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Design Analysis Cover Sheet

Complete only applicable items.

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12. REMARKS

Note: Attachments XII and XXIV are not used.

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00	Initial Issue

Table of Contents:

1. Purpose

This analysis is prepared by the Mined Geologic Disposal System (MGDS) Waste Package Development (WPD) department with the objective of providing a comprehensive, conservative estimate of the consequences of the criticality which could possibly occur as the result of commercial spent nuclear fuel emplaced in the underground repository at Yucca Mountain. The consequences of criticality are measured principally in terms of the resulting changes in radionuclide inventory as a function of the power level and duration of the criticality. The purpose of this analysis is to extend the prior estimates of increased radionuclide inventory (Refs. 5.52 and 5.54), for both internal and external criticality. This analysis, and similar estimates and refinements to be completed before the end of fiscal year 1997, will be provided as input to Total System Performance Assessment - Viability Assessment (TSPA-VA) to demonstrate compliance with the repository performance objectives.

2. Quality Assurance

The Quality Assurance (QA) program applies to this analysis. The work reported in this document is part of the preliminary probabilistic evaluation of the waste package (WP). This activity can affect the proper functioning of the MGDS waste package; the waste package has been identified as an MGDS Q-List item important to safety and waste isolation (Ref. 5.1, pp. 5, 16). The waste package is on the Q-List by direct inclusion by the Department of Energy (DOE) as are the natural barriers of the Topopah Spring Welded (TSw) Hydrogeologic Unit, the Calico Hills Nonwelded (CHn) Hydrogeologic Unit, and the Saturated Zone (SZ) barrier; a QAP-2-3 evaluation has yet to be conducted. The work performed for this analysis is covered by a WPD QAP-2-0 work control Activity Evaluation entitled *Perform Probabilistic Waste Package Design Analyses* (Ref. 5.2). This QAP-2-0 evaluation determined that such activities are subject to *Quality Assurance Requirements and Description* (QARD) (Ref. 5.3) requirements. Applicable procedural controls are listed in the evaluation.

All design inputs which are identified in this document are for preliminary design and shall be treated as unqualified data; these design inputs will require subsequent qualification (or superseding inputs) as the waste package design proceeds. This document will not directly support any construction, fabrication or procurement activity and therefore is not required to be procedurally controlled as TBV (to be verified). In addition, the inputs associated with this analysis are not required to be procedurally controlled as TBV. However, use of any data from this analysis for input into documents supporting procurement, fabrication, or construction is required to be controlled as TBV in accordance with the appropriate procedures.

3. Method

The following methods are used for evaluating the consequences of WP internal criticality:

- The waste package temperature is determined as that at which the evaporation from the water surface (assumed to be just covering the top most assemblies; see Assumption 4.3.16) will just balance the infiltration which is assumed to be the maximum credible, 10

mm/yr (Ref. 5.18, Sect. 7).

- The drift wall temperature is determined by repository scale and drift scale hydrothermal calculations summarized in TSPA-95 (Ref. 5.18).
- The power level of the internal criticality is that necessary to support the rate of heat dissipation to the environment: (1) by radiation to the drift wall and conduction through the rock invert which is driven by the temperature gradient between the waste package and the drift wall; (2) by heating the infiltrating water from the general repository temperature to the waste package temperature; and (3) by evaporation of the water (heat of vaporization) from the surface of the pond within the waste package.
- The duration of the internal criticality is limited by the duration of the peak inflow (to the waste package) of water moderator necessary to maintain the power level.
- The sustainability of this criticality with respect to the balance between fissile species, which are generally consumed by the criticality, and neutron absorbers, which are generally produced by the criticality is verified by using SAS2H (Ref. 5.39) to calculate the species amounts at several times during the criticality, and using these amounts as input to MCNP (Ref. 5.40) to calculate the k_{eff} at each of the times.
- The radionuclide inventory found by using SAS2H is decayed after criticality shutdown for several times up to 999,999 years, using ORIGEN-S (Ref. 5.39).

The following methods are used for evaluating the consequences of criticality external to the WP:

- The average temperature of the critical mass is estimated as the boiling temperature of water at 50 atm. The reason for this estimate is that the most probable place where a reducing zone may occur is in organic material at the base of the tuff (Ref. 5.52), which is typically 500 meters below the water table (Ref. 5.25, Figure 1-6), giving rise to a hydrostatic pressure of 50 atm.
- The maximum power is determined as that required to maintain the average temperature of the critical spherical configuration against heat conduction out from the sphere.
- The maximum sustainable power is determined by assuming that all fissile material transported to the critical mass by the fissile material bearing water from one or more degraded waste packages in the repository is burned (Assumption 4.3.8).
- The duration of the external criticality is determined by the duration of flow of fissile material bearing water from the repository.
- The sustainability of the criticality and the increase in radionuclide inventory are determined by the same methods as were used for the internal criticality, using the computer codes, MCNP (Ref. 5.40), SAS2H, and ORIGEN-S (both Ref. 5.39).

Further detail on the specific analytical methods employed for each step is available in Section 7 of this analysis.

4. Design Inputs

The design inputs identified in this document are for preliminary design and shall be treated as unqualified data; these design input will require subsequent qualification (or superseding inputs) as the waste package design proceeds. This document will not directly support any construction, fabrication, or procurement activity and therefore is not required to be procedurally controlled as TBV.

4.1 Design Parameters

4.1.1 Spent Fuel Assembly Parameters

The fuel assembly upon which this calculation is based is the B&W 15 x 15 fuel assembly. The mechanical parameters for this assembly type are shown in Table 4.1-1. Note that inches are converted to centimeters exactly (2.54 cm/in.); this is not an indication of tolerance (accuracy), but is done for consistency between calculations using English or metric units. The theoretical density of UO_2 is 10.96 g/cm^3 (Ref. 5.39, Table M8.2.1). Non-fuel material compositions of Alloy 825, water, Zircaloy-4, A 516 carbon steel, and 316B6A stainless steel-boron alloy are taken from a QAP-3-9 analysis on material compositions (Ref. 5.5) and used in Attachment VII.

