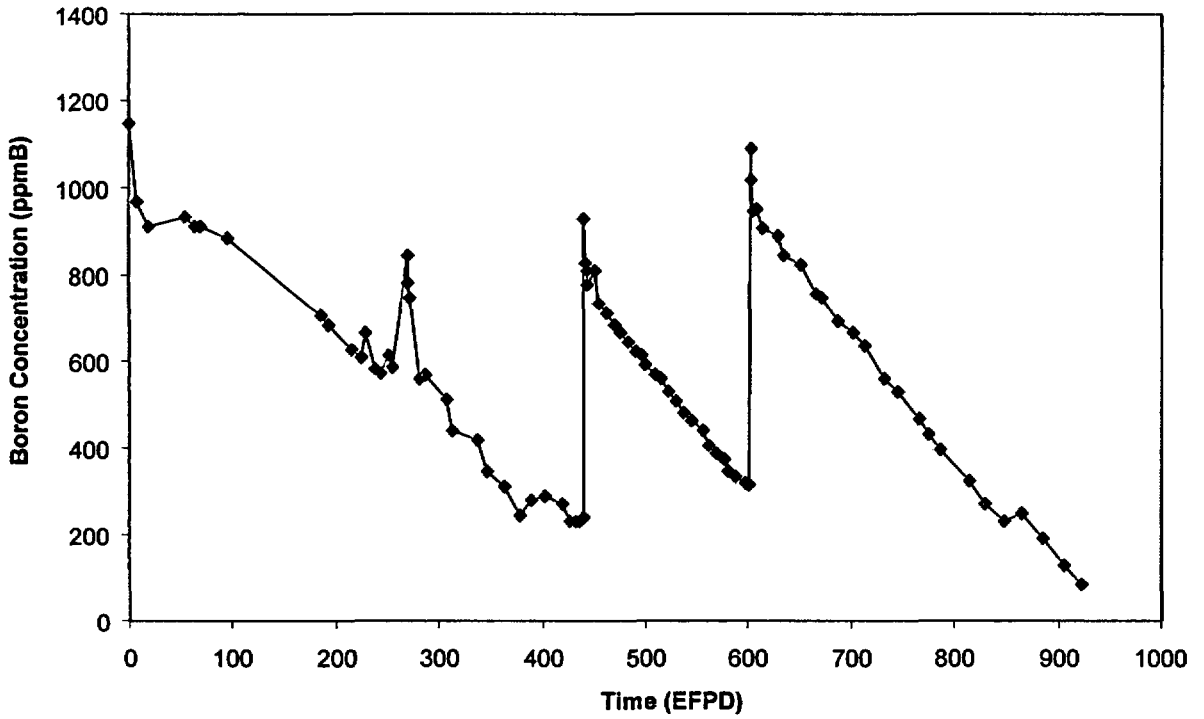
- DTN: MO0003RIB00071.000, Physical and Chemical Characteristics of Alloy 22
- DTN: MO0003RIB00072.000, Physical and Chemical Characteristics of Steel, A 516
- DTN: MO0109RIB00049.001, Waste Package Material Properties: Neutron Absorbing Materials.

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-94b, 1994)
- *Standard Specification for Wrought Zirconium Alloy Seamless Tubes for Nuclear Reactor Fuel Cladding* (ASTM B 811-90, 1991)
- *Standard Practice for Preparing, Cleaning, and Evaluating Corrosion Test Specimens* (ASTM G 1-90, 1999)
- *Practical Handbook of Materials Science* (Lynch 1989).

4.4.1 Boron Letdown Curve for Crystal River Unit 3

The nominal 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 isotopic model is 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	—	—

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

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

4.4.2 Generic Pressurized Water Reactor 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 isotopic model. 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:

- Fuel temperature, 861.3 K
- Moderator temperature, 579.8 K; Density, 0.7556 g/cm^3
- Average specific power, 43.029 MW/MTU
- Moderator boron concentration values are presented in Figure 2 and were interpolated from the nominal values specified in Table 1.

4.4.3 Parameters Used in Demonstration and Validation

The following is a listing of various parameters that were used in demonstrating and validating the model process:

- Commercial reactor critical (CRC) technical information from *Summary Report of Commercial Reactor Critical Analyses Performed for the Disposal Criticality Analysis Methodology* (CRWMS M&O 1998b)
- Radiochemical assay (RCA) technical information from *Calculation of Isotopic Bias and Uncertainty for PWR Spent Nuclear Fuel* (BSC 2002b)
- Depletion parameters for demonstrating bounding parameter selection from *PWR Depletion Parameter Sensitivity Evaluation* (BSC 2001).

5. ASSUMPTIONS

The following assumptions are made by this model report:

It is assumed that the Babcock & Wilcox 15x15 Mk-B2 assembly design is representative of all PWR SNF and is the most limiting PWR fuel assembly design. The basis for this assumption is that a previous analysis for the BR-100 transportation cask established the Babcock & Wilcox 15x15 fuel assembly as one of the most reactive fuel assembly designs (p. II 6-6, B&W Fuel Company 1991). This assumption does not require further confirmation because k_{eff} is dependent upon the global behavior of the neutron population as opposed to a localized behavior, so that the geometric details of the fuel design do not have a strong effect. This assumption is used in Section 7.1.

It is assumed that the Crystal River Unit 3 boron letdown curve is representative of PWR SNF up to 50 GWd/MTU. 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. This assumption does not require further confirmation because it is only used in an example demonstration of how to confirm the model generates conservative isotopes - any boron letdown curve could have been used. This assumption is used in Section 7.1.

It is assumed that the CRC PWR data set (CRWMS M&O 1998b) is an adequate statistical representation of PWR reactor designs. Forty-one startups or restarts were analyzed for four different PWR reactors. The basis for this assumption is that the details of reactor design do not have a strong effect on reactivity. This assumption does not require further confirmation because

the data set follows a normal distribution and contains enough data points to allow a 95/95 confidence interval. This assumption is used in Section 6.1.

It is assumed that the systematic error is the same in k_{eff} calculations for both reactor and waste package environmental conditions. The basis for this assumption is that the systematic error proceeds from the resonance cross section treatment (principally uranium-238) in the Evaluated Nuclear Data File (ENDF). 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, and 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 accounted for. This assumption is used in Section 7.

6. MODEL DISCUSSION

When modeling 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 which 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.

The purpose of the isotopic model is to conservatively calculate isotopic concentrations for commercial SNF waste forms over a long time period. Results from calculations or analyses using this model will be used in the criticality model for evaluating the criticality potential of the waste form configurations. The isotopic model is appropriate for commercial PWR SNF with initial enrichments between 2.0 and 5.0 wt% uranium-235 and burnups between 10 and 50 GWd/MTU.

A listing of corroborating or supporting data, models, or information used to complete the model development activities, along with their sources is provided as follows in Table 2.

Conservative calculations of isotopic concentrations are ensured by choosing bounding parameters for the fuel irradiation. A study of the effects of varying parameters for 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.

Table 2. Supporting Information and Sources for Model Development Activities

Description	Source
Depletion parameter sensitivity study	BSC 2001
Disposal criticality analysis methodology	YMP 2003
CRC analyses results	CRWMS M&O 1998b
Isotopic bias and uncertainty study, and RCA information summary	BSC 2002b
Code-to-code comparison study	BSC 2002c
Representative assembly characteristics	Punatar 2001
General reference to laboratory critical experiments	CRWMS M&O 1999a
General reference to criticality model report	BSC 2003

The isotopic model provides a means for testing the chosen parameters for conservatism. The choice of bounding parameters is left to the discretion of the user of the isotopic model. Example bounding parameter values were chosen in this report so that the model conservatism test procedure could be illustrated. 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 1 in Section 3.5.3.2.10 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 2003)
- 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 (CRWMS M&O 2000a) and k_{eff} values were calculated (using the calculated isotopics) using the MCNP computer code (Briesmeister 1997). 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 3.

Table 3. 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, p. 3-34

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 1998b; BSC 2002b). Further, a code-to-code comparison of SAS2H calculations versus CASMO-3 calculations was previously performed in *Summary Report of Code to Code Comparisons Performed for the Disposal Criticality Analysis Methodology* (BSC 2002c) to ensure that code-dependent issues had been addressed.

Using bounding depletion parameters for the generation of spent fuel assembly isotopics will ensure conservative criticality calculations for PWR SNF in any desired waste package for both preclosure and postclosure. PWR SNF with initial enrichments between 2.0 and 5.0 wt% uranium-235, and burnups between 10 and 50 GWd/MTU were evaluated. Burnable absorbers are simply another depletion parameter for the isotopic model as shown in Section 6.4.6. Separate sets of 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 1998c, 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 was used (illustrated in Attachment I). The fuel assembly design was represented in detail using specifications for the Babcock & Wilcox 15x15 assembly (Punatar 2001).

6.1 COMMERCIAL REACTOR CRITICAL BENCHMARKS

Conventional criticality benchmarks for fresh, unirradiated PWR 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 uranium-235, cause fission, and contribute to the nuclear chain reaction. Neutrons that are captured by other isotopes, such as uranium-238 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 uranium-235 and uranium-238, with a small amount of uranium-234, the desired range of fuel enrichments between about 2.0 and 5.0 wt% uranium-235 have been tested by a number of different critical experiment projects (CRWMS M&O 1998b; CRWMS M&O 1999a; BSC 2003, 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 beginning-of-cycle 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 reactor statepoints using Principal Isotope results, extracted from *Summary Report of Commercial Reactor Critical Analyses Performed for the Disposal Criticality Analysis Methodology* (CRWMS M&O 1998b), are provided in Table 4. Note that all statepoints are for PWR reactors at hot, zero power. Reactor conditions at these statepoints are isothermal, and the geometric configuration of the fuel and control rods are known. Xenon-135 has decayed to essentially zero concentration for these statepoints. These CRC statepoints constitute the only available critical experiments for irradiated fuel. CRC data at full or partial power conditions are not appropriate due to the presence of xenon-135 and three-dimensional effects. Therefore, such data were not included in the presented set of 41 statepoints.

Table 4. Tabulation of CRC Reactivities

Case Name	k_{eff}	σ	Case Name	k_{eff}	σ
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			

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 1998b, p. 42). 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 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 41 data points is calculated 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 Shapiro-Wilks test for normality, and is illustrated in the quantile plot in Figure 3 and the histogram in Figure 4.