Table 4.1-1. Mechanical Parameters of B&W 15x15 Fuel Assembly

Parameter	Value	Units	Metric	Units	Radius (cm)	Ref.
Fuel Rods	208	/assbly	208	/assbly		5.41
Fuel Rods on a Lattice Side	15	/side	15	/side		5.41
Guide Tubes	16	/assbly	16	/assbly		5.41
Instrumentation Tubes	1	/assbly	1	/assbly		5.41
Total Guide + Instrument Tubes	17	/assbly	17	/assbly		-
Clad/Tube Material	ZIRC-4		ZIRC-4			5.41
Fuel Pellet OD	0.3686	inches	0.936244	cm	0.468122	5.41
Fuel Stack Height	141.8	inches	360.172	cm		5.41
Mass of U	1023	lb	464	kg		5.7
Mass of UO_2	1160.64	lb	526.46	kg		5.41
Percent of Theoretical Density	95	%	95	%		5.41
Fuel Clad OD	0.430	inches	1.0922	cm	0.5461	5.41
Clad Thickness	0.0265	inches	0.06731	cm		5.41
Fuel Clad ID*	0.377	inches	0.95758	cm	0.47879	-
Fuel Rod Pitch	0.568	inches	1.44272	cm		5.41
Guide Tube OD	0.530	inches	1.3462	cm	0.6731	5.41
Guide Tube Thickness	0.016	inches	0.04064	cm		5.41
Guide Tube ID*	0.498	inches	1.26492	cm	0.63246	-
Instrumentation Tube OD	0.493	inches	1.25222	cm	0.62611	5.41
Fuel Assembly Envelope	8.536	inches	21.68144	cm		5.41

* The inner diameters (IDs) above are calculated by subtracting 2 × thickness from the outer diameter (OD).

4.1.2 Intact Waste Package Geometry Parameters

The intact waste package geometry parameters used in this analysis are taken from Reference 5.54. The dimensions are listed in Table 4.1-2 below. Figure 4.1-1 depicts the 21 Pressurized Water Reactor (PWR) Advanced Uncanistered Fuel (AUCF) WP, its internals, and the material specifications (Ref. 5.34).

Table 4.1-2. Intact WP Dimensions

Component	Dimension (cm)
Outer barrier length (skirt edge to skirt edge)	533.5
Outer barrier skirt length (both ends)	22.5
Outer barrier inner radii	73.1
Outer barrier outer radii	83.1
Inner barrier length (overall)	466.5
Inner barrier inner radii	71.095
Inner barrier outer radii	73.095
Fuel cell tube opening	22.9
Fuel cell tube thickness	0.5
Fuel cell tube height	457.5
Criticality control panel/plate thickness	0.7
Criticality control panel/plate width	113.4
Criticality control long panel/plate (16 total) length	122.1
Criticality control short panel/plate (16 total) length	73.0
Criticality control panel/plate cutout length (4 per long panel/2 per short panel)	56.7
Criticality control panel/plate cutout width	0.7
Side and corner guide thickness	1.0