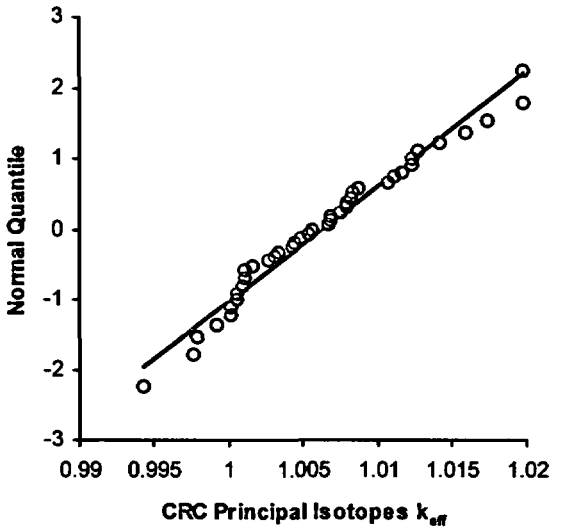


Figure 3. Normal Quantile Plot CRC Data

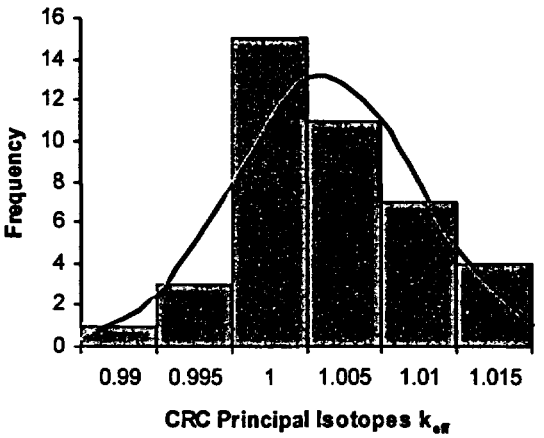


Figure 4. Histogram Plot for CRC Data

The sum of the bias and uncertainty is calculated as illustrated in Equation 3.

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

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 standard deviation associated with the selected Δk_{eff} values as shown in Equation 4

σ_{MCNP} = the standard deviation of the MCNP calculations, calculated as shown in Equation 5

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

where

N = total number of values

x = Δk_{eff} values

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

where

σ_i = the MCNP standard deviation for a CRC case

Bias and uncertainty values were calculated for the CRC data set, as shown in Table 5.

Table 5. Bias and Uncertainty for CRC Data Set

Isotope Set	Bias (β_{ave})	$\sigma_{\Delta k_{eff}}$	σ_{MCNP}	K_b[a]	Sum of Bias and Uncertainty
Principal Isotopes	0.0062	0.0061	0.00045	2.126	-0.0068

NOTE: [a] Multiplier taken from Table A-7 of *Experimental Statistics* (Natrella 1963) for a 95/95 tolerance limit for 40 data points, which is conservative for the 41 data points.

The PWR CRCs show a bias of 0.0062, indicating an overprediction of k_{eff} for SNF of less than one percent. The standard deviation of the data set of 41 CRCs was 0.0061. Thus the sum of the bias and uncertainties at the 95 percent confidence level is -0.0068, or about two-thirds of a percent Δk_{eff}. This Δk_{eff} value of 0.0068 is the criterion that will be used in Section 7.5 to determine if the bounding isotopic parameter set is conservative. Thus, if the bounding parameter set produces an increase in k_{eff} greater than 0.0068, 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 and an accurate k_{eff} could be obtained for the CRC benchmark experiment. 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 without such adjustments in the CRCs, therefore these "compensating errors" do not occur.

6.2 RADIOCHEMICAL ASSAYS

RCA data can provide direct validation 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. This calculation utilizes 74 different radiochemical assayed SNF samples from 22 different fuel assemblies that were irradiated in eight different PWRs. The irradiated fuel samples evaluated span an initial enrichment range of 2.453 wt% through 4.67 wt% uranium-235 enrichment, and burnups from 6.92 GWd/MTU through 55.7 GWd/MTU. The sample parameters are given in Table 6.

Table 6. PWR RCA Parameters

Reactor	Assembly Design	# of Samples/ Assemblies/Rods	Sample Burnups (GWd/MTU)	Initial Enrichments (Wt% U-235)
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 15x15, 20 guide tubes	5/2/5	30.72-31.56	2.556
Mihama	Westinghouse 15x15, 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 15x15, 20 guide tubes, 12 BPRs[c]	4/1/1	16.02-31.66	2.561
Obrigheim	Siemens 14x14	6/5/special[d]	25.93-29.52	3.13
Calvert Cliffs	Combustion Engineering 14x14 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	Babcock & Wilcox 15x15, 16 guide tubes	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

Source: BSC 2002b, pp. 15 and 16

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.

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 7.

Table 7. Number of Samples for Each Isotope[a, b]

Isotope	# of Samples	Isotope	# of Samples	Isotope	# of Samples
U-234	44	Nd-145	31	Eu-155	14
U-235	74	Nd-146	20	Gd-155	22
U-236	74	Nd-148	44	Cm-242	31
U-238	49	Nd-150	20	Cm-243	11
Pu-238	60	Pm-147	3	Cm-244	32
Pu-239	74	Sm-147	22	Am-241	28
Pu-240	74	Sm-148	3	Am-242	6
Pu-241	74	Sm-149	22	Am-242m	27
Pu-242	70	Sm-150	22	Am-243	34
Np-237	31	Sm-151	22	U-232	9
Cs-133	3	Eu-151	22	Pu-236	3
Cs-134	11	Sm-152	22	Ag-109	11
Cs-135	3	Eu-153	22	Mo-95	11
Cs-137	22	Sm-154	3	Tc-99	11
Nd-143	31	Eu-154	3	Ru-101	11
Nd-144	12	Gd-154	3	Rh-103	11

Source: BSC 2002b

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 uranium-233.
[b] Certain isotopes were omitted from the Three Mile Island sample MCNP calculations for having concentrations less than 0.0001 wt% in either the measured or calculated composition. Among these were the isotopes Eu-151 and Am-242m in the assembly NJ05YU MCNP calculations, and the isotopes Eu-151, Am-242m, Mo-95, Tc-99, Ru-101, and Rh-103 in the NJ070G MCNP cases. In addition, the isotopes Nd-146 and Nd-150 were also omitted since the MCNP cross section libraries for these isotopes were not available, and their concentrations were very small (< 0.1 wt%) (BSC 2002b, p. 75).

6.2.1 RCA Data

The method used to determine the Δk_{eff} for RCAs compared to SAS2H calculations is illustrated in Figure 5. All k_{eff} calculations were performed in a waste package geometry corresponding to that illustrated in Attachment I.

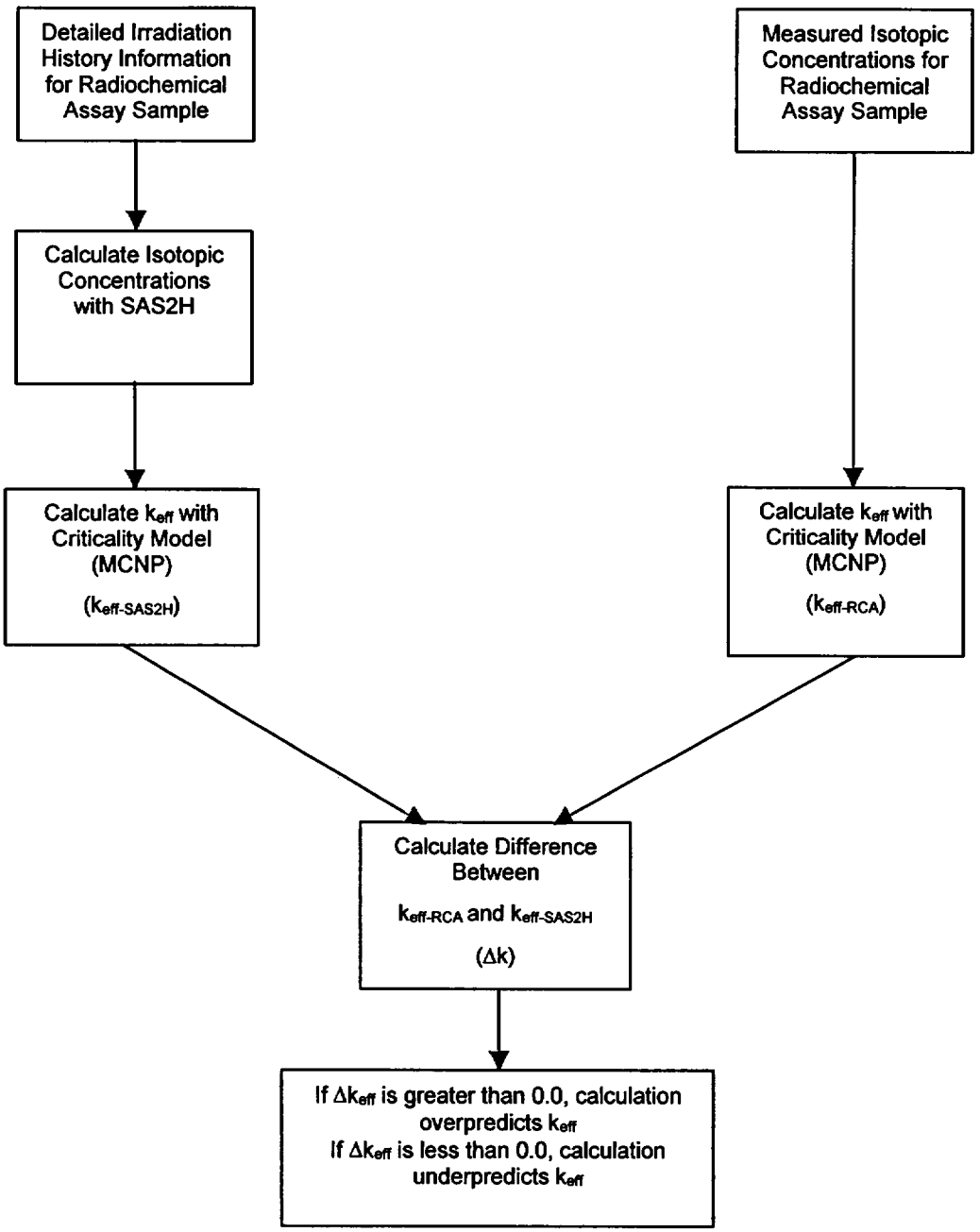


Figure 5. Isotopic Bias and Uncertainty Methodology Calculations

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 whatever isotopes were provided from the RCA measurement. The reactivity data were obtained from *Calculation of Isotopic Bias and Uncertainty for PWR Spent Nuclear Fuel* (BSC 2002b) and are presented in Table 8.

Table 8. 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	0.89999	0.00065	0.90370	0.00066	0.0037
S2	0.84278	0.00065	0.85382	0.00058	0.0110
S3	0.84184	0.00070	0.83362	0.00064	-0.0082
S4	0.80356	0.00065	0.81954	0.00059	0.0160
Calvert Cliffs Samples					
S1	0.78255	0.00066	0.79983	0.00063	0.0173
S2	0.71470	0.00054	0.73699	0.00054	0.0223
S3	0.66405	0.00057	0.70409	0.00061	0.0400
S4	0.86583	0.00058	0.87305	0.00070	0.0072
S5	0.81840	0.00054	0.82769	0.00068	0.0093
S6	0.77655	0.00058	0.80050	0.00060	0.0240
S7	0.73356	0.00062	0.74997	0.00051	0.0164
S8	0.70428	0.00062	0.72507	0.00056	0.0208
S9	0.66719	0.00056	0.70013	0.00043	0.0329
Obrigheim Samples					
S1	0.85505	0.00064	0.86987	0.00065	0.0148
S2	0.84625	0.00067	0.86604	0.00060	0.0198
S3	0.84397	0.00063	0.86043	0.00068	0.0165
S4	0.84197	0.00067	0.85835	0.00076	0.0164
S5	0.83919	0.00064	0.85416	0.00070	0.0150
S6	0.83625	0.00065	0.85261	0.00074	0.0164
Trino Vercelles Samples					
S1	0.96939	0.00042	0.96796	0.00041	-0.0014
S2	0.91153	0.00040	0.91402	0.00044	0.0025
S3	0.90525	0.00043	0.90988	0.00044	0.0046
S4	0.92571	0.00043	0.92629	0.00046	0.0006
S5	0.92112	0.00044	0.92127	0.00045	0.0001
S6	0.89143	0.00042	0.89537	0.00040	0.0039
S7	0.87572	0.00040	0.88437	0.00041	0.0086
S8	0.87610	0.00042	0.88022	0.00042	0.0041
S9	0.88155	0.00043	0.88399	0.00039	0.0024
S10	0.87497	0.00039	0.87949	0.00039	0.0045
S11	0.88200	0.00039	0.88390	0.00042	0.0019
S12	0.87488	0.00040	0.87941	0.00043	0.0045
S13	0.88316	0.00041	0.88347	0.00042	0.0003
S14	0.87661	0.00038	0.87985	0.00044	0.0032
Turkey Point Samples					
S1	0.82837	0.00063	0.82882	0.00061	0.0004
S2	0.82745	0.00072	0.82946	0.00055	0.0020
S3	0.82973	0.00074	0.82370	0.00065	-0.0060
S4	0.82861	0.00065	0.82580	0.00066	-0.0028
S5	0.82373	0.00062	0.82584	0.00063	0.0021

Table 8. 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	0.79427	0.00040	0.78589	0.00043	-0.0084
S2	0.76666	0.00036	0.74607	0.00037	-0.0206
S3	0.76392	0.00037	0.74358	0.00038	-0.0203
S4	0.78481	0.00039	0.77115	0.00037	-0.0137
S5	0.76131	0.00041	0.74420	0.00039	-0.0171
S6	0.75841	0.00040	0.74303	0.00036	-0.0154
S7	0.72665	0.00035	0.73561	0.00035	0.0090
S8	0.72596	0.00036	0.73450	0.00037	0.0085
Mihama Samples					
S1	1.01289	0.00073	1.00702	0.00076	-0.0059
S2	1.02653	0.00065	1.02003	0.00076	-0.0065
S3	0.97472	0.00070	0.95840	0.00070	-0.0163
S4	0.93623	0.00068	0.92008	0.00066	-0.0162
S5	0.97662	0.00063	0.96466	0.00069	-0.0120
S6	0.87379	0.00065	0.85522	0.00065	-0.0186
S7	0.86657	0.00059	0.84160	0.00071	-0.0250
S8	0.83131	0.00071	0.82998	0.00071	-0.0013
S9	0.83990	0.00063	0.83833	0.00067	-0.0016
Three Mile Island Samples					
YU1	0.74658	0.00056	0.79167	0.00063	0.0451
YU2	0.74501	0.00063	0.79798	0.00056	0.0530
YU3	0.75571	0.00064	0.80272	0.00058	0.0470
YU4	0.75778	0.00059	0.79254	0.00068	0.0348
YU5	0.77382	0.00050	0.83197	0.00062	0.0582
YU6	0.77125	0.00064	0.80872	0.00062	0.0375
YU7	0.73462	0.00053	0.77018	0.00057	0.0356
YU8	0.72223	0.00061	0.76972	0.00061	0.0475
YU9	0.72601	0.00055	0.77867	0.00057	0.0527
YU10	0.75337	0.00059	0.77058	0.00054	0.0172
YU11	0.75135	0.00054	0.79448	0.00057	0.0431
S1	0.97173	0.00068	0.98959	0.00074	0.0179
S2	0.94074	0.00071	0.97017	0.00071	0.0294
S3	0.96219	0.00084	0.99217	0.00069	0.0300
S4	0.98469	0.00066	1.00203	0.00077	0.0173
S5	0.97323	0.00067	0.98907	0.00067	0.0158
S6	0.99642	0.00072	1.00822	0.00075	0.0118
S7	0.98786	0.00075	1.00925	0.00067	0.0214
S8	0.97200	0.00077	0.99026	0.00071	0.0183

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] Δk = SAS2H k_{eff} – RCA k_{eff}.

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 does not follow a normal distribution, which was tested using the Shapiro-Wilks test for normality, and is illustrated in the quantile plot in Figure 6 and the histogram in Figure 7.

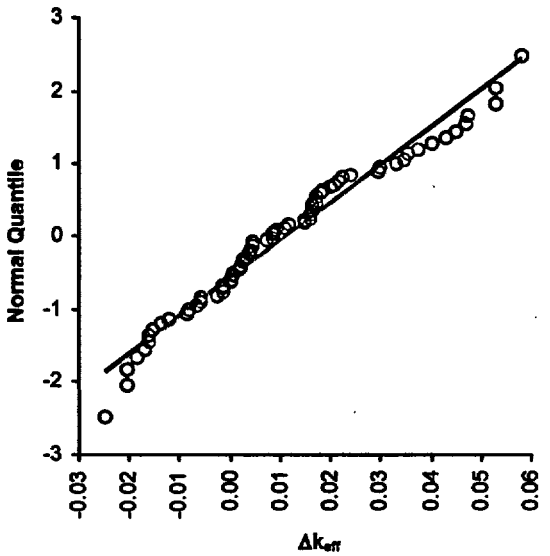


Figure 6. Normal Quantile Plot for RCA and SAS2H Data

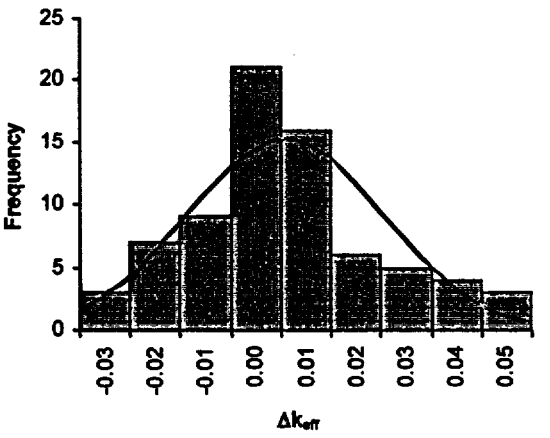


Figure 7. Histogram Plot for RCA and SAS2H Data

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 lower limit and uncertainty is calculated as illustrated in Equation 6.

$$\textit{Lower Limit and Uncertainty} = -0.0250 - \sigma_L \quad \text{(Eq. 6)}$$

where

-0.0250 is determined from the one-sided distribution free tolerance limit for 74 data points with 95 percent confidence, corresponding to an index value of 1 from Table A-31 of *Experimental Statistics* (Natrella 1963), which equates to the minimum Δk value

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 9. Table 9 shows that on average, the calculated SAS2H isotopics cause MCNP to overpredict k_{eff} relative to the RCA measured isotopics.

Table 9. Isotopic Bias and Uncertainty Values

Isotope Set	Average Δk_{eff} (bias)	σ_L	Lower Limit and Uncertainty
All Available Isotopes	0.0108	0.0009	-0.0259

This Δk_{eff} value of 0.0259 is the criterion that will be used in Section 7.5 to determine if the bounding isotopic parameter set is conservative. Thus, if the bounding parameter set produces an increase in k_{eff} greater than 0.0259, 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 assembly isotopics. Another code, CASMO-3 (referred to as GRCASMO-3), has a two-dimensional representation of the assembly. Table 10 presents a summary of the results of a comparison (BSC 2002c) of the SAS2H code sequence to the GRCASMO-3 isotopic depletion code for the Calvert Cliffs 1 and Turkey Point 2 assays. The measured isotopic concentrations obtained from RCAs discussed in Section 6.2.1 were used as the basis, or "correct numbers" for these comparisons.

Table 10. 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
U^{234}	-0.6	-12.6	2.2	-10.0
U^{235}	-1.7	-4.3	-1.2	-1.2
U^{236}	2.9	-0.8	2.6	-0.4
U^{238}	-0.7	-0.6	-0.2	-0.02
Np^{237}	3.7	-0.8	*	*
Pu^{238}	-5.4	-12.2	-2.2	-1.1
Pu^{239}	-13.9	-4.3	4.3	-1.7
Pu^{240}	4.7	-2.1	1.6	-0.4
Pu^{241}	-2.2	-5.1	-0.8	-0.4
Pu^{242}	16.6	-9.0	2.3	-4.8
Am^{241}	-5.3	-9.9	*	*
Nd^{143}	1.8	0.3	*	*
Nd^{145}	-0.2	-2.7	*	*
Sm^{149}	-35.5	-33.4	*	*
Sm^{150}	0.0	-5.5	*	*
Sm^{152}	14.9	0.6	*	*
Eu^{153}	0.8	-0.2	*	*

Source: BSC 2002c, p. 4-58

NOTE: * Measurement not made for this isotope.
Percentage difference calculated as follows: 100 x (C/M-1) where C represents calculated value, and M is measured value.