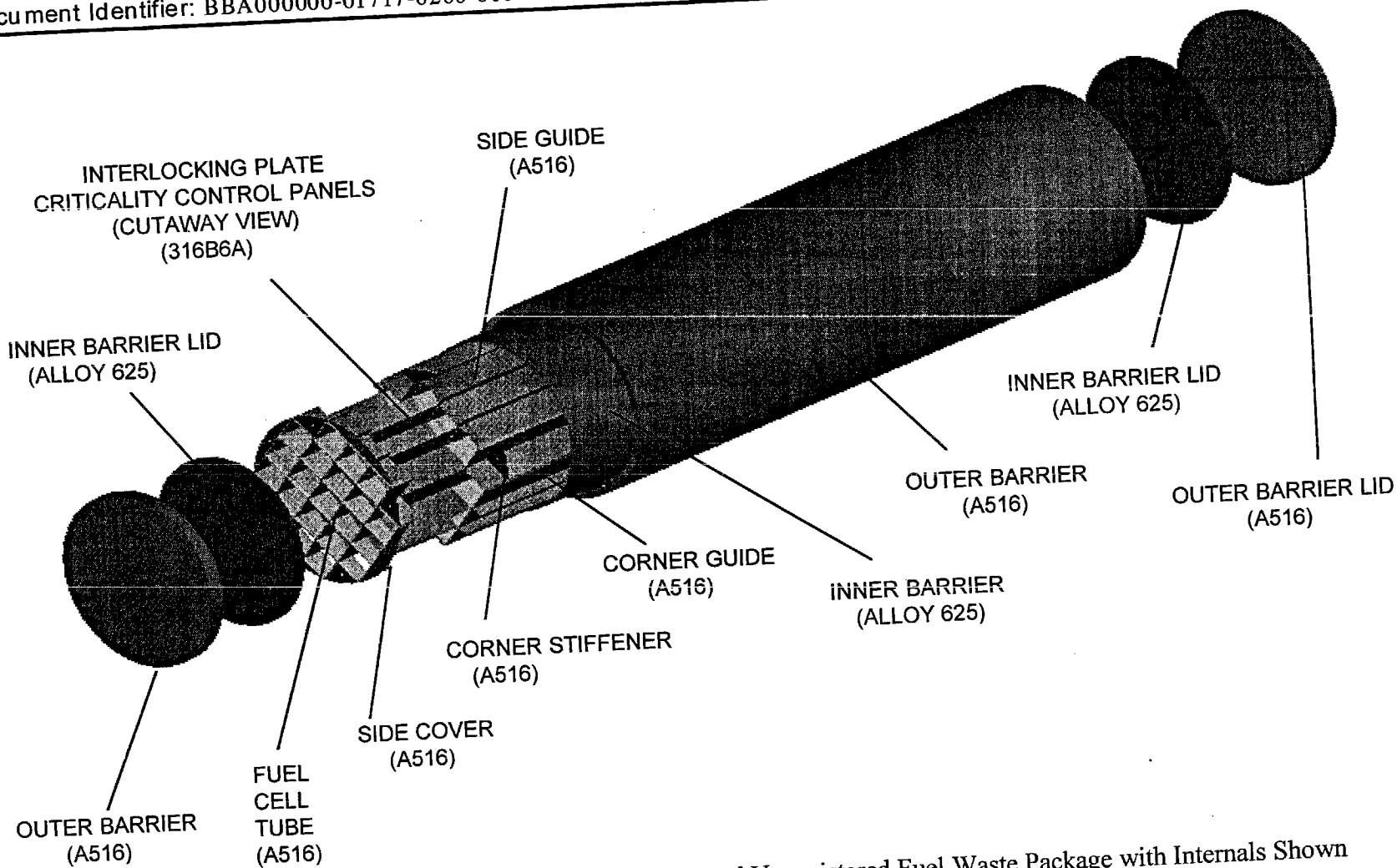

Figure 4.1-1. Advanced Uncanistered Fuel Waste Package with Internals Shown

4.1.3 Isotope Atomic Weights

The atomic weights of isotopes are listed in Table 4.1-3 below (Ref. 5.43 unless otherwise noted) and are used in the number density calculations discussed in Sections 7.2.1 and 7.4.4.

Table 4.1-3. Atomic Weights in g/mole (Ref. 5.43)

Isotope	MCNP ID	Atomic Weight
O-16	8016.50C	15.994915
nat. Mo	42000.50C	95.94
Mo-95	42095.50C	94.905839
Tc-99	43099.50C	98.90627501*
Ru-101	44101.50C	100.905576
Rh-103	45103.50C	102.905511
Ag-109	47109.50C	108.904756
nat. Cd	48000.50C	112.4
Xe-131	54131.50C	130.905069**
Xe-135	54135.50C	134.9063***
Cs-133	55133.50C	132.905355
Cs-135	55135.50C	134.90577
Nd-143	60143.50C	142.909779
Nd-145	60145.50C	144.912538
Sm-147	62147.50C	146.914867
Sm-149	62149.50C	148.91718
Sm-150	62150.50C	149.917276
Sm-151	62151.50C	150.919919
Sm-152	62152.50C	151.919756
Eu-151	63151.55C	150.919838
Eu-153	63153.55C	152.921242
Eu-154	63154.50C	153.923053
Gd-155	64155.50C	154.922664
Gd-157	64157.50C	156.924025
U-233	92233.50C	233.039522
U-234	92234.50C	234.040904
U-235	92235.50C	235.043915
U-236	92236.50C	236.045637
U-238	92238.50C	238.05077
Np-237	93237.55C	237.048056
Pu-238	94238.50C	238.049511
Pu-239	94239.55C	239.052146
Pu-240	94240.50C	240.053882
Pu-241	94241.50C	241.056737
Pu-242	94242.50C	242.058725
Pu-243	94243.35C	243.061972
Am-241	95241.50C	241.056714
Am-242m	95242.50C	242.059502
Am-243	95243.50C	243.061367
Cm-243	96243.35C	243.06137
Cm-245	96245.35C	245.065371

* From Reference 5.5

** From Reference 5.33

***Linearly interpolated from Atomic Weights of Xe-134 and Xe-136 in Reference 5.33.

Avogadro's Number [N_A] = 0.602252 $(g\text{-}mol)^{-1} \times 10^{24}$ (Ref. 5.43, p. 933).

4.1.4 Far-Field Tuff Composition and Characteristics

The composition and characteristics of the far field tuff are shown in Table 4.1-1 (Ref. 5.48, p. 16 unless noted otherwise).

Table 4.1-4. Calico Hills/Prow Pass Nonwelded-Zeolitic Tuff

Parameter	Value
Mean Density 198 samples	1.746 g/cm^3 *
Mean Porosity 127 samples (Max = 0.470**)	0.306*
Estimated Average Thermal Conductivity	1.38 W/m·K***
SiO_2 Wt%	69.1
TiO_2 Wt%	0.11
Al_2O_3 Wt%	13.4
Fe_2O_3 Wt%	1.13
MnO Wt%	0.05
MgO Wt%	0.94
CaO Wt%	3.22
Na_2O Wt%	1.23
K_2O Wt%	2.64
P_2O_5 Wt%	0.01
LOI (volatile) Wt%	8.90
Total Wt%	100.7

* Average values obtained form the data in Reference 5.47, p. 7-11.

** Previous evaluation of the porosity data for this tuff indicated that the 47% porosity data point was a statistical outlier (Ref. 5.47, p. 7-10) which was probably anomalous, so that the maximum of the sample should have been the maximum of the remaining 126 elements, 40% porosity.

*** Estimate is from Reference 5.31, p. 6 and is based on the average of two values from the Calico Hills tuff unit.

In addition to the above major-element concentrations, 25 trace-element concentrations were identified by parts per million (ppm) by weight (Ref. 5.48, Appendix C). Some of these trace elements have high absorption cross sections, for example, Eu, Hf, Sm, etc. Previous evaluation (Ref. 5.55, p. 5) indicated that none of these elements is contained in sufficient concentrations in the tuff, with an adequate confidence in the nominal value, to be included.