Review of the comparison table shows good agreement for the better-known actinides of uranium-235, uranium-236, and uranium-238. SAS2H more accurately predicts the uranium-235 contents, while GRCASMO-3 is better at predictions of plutonium-239. The prediction of plutonium-242 is challenging for depletion codes due to the number of neutron captures required to produce this heavy isotope, but the actual quantity of plutonium-242 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 11 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 11. 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 2002c, p. 4-59

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

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

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 fuel assemblies. The scope of this calculation covers an initial enrichment range of 2.0 through 5.0 wt% uranium-235 and a burnup range of 10 through 50 GWd/MTU. An infinite lattice of fuel was used for all calculations, and results were normalized to the average value of k_∞ of each data series.

An example set of depletion parameters chosen based on nominal reactor operating values was used for the sensitivity variations, as described in *PWR Depletion Parameter Sensitivity Evaluation* (BSC 2001). The base case parameters are provided in Table 12. The moderator material specification contains soluble boron.

Table 12. Nominal SAS2H 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)

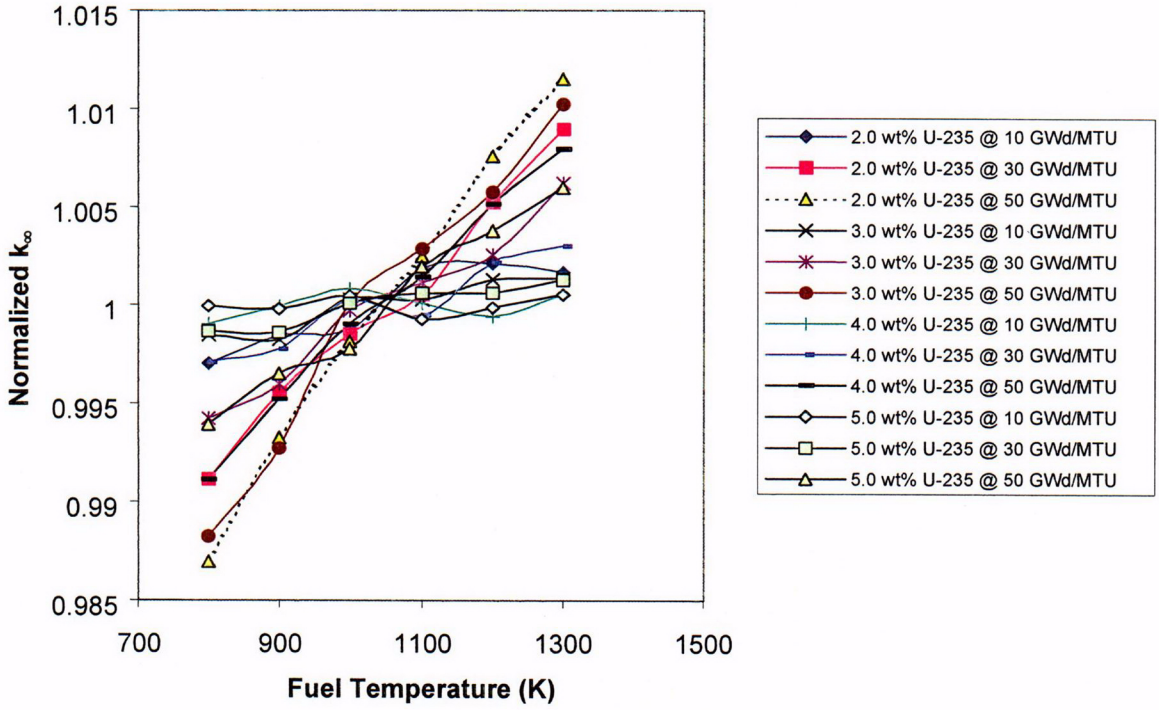
Source: BSC 2001, Table 2

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 radius of 0.9398 cm (Punatar 2001, pp. 2-5 and 3-1).

The 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

The fuel temperature effects were evaluated in order to determine the sensitivity of Doppler broadening of primarily the uranium-238 resonance absorption cross section. Normalized k_∞ values are graphically illustrated in Figure 8. Values were normalized to the average k_∞ of each burnup/enrichment pair.



Source: BSC 2001, p. 39

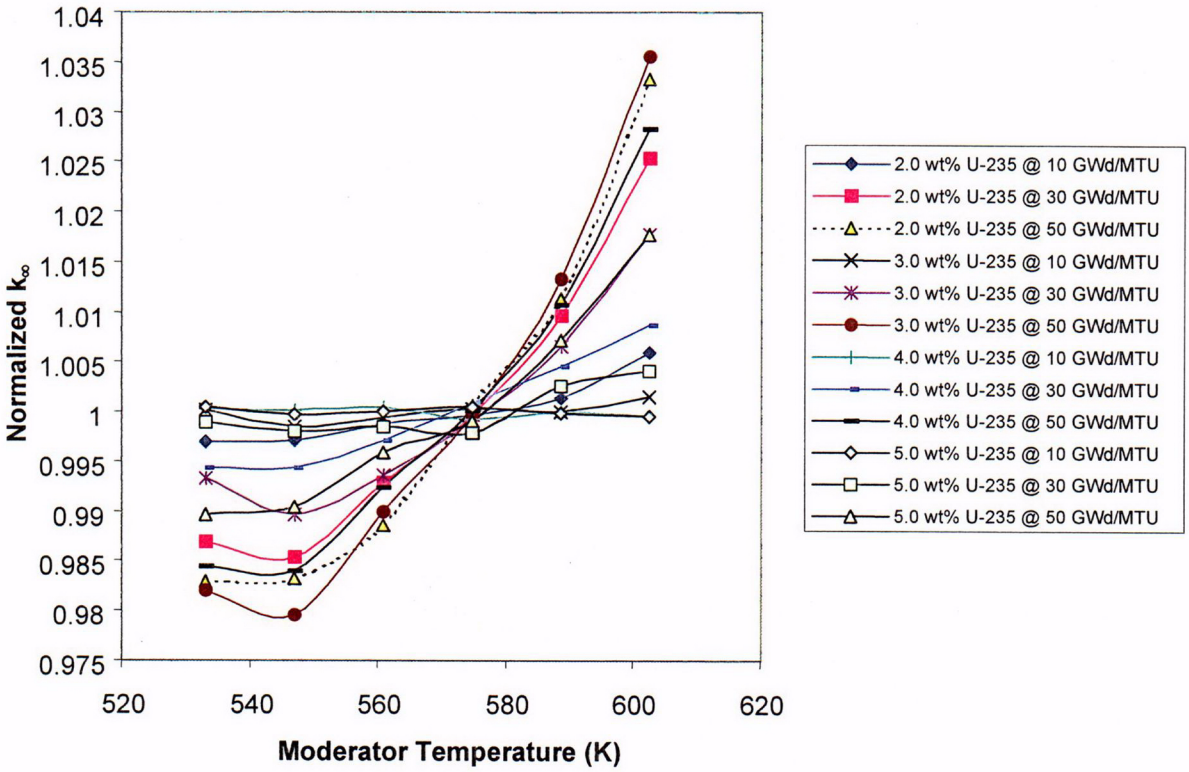
Figure 8. Fuel Temperature Results (5-Year Cooling Time)

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 reactivity.

6.4.2 Moderator Temperature Effects

6.4.2.1 Non-Borated Moderator

The moderator temperature sensitivity effects were evaluated in order to determine the sensitivity of moderation primarily affecting the neutron energy spectrum. This set of cases was performed with non-borated moderator present in order to independently evaluate the spectral effects from moderator density changes. Normalized k_∞ values are graphically illustrated in Figure 9. Values were normalized to the average k_∞ of each burnup/enrichment pair.



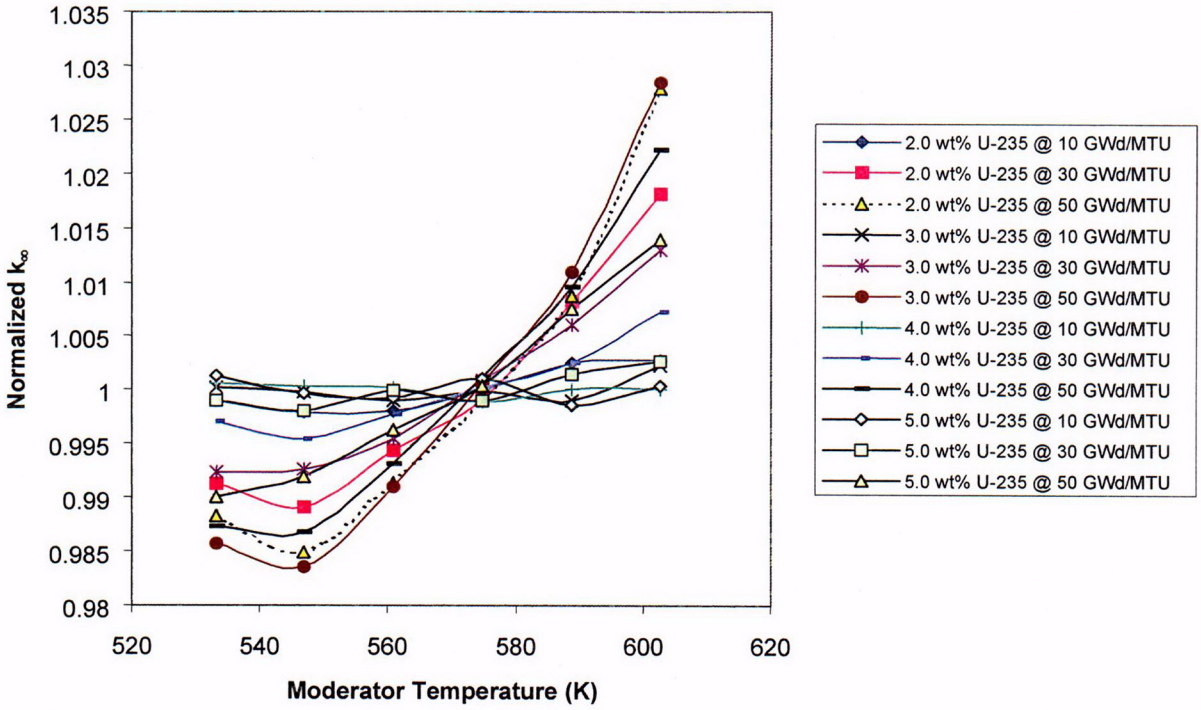
Source: BSC 2001, p. 41

Figure 9. Moderator Temperature Effects with No Soluble Boron (5-Year Cooling Time)

The moderator temperature may have a substantial effect upon the calculated reactivity of SNF. Higher moderator temperature results in a greater reactivity.

6.4.2.2 Nominal Borated Moderator

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 10. Values were normalized to the average k_∞ of each burnup/enrichment pair.



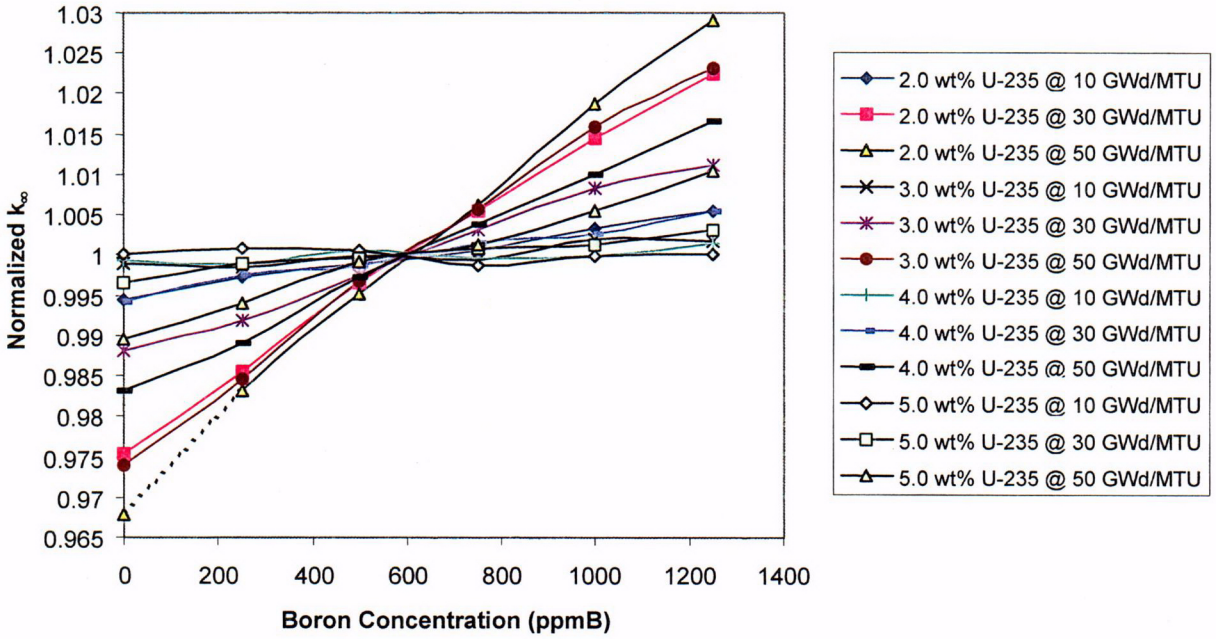
Souce: BSC 2001, p. 44

Figure 10. Moderator Temperature Effects (5-Year Cooling Time)

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

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 11. Values were normalized to the average k_∞ of each burnup/enrichment pair.



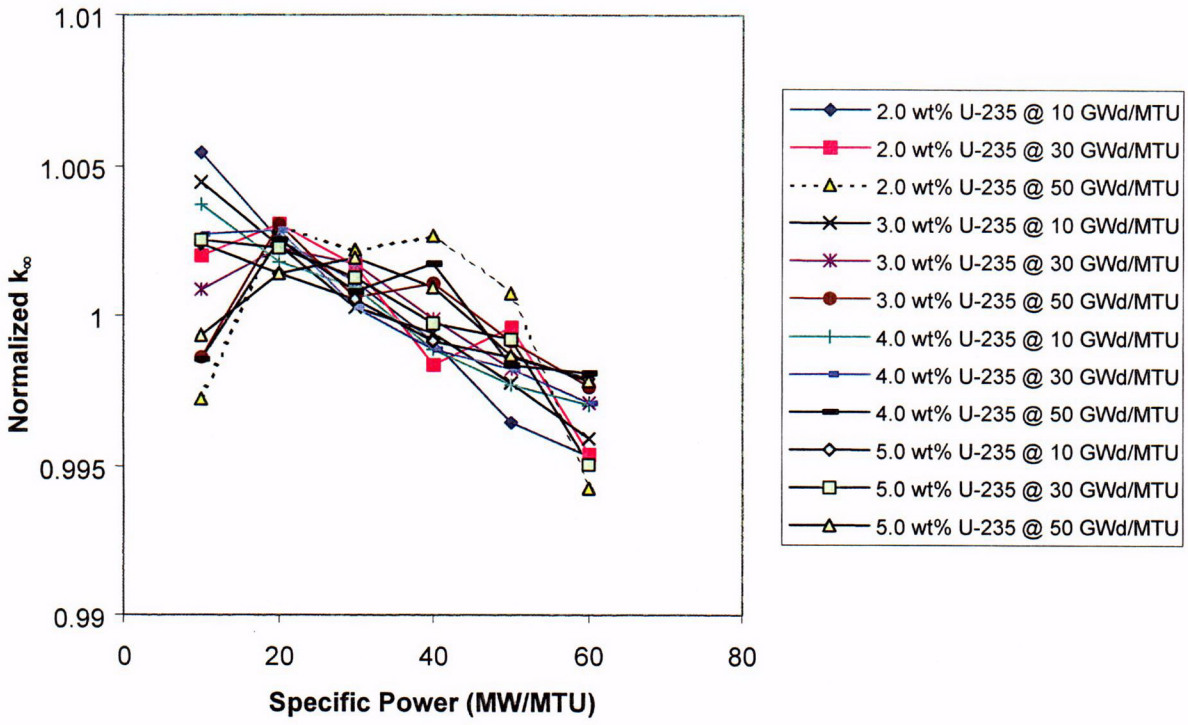
Source: BSC 2001, p. 46

Figure 11. Boron Concentration Effects (5-Year Cooling Time)

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

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 12. Values were normalized to the average k_∞ of each burnup/enrichment pair.



Source: BSC 2001, p. 49

Figure 12. Specific Power Effects (5-Year Cooling Time)

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 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 13. Thus, 30 MW/MTU is the lowest practical specific power and is chosen as the bounding depletion parameter.

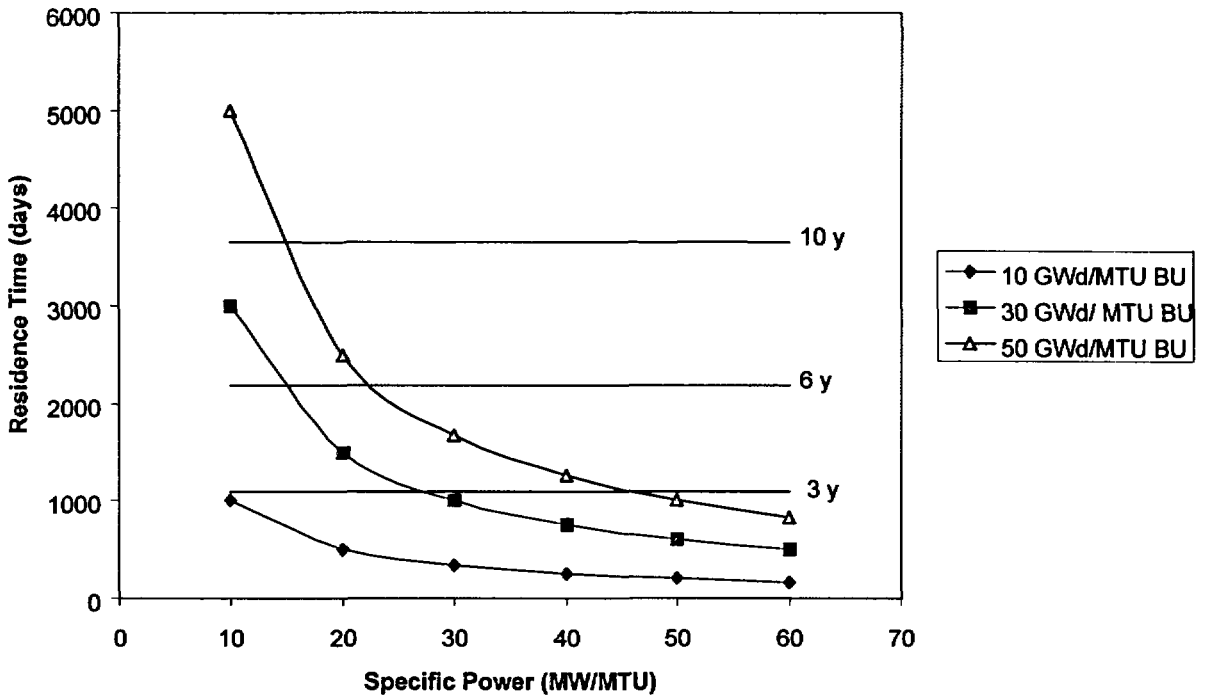


Figure 13. Time Required to Achieve Target Burnup versus Specific Power

6.4.5 Homogenized Spacer Grid Effects

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 13.

Table 13. Homogenized Spacer k_∞ Sensitivity Results With 5-Year Cooling Time

Wt% U-235	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	

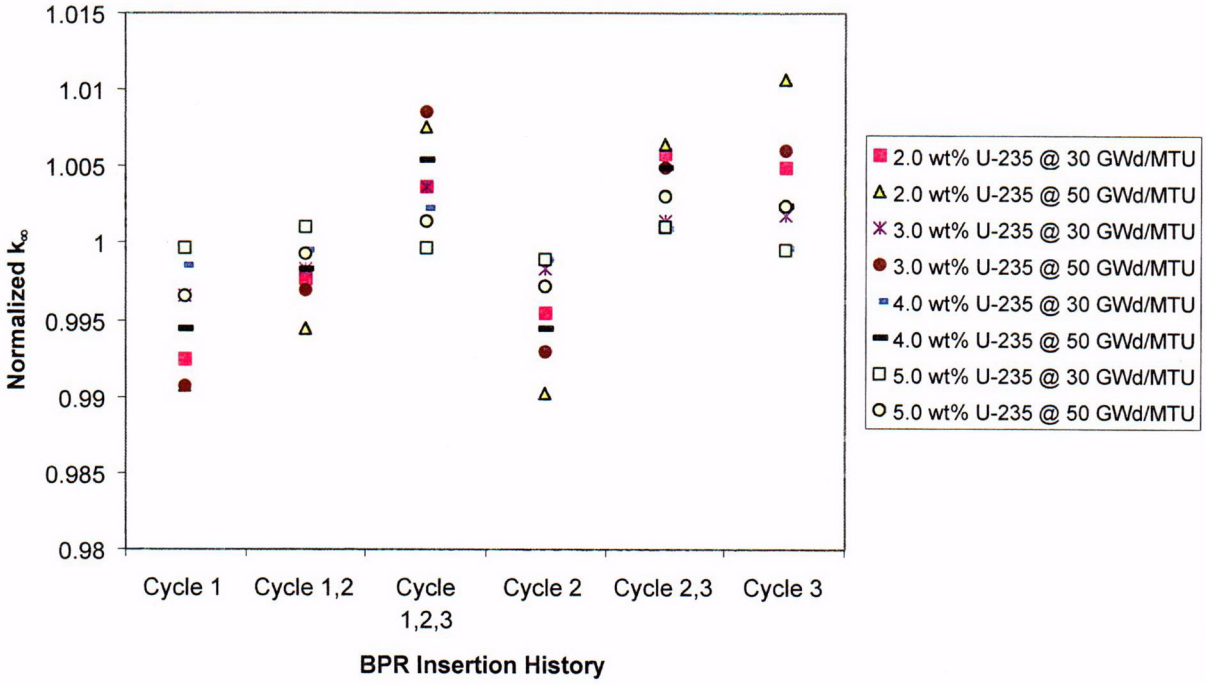
Source: BSC 2001, p. 50

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.