4.1.5 Properties of Saturated Liquid Water

Table 4.1-5. Properties of Saturated Water (Ref. 5.20, p. 656)

Temperature (°F)	Pressure (psia)	Specific Volume (ft^3/lb)
500	680.0	0.02043
510	743.5	0.02067

4.2 Criteria

This design analysis provides preliminary input for criticality analyses which evaluate whether waste package designs meet the repository criticality control design criteria from requirement documents. The *Mined Geological Disposal System Requirements Document* (Ref. 5.11) and the *Engineered Barrier Design Requirements Document* (EBDRD, Ref. 5.12) have criteria which pertain to criticality analyses. Reference 5.12 is the lower level document and contains all of the criteria listed in Reference 5.11. These requirements also apply to accumulations of fissile material in the far-field because far-field consequences can have an impact on the WP design. The WP is the source for material in the far-field and mitigation of significant consequences in the far-field may require some modification of the WP (Engeneered Barrier) design. The criteria cited in Reference 5.12 that have bearing on this analysis include the following:

4.2.1 From the EBDRD (Ref. 5.12);

"**3.2.2.6 CRITICALITY PROTECTION**

A. The Engineered Barrier Segment shall be designed to ensure that a nuclear criticality accident is not possible unless at least two unlikely, independent, and concurrent or sequential changes have occurred in the conditions essential to nuclear criticality safety. Each system shall be designed for criticality safety under normal and accident conditions. The calculated effective multiplication factor must be sufficiently below unity to show at least a five percent margin, after allowance for the bias in the method of calculation and the uncertainty in the experiments used to validate the methods of calculation.
[MGDS-RD 3.2.2.6.A][10CFR60.131(b)(7)]

B. To mitigate the potential for nuclear criticality, the Engineering Barrier Segment shall be designed and constructed to comply with the nuclear criticality requirements specified by DOE order 6430.1A, 1300-4.
[MGDS-RD 3.2.2.6.B] [DOE Order 6430.1A, 1300-4]"

4.2.2 From the EBDRD (Ref. 5.12);

"**3.7.1.3 INTERNAL STRUCTURE REQUIREMENTS**

A. The internal structure shall provide separation of the waste forms such that

nuclear criticality shall not be possible unless at least two unlikely, independent, and concurrent or sequential changes have occurred in the conditions essential to nuclear criticality safety. The calculated effective multiplication factor (k_{eff}) must be sufficiently below unity to show at least a five percent margin after allowance for the bias in the method of calculation and the uncertainty in the experiments used to validate the methods of calculation (TBD).
[MGDS-RD 3.2.2.6.A] [10CFR60.131(b)(7)]"

The present DOE Office of Civilian Radioactive Waste Management (OCWRM) and Civilian Radioactive Waste Management System (CRWMS) Management and Operating Contractor (M&O) position is that the requirement cited in the above criteria based on 10CFR60.131(b)7, being primarily of a deterministic nature, is not appropriate for postclosure disposal criticality. Instead, the probability or risk based approach has been recommended to the U.S. Nuclear Regulatory Commission (NRC) in the following two letters:

4.2.3 From Ronald A. Milner, Director, Office of Program Management and Integration, OCRWM, to the NRC, Docketing and Service Branch, dated June 16, 1995, which included the specific recommendation to apply the above requirements only to preclosure, and create the following new requirement for postclosure criticality:

"Postclosure criticality safety. The engineered barrier system shall be designed such that the probability and consequences of nuclear criticality provide reasonable assurance that the performance objective of §60.112 is met." (Ref. 5.4)

4.2.4 From Stephan J. Brocoum, Assistant Manager for Suitability and Licensing, OCRWM, to Michael J. Bell, Chief, Engineering and Geosciences Branch, Division of Waste Management, Office of Nuclear Material Safety and Safeguards, NRC, which referred to the above referenced letter, and specifically commented as follows:

"The DOE, therefore, requests that consideration be given to the DOE's proposed revision to 10CFR60.131(b)7 that would allow disposal criticality to be evaluated with risk-based methods." (Ref. 5.6)

The analyses in this document are intended to provide values of, and justification for, consequence parameters (specifically increased radionuclide inventory) plus probability information which will be used as part of TSPA-License Application (LA) to demonstrate compliance with the performance objective of §60.112 (or, as appropriate, other applicable performance objectives in effect or proposed by the NRC at the time the TSPA-LA analysis is performed). The "TBD" items identified in the above criteria will not be carried to the conclusions of this analysis based on the rationale that the conclusions are for preliminary design, and will not be used as input in design documents supporting construction, fabrication, or procurement.

4.3 Assumptions

All assumptions identified in this section will require verification (or superseding assumptions) as the waste package design proceeds and should be treated as unconfirmed items for preliminary design. For this preliminary design, that will not be used to support procurement, fabrication, or construction, the assumptions are clearly identified and traceable to a source, but are not procedurally controlled as TBV.

4.3.1 Principal Isotope (PI) burnup credit is assumed to be an acceptable method to account for reduced reactivity of SNF in criticality evaluations. The basis for this assumption is CDA Key 009 (Ref. 5.44). This assumption is used throughout Section 7.

4.3.2 The reference PWR fuel physical assembly selected for conceptual development is the B&W 15 x 15 fuel type, which has been established as one of the more reactive PWR fuel designs under intact fuel assembly and fixed basket geometry conditions (Ref. 5.16, p. II.A.3-35). This assumption is used throughout Section 7.

4.3.3 The design basis spent nuclear fuel (SNF) characteristics within the physical assembly are 3.0% U-235 enrichment, 20 GWd/MTU burnup, as established by the M&O (Ref. 5.10, Section 5). This SNF composition is assumed to be more stressing with respect to criticality than 96-97% of the SNF inventory. This SNF composition is representative only. It does not necessarily match any composition for a B&W assembly type specified in the previous assumption. This assumption is used throughout Section 7.

4.3.4 For SNF, the list of "Principal Isotopes" previously established (Ref. 5.46, p. 4-4) for long-term criticality control was used. The 29 principal isotopes are shown in Table 4.3-1. This assumption is used in Sections 7.3.2 and 7.4.

Table 4.3-1. Principal Long-Term Burnup Credit Isotopes

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

4.3.5 It is assumed that the cooling of the external criticality in the saturated zone will be primarily by conduction. The basis for this assumption is that the maximum cooling possible from the next largest physical mechanism, advective flow through the criticality zone, is much smaller than the rock conduction, as is seen from the following calculation:

The maximum advective heat transfer is approximated by the mean advective flow

(Darcy velocity) in the saturated zone (2 meters/yr, Ref. 5.18, p. 7-21) multiplied by the cross-section area of the critical zone (1.4 m radius, which is 6.16 m^2 cross-section), multiplied by the heat capacity of water (aproximated by 4200 Joules/kg·K, Ref 5.14, which is also $4.2x10^6$ Joules/m^3·K), multiplied by maximum temperature change between the critical mass and the far-field heat sink, and divided by the number of seconds in a year ($31.5x10^6$). The maximum change in temperature between the critical sphere and the far field is given in Attachment I, and in Section 7.3.2, as $P/(4\pi kR)$, where k is the thermal conductivity (1.38 W/m·K, Ref. 5.31, p. 6), P is the power generated by the critical sphere, and R is the radius, 1.4 m, given above. The resulting conservative estimate of advective heat transfer is 0.07P, which means that it can be no more than 7% of the conductive heat transfer. This assumption is used in Section 7.3.2.

4.3.6 It is assumed that the maximum power from the worst case external criticality will occur in the saturated zone, at the base of the tuff and will be at a pressure of 50 atmospheres. The basis for this assumption is that the reducing material from original organic deposits could not have been emplaced while the tuff was being deposited, and can, therefore, be found only at the base of the tuff, which is approximately 500 meters below the water table (Ref. 5.25, Figure 1-6), at which the hydrostatic pressure is approximately 50 atmospheres. A rapid onset of criticality could, of course, result in a temporary overpressure, but that possibility is not considered according to the steady state assumption (Assumption 4.3.7, below). This assumption is used in Section 7.3.3.

4.3.7 It is assumed that the criticality is in a steady state so that the time independent heat conduction equation can be used to establish the relation between criticality power and temperature. The basis for this assumption is that over the thousands of years (conservative estimate of reactor duration) the short period fluctuations will average out. This assumption is used in Section 7.3.2 and in Attachment I.

4.3.8 First, it is assumed that the sustainable criticality power for the external criticality is limited by the fuel replenishment rate from the infiltration of fissile material bearing water from the repository. (This is lower than the maximum power identified in Assumption 4.3.6, above and described in Section 7.3.3.) Secondly, it is further assumed that the incoming fissile material can only provide that portion of the fissile material which is above 1.37%, as is explained in Section 7.3.4 of this analysis and Section 7.7 of Reference 5.52, where the argument was initially presented. The basis for the first part of this assumption is that the criticality will begin when k_{eff} just reaches 1, so that any amount of fissile material consumed must be replaced by fresh fissile material in order to sustain the criticality. The basis for the second part of this assumption is given in Section 7.3.4 of this analysis and Section 7.7 of Reference 5.52. This assumption is used in Section 7.3.4.

4.3.9 The SAS2H module in SCALE4.3 (Ref. 5.39) is assumed to be applicable to analysis of accumulations of fissile material in tuff. The basis of this assumption is that the 44 group cross section library used in these calculations likely provides enough detail to cover the more thermal spectrum (compared to PWRs) of the external accumulations adequately.

This assumption will require future verification. This assumption was used in a previous analysis (Ref. 5.53) to generate the data used in Section 7.2.2, and is also used in Section 6.1.

4.3.10 The SAS2H and ORIGEN-S modules in SCALE4.3 are assumed to provide reasonable predictions of isotopic compositions for a low power criticality event over several thousand years. The basis of this assumption is the demonstration in Section 7.4.2 that no nonconservative trends exist by comparing the results of 100 year and 1000 year time steps. This assumptions will require future verification. This assumption is used in Sections 6.1, 7.2.1, 7.2.2, 7.4.3, and 7.4.4.

4.3.11 For external criticality, water infiltration has provided the mechanism for waste package and SNF degradation, as well as the mechanism for actinide transport to the far field environment. This assumption is used throughout Sections 7.3 and 7.4.

4.3.12 The material compositions for tuff in the far field is assumed to be represented by the major constituents of Calico Hills/Prow Pass nonwelded-zeolitic tuff taken from References 5.47 and 5.48. Portions of these formations fall within the saturated zone. This assumption is used throughout Sections 7.3 and 7.4.

4.3.13 The accumulation of UO_2 in saturated tuff is assumed to be represented by a spherical homogeneous mixture of UO_2/tuff/water. Fracture distributions and densities in the tuff, size and density of potential uranium deposits, and presence and composition of reducing zones within the tuff are unknown. This assumption is used throughout Sections 7.3 and 7.4.

4.3.14 The power level of the internal criticality is that necessary to support the rate of heat dissipation to the environment: (1) from the lower half of the waste package, by conduction through the rock invert which is driven by the temperature gradient between the waste package and the drift wall; (2) from the upper half of the waste package, which is assumed to be uncovered, by radiation from the package surface to the drift wall; (3) by evaporation of the water from the surface of the pond within the waste package. This assumption was used in Reference 5.54, which is the basis for information provided in Sections 7.1 and 7.2.

4.3.15 In determining the temperature gradient for Assumption 4.3.14, the drift wall temperature is determined by repository scale and drift scale hydrothermal calculations summarized in TSPA-95 (Ref. 5.18). This assumption is used throughout Sections 7.1 and 7.2.