The tabulated k_∞ differences indicate that the spacer grids have relatively little effect upon the calculated reactivity of SNF.

6.4.6 Burnable Poison Rod Assembly Insertion Results

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 14.



Source: BSC 2001, p. 53

Figure 14. Burnable Poison Rod Insertion History Effects (5-Year Cooling Time)

Figure 14 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 model 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.

6.4.7 Depletion Time Step Results

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 14.

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.

Table 14. Depletion Time Step k_∞ Sensitivity Results With 5-Year Cooling Time

Burnup (GWd/ MTU)	Time Step Length (days)	2.0 wt% U-235		3.0 wt% U-235		4.0 wt% U-235		5.0 wt% U-235	
		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

Source: BSC 2001, p. 54

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

6.5 BOUNDING PARAMETERS

The isotopic model must be capable of predicting conservative reactivities for a variety of PWR 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 PWR waste packages.

Section 6.1 showed that the overall bias for criticality calculations for SNF, based upon CRCs, is 0.0062. Section 6.2, RCAs, showed that isotopic concentrations calculated by SAS2H were reasonable, with a reactivity bias of +0.0108. These values indicate the non-existence of "compensating errors." Further, a code-to-code comparison of SAS2H and GRCASMO-3 in Section 6.3 showed that both codes generate similar results, and SAS2H therefore appears to be a reasonable tool to calculate the isotopic concentrations of PWR SNF.

Example SAS2H depletion parameters were chosen to illustrate the isotopic model test for conservatism. The chosen bounding parameters are as follows:

- Fuel temperature, 1200 K
- Moderator temperature, 625°F (602.6 K)
- Moderator density, 0.6516 g/cm^3
- Boron concentration, 950 parts per million boron by mass, constant (no boron letdown curve)
- Specific power, 30 MW/MTU
- Irradiation timestep, 80 days (or less)
- No spacer grids modeled.

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 for illustration of the isotopic model.

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. VALIDATION

This section presents a systematic approach for validation of the bounding parameter calculational method used to determine the isotopic concentrations of SNF. The validation approach is to calculate the reactivity for a nominal fuel assembly with nominal PWR 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 PWR CRCs (-0.0068 from Table 5). 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 (-0.0259, from Table 9) could be used.

The bounding parameters are only applicable to commercial PWR SNF.

A listing of corroborating or supporting data, models, or information used to complete the model validation activities, along with their sources, is provided in Table 15.

Table 15. Supporting Information and Sources for Model Validation Activities

Description	Source
Representative assembly characteristics	Punatar 2001
Equation for fresh fuel compositions	Bowman et al. 1995
Material composition for Zircaloy-4	ASTM B 811-90 1991
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 (SB-575 N06022)	DTN: MO0003RIB00071.000
Material composition for SA-240 S31600	ASM International 1987, p. 931; ASME 1998, Section II, SA-240
Material composition for Neutronit A978	DTN: MO0109RIB00049.001
Material composition for Al 6061	ASM International 1990
Density of Al 6061 and Stainless Steels 304 and 316	ASTM G 1-90 1999
Material composition for Grade 70 Carbon Steel Type A516	DTN: MO0003RIB00072.000
Material composition for Stainless Steel Type 304	ASTM A 240/A 240M-94b 1994
Material composition for Inconel 718	Lynch 1989
General reference to principal isotopes	YMP 2003
General reference to SCALE manual	CRWMS M&O 2000a
Density of Al 6061	ASME 1995

7.1 NOMINAL DEPLETION PARAMETER SELECTION

The 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 Babcock & Wilcox 15x15 fuel assemblies for which the operating temperatures, boron letdown curve, irradiation power levels, and exposure times are known. The depletion parameters obtained from *Summary Report of Commercial Reactor Criticality Data for Crystal River Unit 3* (Punatar 2001), were as follows:

- Fuel temperature, 861.3 K.
- Moderator temperature, 579.8 K (note that the fuel cladding temperature was 60 K greater than the moderator temperature).
- Moderator density, 0.7556 g/cm^3
- Specific power, 43.029 MW/MTU.
- Moderator boron concentration values are presented in Table 16 and were interpolated from the nominal values specified in Section 4.
- 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).

Table 16. 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

NOTE: [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 which 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 models, Path A and Path B, to calculate energy dependent spatial neutron flux distributions necessary to perform cross section cell-weighting calculations.

7.2 DEPLETION PARAMETERS

A set of depletion parameters based on bounding reactor operating 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 17 for each of the burnups evaluated.

Table 17. Nominal SAS2H Base Case Depletion Time Steps

Burnup (GWd/MTU)	Power (MW)	Time Step (days)
10	0.77244	66.667
20	0.77244	74.074
30	0.77244	55.556
40	0.77244	74.074

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 uranium-234, uranium-235, uranium-236, and uranium-238. The fresh fuel compositions for each uranium-235 enrichment used in this evaluation are specified in Table 18, and were calculated using Equation 8 (Bowman et al. 1995, p. 20) for each isotope based on the uranium-235 wt%. The material specification for Inconel 718 is specified in Table 19.

Table 18. SAS2H Fresh Fuel Compositions

Enrichment (wt% U-235)	Wt% U-234	Wt% U-235	Wt% U-236	Wt% U-238
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 19. 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		

Source: Lynch 1989, p. 496

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

The 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 20.

Table 20. 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		

Source: ASTM B 811-90 1991, p. 2, Table 2

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

The fuel rod fill gas material was specified as helium. The helium material temperature was allowed to default to 293 K.

7.4 MCNP MODEL

The MCNP model was for the representative 21 PWR waste package as shown in Attachment I. The waste package is treated as fully flooded and at room temperature, containing Babcock & Wilcox 15x15 fuel assemblies.

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 21 PWR waste

package follows the same description as that shown in the sketch of Attachment I. This waste package is 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 21). 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 1998, Section II, SA-240, Table 1), as described in Table 22. The fuel basket plates were represented as Neutronit A978 with 1.62 wt% boron as described in Table 23. The thermal shunts were represented as aluminum 6061 (as described in Table 24), and the basket side and corner guides were represented as Grade 70 Carbon Steel Type A516 (as described in Table 25). 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 wt% in the material of interest by the natural weight fraction of the isotope in the elemental state to obtain the wt% 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).

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

where

I is the total number of isotopes in the natural element

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

Table 21. Alloy 22 (SB-575 N06022) Material Composition

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

Source: DTN: MO0003RIB00071.000

NOTES: [a] ZAID = MCNP material identifier.

Table 22. Material Specifications for SA-240 S31600

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

Source: ASM International 1987, p. 931; ASME 1998, Section II, SA-240, Table 1; and ASTM G 1-90 1999, p. 7, Table X1

NOTES: [a] ZAID = MCNP material identifier.

Table 23. Material Specifications for Neutronit A978 with 1.62 wt% Boron

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

Source: DTN: MO0109RIB00049.001; Audi and Wapstra 1995

NOTES: [a] ZAID = MCNP material identifier.

Table 24. 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
Fe-54	26054.60c	0.0396	Cr-50	24050.60c	0.0081
Fe-56	26056.60c	0.6433	Cr-52	24052.60c	0.1632
Fe-57	26057.60c	0.0151	Cr-53	24053.60c	0.0189
Fe-58	26058.60c	0.0020	Cr-54	24054.60c	0.0048
Cu-63	29063.60c	0.1884	Ti-nat	22000.50c	0.1500
Cu-65	29065.60c	0.0866	Al-27[b]	13027.50c	96.9300
Mn-55	25055.50c	0.1500	Density[c] = 2.7065 g/cm^3		

Source: ASM International 1990, p. 102

NOTES: [a] ZAID = MCNP material identifier.
[b] Zn cross-section data unavailable; therefore, it was substituted as Al-27.
[c] ASTM G 1-90 1999, p. 7, Table X1 indicates 2.7 g/cm^3; ASME 1995, Table NF-2 indicates a converted value from 0.098 lb/in^3 of 2.713 g/cm^3; therefore the midpoint was used.

Table 25. Grade 70 Carbon Steel Type A516 Composition

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

DTN: MO0003RIB00072.000

NOTE: [a] ZAID = MCNP material identifier.

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 modeled with material compositions that represent the homogenization of all of the components in the regions. Table 26 presents the material composition of Stainless Steel Type 304. Table 27 presents the material composition of Zircaloy-4. Table 28 presents the material composition of Inconel 718. Equations 14 and 15 were used for determining the end-fitting material volume fractions. Table 29 presents the component material volume fractions for the upper and lower end-fitting regions for the Babcock & Wilcox 15x15 assembly design. Table 30 presents the upper and lower end-fitting homogenized material compositions for the Babcock & Wilcox 15x15 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.

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

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

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

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

$$\left(\begin{array}{l} \textit{End} - \textit{Fitting Material} \\ \textit{Volume} \end{array} \right) = \sum \frac{mass_i}{density_i} \quad \text{(Eq. 14)}$$

where

i represents a common material such as Stainless Steel Type 304

$$(Volume\ Fraction)_i = \frac{\left(\begin{matrix} End - Fitting\ Material \\ Volume \end{matrix}\right)_i}{\left(\begin{matrix} Total\ End - Fitting \\ Volume \end{matrix}\right)} \qquad \text{(Eq. 15)}$$

where

i represents a common material such as Stainless Steel Type 304

Table 26. Stainless Steel Type 304 Material Composition

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

Source: ASTM A 240/A 240M-94b 1994, p. 2, Table 1

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.