4.3.16 In determining the temperature gradient for Assumption 4.3.14, the waste package temperature is assumed to be just large enough that the evaporation from the water surface (assumed to just cover the top most assemblies) will just balance the water inflow to the package which is assumed to be at the maximum high infiltration rate 10 mm/yr (Ref. 5.18, TSPA-95). The basis for this assumption is that the internal criticality is moderator limited, so that it is necessary to maintain the water level in order to maintain

the criticality. It turns out that even for this maximum possible infiltration rate, this waste package temperature is significantly less than the boiling temperature. This assumption is stated in Section 3.0, and is used throughout Sections 7.1, 7.2, and 7.3.4.

4.3.17 The duration of the internal criticality is limited by the peak inflow of water necessary to maintain the power level estimated according to Assumption 4.3.14. The basis for this assumption is the same as the basis for Assumption 4.3.16 to which it is closely related. This assumption is used throughout Sections 7.1 and 7.2.

4.3.18 The fresh fuel bias and uncertainty for MCNP is approximately 0.015 (Ref. 5.45, p. 6-221). The preliminary SNF bias and uncertainty is approximately 0.06 (Ref. 5.45, p. 6-221). These uncertainties were used in a prior unverified analysis. This assumption is used throughout Section 7.

4.3.19 The deterministic based requirements in the EBDRD (Ref. 5.12) are assumed not to apply to postclosure disposal criticality. The basis is the ongoing interaction between DOE and NRC to change the requirements to allow a probabilistic approach to postclosure disposal criticality as indicated in Section 4.2. This assumption is used throughout Section 7.

4.3.20 It is assumed that the mobilization (removal from the waste package) of the fissile material is much slower than the dissolution of the SNF. The consequence of this assumption is that the removal of the fissile material from the waste package is limited by the water flux through the waste package, or incident on the waste package. The basis of this assumption is the analysis given in Reference 5.52, Section 7.2. This assumption is used in Section 7.3.4.

4.4 Codes and Standards

American National Standard on "Criticality Safety Criteria for the Handling, Storage, and Transportation of LWR Fuel Outside Reactors", ANSI/ANS-8.17, 1984.

5. References

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5.2 Activity Evaluation, *Perform Probabilistic Waste Package Design Analyses*, Document Identifier Number (DI#) BB0000000-01717-2200-00030 REV 02, CRWMS M&O

5.3 *Quality Assurance Requirements and Description*, DOE/RW-0333P, REV 5, Department of Energy (DOE) Office of Civilian Radioactive Waste Management (OCRWM)

5.4 Letter, R.A. Milner to Secretary, U.S. NRC Docketing and Service Branch, Transmitting DOE comments regarding NRC-proposed revisions to 10 CFR Part 60 Regulations for Design Basis Events, June 16, 1995

5.5 *Material Compositions and Number Densities for Neutronics Calculations*, DI# BBA000000-01717-0200-00002 REV 00, CRWMS M&O

5.6 Letter, S.J. Brocoum to M.J. Bell, Providing DOE acknowledgment of receipt of NRC comments on the Annotated Outline for the Disposal Criticality Analysis Topical Report, April 12, 1996

5.7 *Characteristics of Potential Repository Wastes*, DOE/RW-0184-R1, Volume 1, p. 2A-8, July 1992, DOE OCRWM

5.8 *Initial Waste Package Probabilistic Criticality Analysis: Uncanistered Fuel*, DI# B00000000-01717-2200-00079 REV 01, CRWMS M&O

5.9 *Initial Waste Package Probabilistic Criticality Analysis: Multi-Purpose Canister With Disposal Container*, DI# B00000000-01717-2200-00080 REV 01, CRWMS M&O

5.10 *Mined Geologic Disposal System Advanced Conceptual Design Report, Volume III of IV, Engineered Barrier Segment/Waste Package*, DI#: B00000000-01717-5705-00027 REV 00, CRWMS M&O.

5.11 *Mined Geologic Disposal System Requirements Document*, DOE/RW-0404P REV 02/ICN 01, DOE OCRWM

5.12 *Engineered Barrier Design Requirements Document*, YMP/CM-0024, REV 0, ICN 1, Yucca Mountain Site Characterization Project

5.13 *Characteristics Database LWR Radiological PC Database*, Version 1.1, CSCI A00000000-02268-1200-20002, CRWMS M&O

5.14 Holman, J.P., *Heat Transfer*, 7th Edition, McGraw-Hill Publishing Company, 1990

5.15 *User Manual for the CDB_R*, DI#: A00000000-01717-2002-20002 REV 01, CRWMS M&O

5.16 *Multi-Purpose Canister (MPC) Implementation Program Conceptual Design Phase Report, Volume II.A - MPC Conceptual Design Report*, DI# A20000000-00811-5705-00002 REV 00, CRWMS M&O

5.17 *CRC Handbook of Chemistry and Physics*, 66th Edition, CRC Press, 1985

5.18 *Total System Performance Assessment - 1995: An Evaluation of the Potential Yucca Mountain Repository*, DI# B00000000-01717-2200-00136 REV 01, CRWMS M&O

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5.25 *Performance Assessment of the Direct Disposal in Unsaturated Tuff of Spent Nuclear Fuel and High-Level Waste Owned by U.S. Department of Energy*, Sandia National Laboratory, SAND94-2563/2, March 1995

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5.31 *Emplacement Scale Thermal Evaluations of Large and Small WP Designs*, DI# BB0000000-01717-0200-00009 REV 00, CRWMS M&O

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5.33 *Nuclides and Isotopes*, Fourteenth Edition, General Electric Company, 1989

5.34 *Material of 21 PWR AUCF Waste Container*, Interoffice Correspondence LV.WP.HW.03/96.059, Helen Wang, March 13, 1996, CRWMS M&O

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5.39 *SCALE 4.3, RSIC Computer Code Collection*, CCC-545, Oak Ridge National Laboratory, October 1995

5.40 *MCNP 4A - Monte Carlo N-Particle Transport Code System*, CSCI# 30006 v4A, RSIC Computer Code Collection, CCC-200, Oak Ridge National Laboratory, February 1994

5.41 *Preliminary Waste Form Characteristics Report Version 1.0*, UCRL-ID-108314 Rev 1, Lawrence Livermore National Laboratory, December 1994

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5.43 Benedict, Manson, et al., *Nuclear Chemical Engineering*, Second Edition, McGraw-Hill Book Company, New York, 1981

5.44 *Controlled Design Assumptions (CDA) Document*, DI# B00000000-01717-4600-00032 REV 03, CRWMS M&O (TBV-221-DD)

5.45 *Initial Summary Report for Repository/Waste Package Advanced Conceptual Design*, DI# B00000000-01717-5705-00015 REV 00, CRWMS M&O

5.46 *Disposal Criticality Analysis Technical Report*, DI# B00000000-01717-5705-00020 REV 00, CRWMS M&O

5.47 *Total-System Performance Assessment for Yucca Mountain - SNL Second Iteration (TSPA-1993), Volume 1*, SAND93-2675, April, 1994

5.48 *Chemistry of Diagenetically Altered Tuffs at a Potential Nuclear Waste Repository, Yucca Mountain, Nye County, Nevada*, LA-10802-MS, Los Alamos National Laboratory, October, 1986

5.49 *SCALE4.3 and MCNP4A Installation*, Interoffice Correspondence LV.WP.JWD.06/96.135, J. Wesley Davis, June 11, 1996, CRWMS M&O

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5.52 *Probabilistic External Criticality Evaluation*, DI# BB0000000-01717-2200-00037 REV 00, CRWMS M&O

5.53 *SAS2H Generated Isotopic Concentrations for B&W 15x15 PWR Assembly*, DI# BBA000000-01717-0200-00012 REV 01, CRWMS M&O

5.54 *Second Waste Package Probabilistic Criticality Analysis: Generation and Evaluation of Internal Criticality Configurations*, DI# BBA000000-01717-2200-00005 REV 00, CRWMS M&O

5.55 *Preliminary Criticality Analysis of Degraded SNF Accumulations External to a Waste Package*, DI# BBA000000-01717-0200-00016 REV 00, CRWMS M&O

5.56 *Validation of the Scale System for PWR Spent Fuel Isotopic Composition Analyses*, Oak Ridge National Laboratory, ORNL/TM-12667, March 1995

6. Use of Computer Software -

6.1 Scientific and Engineering Software

SCALE 4.3 (Ref. 5.39), which includes the SAS2H and ORIGEN-S modules used in this report, has not been qualified according to QA procedures. The SAS2H and ORIGEN-S results for external criticalities of this analysis, therefore, shall be treated as unqualified data. SCALE 4.3 was run on HP Series 735 Workstations. SCALE 4.3 is an appropriate tool to be utilized to determine the composition and characteristics of PWR spent fuel and has been demonstrated to run correctly on the HP 735 workstations (Ref. 5.49). This code has been validated for this application by ORNL (Ref. 5.56). The application of SAS2H to accumulations of fissile material in tuff and to long term low power depletion due to a criticality event does not fall within the ORNL range of validation and must be validated in the future. The 44 group cross section library used in these calculations likely provides enough detail to cover the more thermal spectrum of the external accumulations adequately (Assumption 4.3.9). In addition, the ability to cover the long term low power depletion calculations is checked in this report (Section 7.4.2) by comparing the results from two different time step sizes (100 and 1000 years; Assumption 4.3.10).

MCNP4A (Ref. 5.40; CSCI# 30006 v4A) was run on HP 735 Workstations. MCNP4A is qualified according to QA procedures and was obtained from the SCM in accordance with appropriate procedures. MCNP4A is utilized to determine the criticality potential SNF and of fissile material accumulations in the far field environment external to the repository and is an appropriate tool for these purposes, and was used within the range of validation.

The results from MCNP cases are reported as $k_{eff} \pm 2\sigma$. k_{eff} is the final estimated combined collision/absorption/track-length k_{eff} reported in MCNP. 2σ is twice the standard deviation of the calculated value and $k_{eff} \pm 2\sigma$ approximately represents the 95% confidence interval of the result.

There are biases and uncertainties associated with a criticality calculation. How these biases and uncertainties are treated in criticality calculations is covered in the American National Standard on "Criticality Safety Criteria for the Handling, Storage, and Transportation of LWR Fuel Outside Reactors" (see Section 4.4). The fresh fuel bias and uncertainty for MCNP is approximately 0.015 (Ref. 5.16, p. II.A.3-35). The fresh fuel bias and uncertainty is appropriate for application to the external accumulations of fissile material investigated in this analysis.

The CDB LWR Radiological PC Database (CDB-R, Ref. 5.13), CSCI: A00000000-02268-1200-20002 v1.1, was used to obtain the radiological characteristics of the thermal/shielding DBF. The CDB has been qualified by the Office of Civilian Radioactive Waste Management for use in work subject to the requirements of the QARD (Ref. 5.3). The CDB was installed on an IBM-compatible PC in accordance with the User Manual for the CDB-R (p. 1, Ref. 5.15) and was obtained in accordance with the QAP-SI series procedures. Use of the SNF radionuclide inventories from the CDB is appropriate for this design analysis and is within the range of validation performed for the CDB.

6.2 Computational Support Software

LOTUS 1-2-3, Release 4.01 for Windows was used to calculate the isotopic number densities for the spent nuclear fuel and tuff/water/UO_2 mixtures investigated. Details of the equations and used of the spreadsheet are provided in Section 7.