Table 27. Zircaloy-4 Material Composition

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

Source: ASTM B 811-90 1991, p. 2, Table 2

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

Table 28. Inconel 718 Material Composition

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

Source: Lynch 1989, p. 496

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

Table 29. End-Fitting Component Material Volume Fractions for Babcock & Wilcox 15x15 Assembly Design

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

7.4.4 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. 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 compact disc in Attachment III.

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 27). The upper and lower fuel rod plenum regions were represented as containing Stainless Steel Type 304 springs. Table 31 contains the upper and lower fuel rod plenum volume fractions, and Table 32 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 30. End-Fitting Homogenized Material Compositions for Babcock & Wilcox 15×15 Assembly Design

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

NOTES: [a] ZAID = MCNP material identifier.

Table 31. Fuel Rod Plenum Material Volume Fractions

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

Source: Punatar 2001, Section 2

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

Table 32. Fuel Rod Plenum Homogenized Material Compositions for Babcock & Wilcox 15×15 Assembly Design

Element/Isotope	ZAID[a]	Wt% of Element/Isotope in Material Composition	
		Upper Fuel Rod Plenum	Lower Fuel Rod Plenum
C-nat	6000.50c	0.0124	0.0131
N-14	7014.50c	0.0413	0.0436
Si-nat	14000.50c	0.3096	0.3270
P-31	15031.50c	0.0186	0.0196
S-32	16032.50c	0.0124	0.0131
Cr-50	24050.60c	0.3302	0.3485
Cr-52	24052.60c	6.6148	6.9806
Cr-53	24053.60c	0.7644	0.8067
Cr-54	24054.60c	0.1935	0.2042
Mn-55	25055.50c	0.8257	0.8720
Fe-54	26054.60c	1.5943	1.6829
Fe-56	26056.60c	25.9299	27.3712
Fe-57	26057.60c	0.6099	0.6438
Fe-58	26058.60c	0.0820	0.0865
Ni-58	28058.60c	2.7744	2.9298
Ni-60	28060.60c	1.1053	1.1672
Ni-61	28061.60c	0.0489	0.0516
Ni-62	28062.60c	0.1581	0.1670
Ni-64	28064.60c	0.0418	0.0442
O-16	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

NOTES: [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 able 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 19. In Equations 16 and 17 the atomic mass values (A) come from work by Audi and Wapstra (1995).

$$\frac{U\ Mass}{mol\ UO_2} = \left[\begin{matrix}(A)(U^{234}wt\%)+(A)(U^{235}wt\%)+\\(A)(U^{236}wt\%)+(A)(U^{238}wt\%)\end{matrix}\right](0.01) \quad \text{(Eq. 16)}$$

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.

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

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

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

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

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

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.

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

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.

7.5 RESULTS

The reactivity of several k_{eff} calculations using bounding versus nominal isotopic parameters is shown in Table 33. The data points were chosen to represent enrichment and burnup values that would be likely for PWR SNF. The calculated Δk_{eff} values are shown in Table 33 and plotted in Figure 15. 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 33. Δk_{eff} versus Burnup for Different Enrichments

Burnup (GWd/MTU)	Initial Enrichment (Wt% U-235)					
	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.

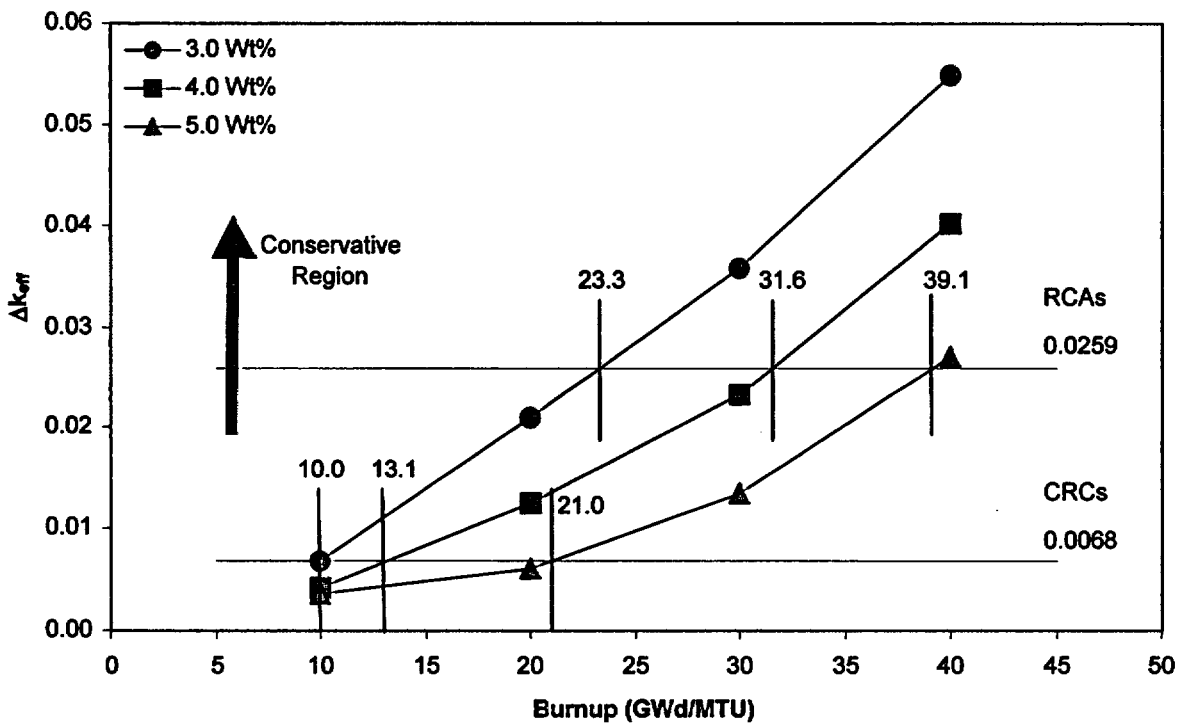


Figure 15. Δk_{eff} Values for Bounding versus Nominal Parameters

Figure 15 shows the bias plus uncertainty for the CRCs as a horizontal line at 0.0068 (from Table 5) and the lower limit and uncertainty from the RCAs at 0.0259 (from Table 9). Inspection of the figure indicates that the CRC bounding depletion parameter set is conservative for a 3.0 wt% enriched fuel assembly if the burnup exceeds 10.0 GWd/MTU, for a 4.0 wt%

C07

enriched fuel assembly if the burnup exceeds 13.1 GWd/MTU, and for a 5.0 wt% enriched fuel assembly if the burnup exceeds 21.0 GWd/MTU. The conservative cutoff values using the RCA lower limit and uncertainty are at 23.3 GWd/MTU for the 3.0 wt% enriched fuel, 31.6 GWd/MTU for the 4.0 wt% enriched fuel, and 39.1 for the 5.0 wt% 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.

8. CONCLUSIONS

The *Isotopic Model Report* documents the isotopic model and its validation. The validation uses current data for pressurized water reactor spent nuclear fuel and provides a validated model that may be updated as additional data becomes available. The isotopic model 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 isotopic model will produce isotopic concentrations that will ensure the calculation of conservative reactivities for typical commercial PWR SNF with initial enrichments between 2.0 and 5.0 wt% uranium-235, and burnups between 10 and 50 GWd/MTU. A set of bounding isotopic depletion parameters can be 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 Figure 15. The isotopic model 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 model is only applicable to commercial PWR SNF. The isotopic model causes the Δk_{ISO} isotopic value required by *Disposal Criticality Analysis Methodology Topical Report* (YMP 2003, Section 3.5.3.2.10) to be greater than or equal to zero, then set to zero, because the isotopic model bounding parameters produce conservative results over the range of applicability.

The isotopic model process documented in this report contributes to or meets the acceptance criteria stated in Section 4.2 through the development of conservative isotopic concentrations for criticality evaluations. The isotopic model is a process rather than a mathematical model, therefore data output is not developed.

Two open items from Reamer (2000) were addressed in the *Isotopic Model Report*. They were open items 7 and 11, as listed in Section 4.2. Open item 7 is addressed in Section 6.3 by a comparison against a two-dimensional code which results in comparable results to the one-dimensional SAS2H. Open item 11 is addressed in Sections 6.1, 6.2, 6.6, and Figure 15 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, and testing a set of isotopics generated

under bounding operating parameters to determine where conservative isotopics are assured (Figure 15).

9. INPUTS AND REFERENCES

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9.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

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9.3 SOURCE DATA LISTED BY DATA TRACKING NUMBER

MO0003RIB00071.000. Physical and Chemical Characteristics of Alloy 22. Submittal date: 03/13/2000.

MO0003RIB00072.000. Physical and Chemical Characteristics of Steel, A 516. Submittal date: 03/13/2000.

MO0109RIB00049.001. Waste Package Material Properties: Neutron Absorbing Materials. Submittal date: 09/17/2001.

9.4 SOFTWARE CODES

Software Code: MCNP. 4B2LV. HP. 30033 V4B2LV.

Software Code: SCALE. V4.4A. HP. 10129-4.4A-00.

10. ATTACHMENTS

The description of the attachments is provided in Table 34.

Table 34. Attachment Listing

Attachment	No. of Pages	Description
I	4	21 PWR waste package sketch
II	4	Description of SAS2H input files, SAS2H outputs, MCNP inputs, and MCNP outputs contained in Attachment III
III	N/A	Compact Disc attachment containing information listed in Attachment II

ATTACHMENT I

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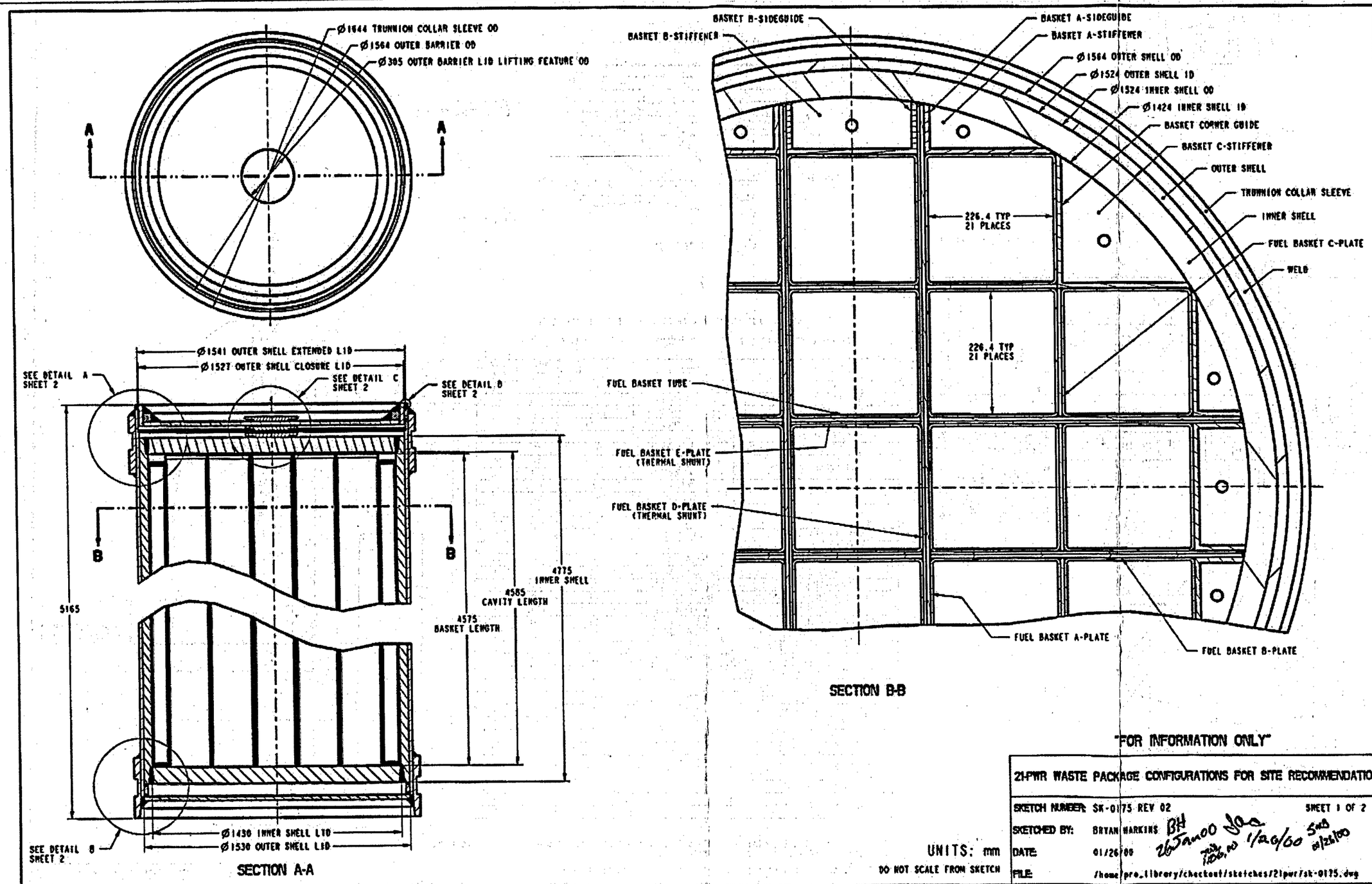
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Ø1564 OUTER BARRIER OD
Ø305 OUTER BARRIER LID LIFTING FEATURE OD
A
A
Ø1541 OUTER SHELL EXTENDED LID
Ø1527 OUTER SHELL CLOSURE LID
SEE DETAIL A SHEET 2
SEE DETAIL C SHEET 2
SEE DETAIL B SHEET 2
B
B
5165
4775 INNER SHELL
4585 CAVITY LENGTH
4575 BASKET LENGTH
Ø1430 INNER SHELL LID
Ø1530 OUTER SHELL LID
SEE DETAIL B SHEET 2
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
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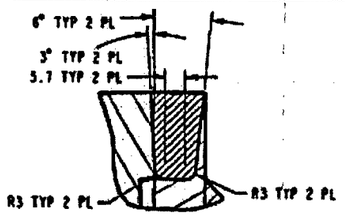
UNITS: mm
DO NOT SCALE FROM SKETCH



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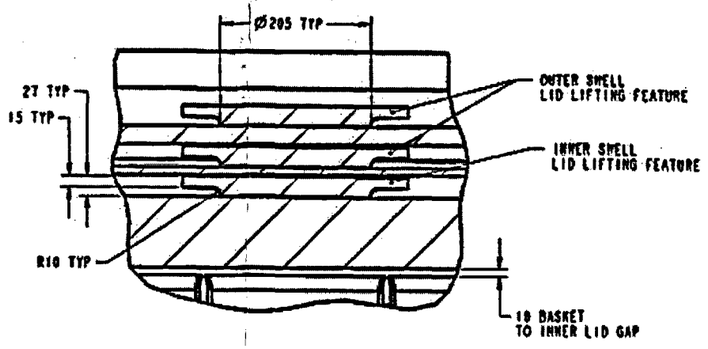

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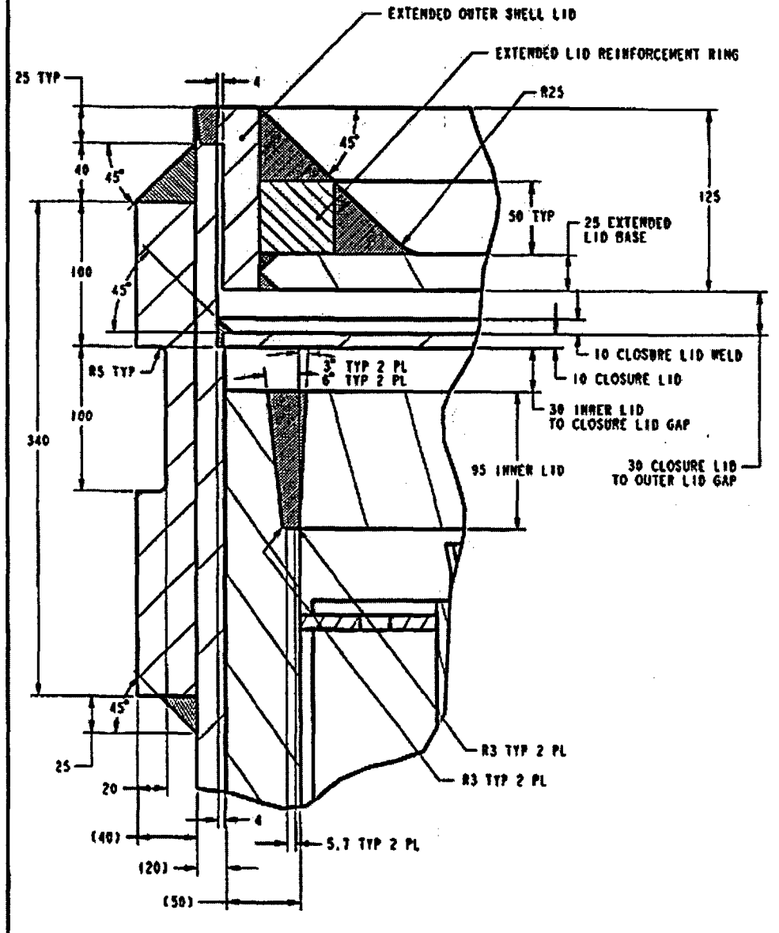
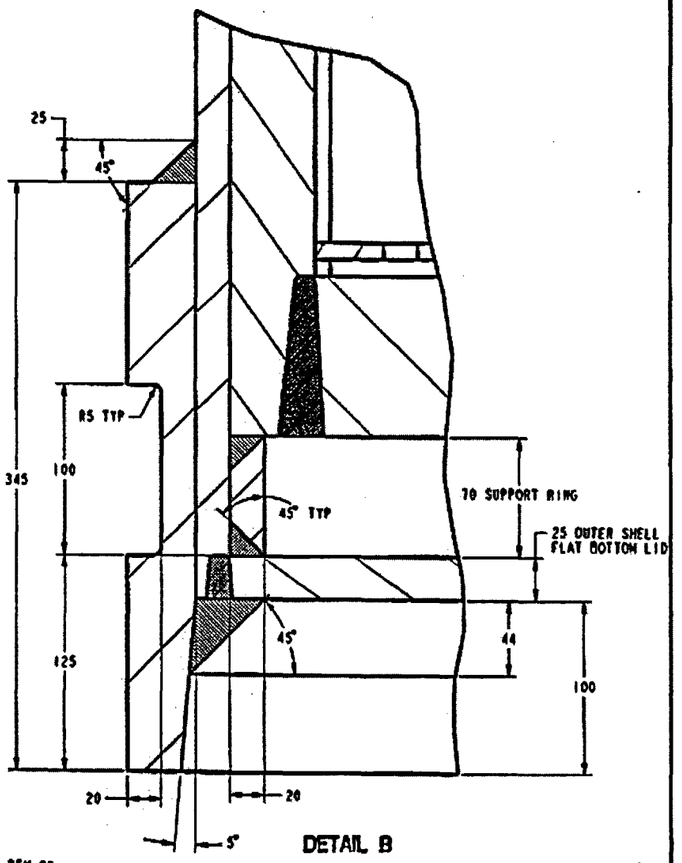


DETAIL A

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 PER
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	87	886	98
FUEL BASKET B-PLATE	NEUTRONIT A 978	7	85	8
	&SA-516 K02700	87	886	88
FUEL BASKET C-PLATE	NEUTRONIT A 978	7	44	16
	&SA-516 K02700	87	845	816
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	-	126	**
WASTE PACKAGE ASSEMBLY	-	-	26035	1
	-	-	826059	81
PWR FUEL ASSEMBLY	-	-	773.4*	21
WP ASSEMBLY WITH SNF	-	-	42277	1
	-	-	842301	81



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

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ATTACHMENT II

This attachment contains a listing and description of the zip file contained on the attachment CD of this report. The CD was written using ROXIO Easy CD Creator 5 Basic installed on CRWMS M&O tag number 150527 central processing unit, and can be viewed on most standard CD-ROM drives. The zip archive was created using WINZIP 8.1. The zip file attributes on the CD are as follows:

Archive Filename	File Size (bytes)	File Date	File Time
Att.zip	5,465,107	05/15/2003	9:35a

There are 168 total files (not including folders) contained in a unique directory structure. Upon file extraction, the file naming system corresponds as follows for the SAS2H cases:

- *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 temporary 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.
- *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.

//*X.XatYY/*: this is a third level subdirectory where the X.X represents the initial uranium-235 enrichment in terms of wt% uranium-235 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 uses a 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 wt% uranium-235 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.

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