7. Design Analysis -

This design analysis is presented in five sections. Sections 7.1 and 7.2 deal with internal criticality. The first gives the basic parameters of the criticality, and the second gives the results of the neutronics evaluation; increase in radionuclide inventory and change in k_{eff}. Sections 7.3 and 7.4 deal with external criticality in the same way as the internal criticality sections. Section 7.5 summarizes the previous estimates of probability associated with the critical configurations and lists the data items expected to be obtained within the next year to improve these estimates.

7.1 Internal Criticality, Basic Parameters

7.1.1 Waste Package Nominal Criticality Configuration

The purpose of this section is to summarize the 21 PWR AUCF WP internal degraded configuration for which the consequences of criticality have been modeled, and provide a brief summary of the progression of WP degradation from the initial configuration to the configuration for which criticality may be of concern. Further detail on the information presented here can be found in the *Second Waste Package Probabilistic Criticality Analysis: Generation and Evaluation of Internal Criticality Configurations* (Ref. 5.54) and the *Emplaced Waste Package Structural Capability Through Time Report* (Ref. 5.50).

7.1.1.1 Basket Collapse

This section discusses the four primary basket components responsible for maintaining the initial configuration of the WP, and the anticipated changes in the WP configuration which will occur as a result of their degradation following WP breach. These are the side and corner guides, the neutron absorber plates, fuel cell tubes, and the fuel assemblies themselves. Prior to WP breach, the interior of the WP is filled with an inert gas, and no degradation of the internal components would be expected. The inert environment is lost on first pit penetration of both WP barriers, which TSPA-95 (Ref. 5.18, Sect. 5) predicted would occur for a majority of WPs (typically 80% or more) within 2000 to 10,000 years after emplacement under most of the 83 MTU/acre scenarios. However, those scenarios which considered that the remaining carbon steel could provide cathodic protection for the inner barrier showed much longer times to first pit penetration (in the 10,000 to 100,000 year time frame)

The AUCF WP side and corner guides are fabricated from 10 mm thick carbon steel plates. Reference 5.50 indicates that the side guide will fail by bending at a thickness of 2.9 mm if there is no backfill loading the basket. Reference 5.50 estimated that this failure would occur within 60 to 340 years following WP breach for the 83 MTU/acre case without backfill using the TSPA-95 carbon steel corrosion model. Failure of the side guides will cause the bottom row of fuel assemblies to shift downward to touch the inside of the inner barrier. As the criticality control plate assemblies also rest on the top of the side guides, the entire basket structure should also shift downward. Since the corner guides are under less loading, their failure should occur shortly after failure of the side guides. Failure of the corner guides will result in the assemblies on the end of the second row from the bottom to shift downward to touch the inside of the inner barrier.

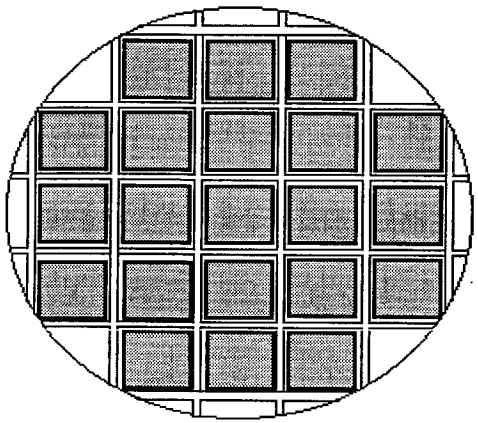
The assemblies above them should remain in place until sufficient degradation of the neutron absorber plates which support them has occurred.

The fuel cell tubes are also fabricated from carbon steel and have a wall thickness of 5 mm. The tubes will fully degrade before the failure of the side guides or the criticality control plates. In analyzing the criticality control plates, it was determined that the plates could maintain the basket and SNF assembly configuration without structural support from the tubes. Failure of the tubes will, therefore, not cause collapse of the basket, so no specific analysis was performed for the tubes. However, the remaining corrosion products occupy a greater volume than the original tubes and are fairly insoluble. Thus their presence may have some impact on WP internal criticality.

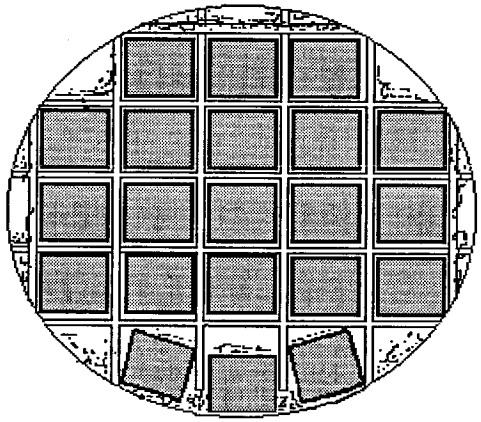
The AUCF WP neutron absorber plates are fabricated from 7 mm thick borated Type 316L stainless steel plates. Reference 5.50 found that the horizontal absorber plates will bend once 2.5 mm of thinning has occured, and the vertical plates will buckle after 5.36 mm of material is removed. Reference 5.50 made a preliminary estimate that it will take 2000 to 8500 years following breach of the WP for general corrosion of both sides of the neutron absorber plates to remove the 2.5 mm of material that would be required for bending to occur. It was estimated to take 4300 to 18,000 years to remove the 5.36 mm of material that would be required for buckling of the vertical plates. Bending will occur first at the ends of horizontal long criticality plates, causing the assemblies in the two side columns to drop down. Final collapse of the basket will occur due to bending of the horizontal plates supporting the assemblies (which would be expected to occur at a time later than the bending of the ends because the plates are supported on two sides) or buckling of the vertical plates. Final collapse will leave the center three columns of fuel assemblies resting on the bottom of the inner barrier.

Finally, Reference 5.50 also evaluated possible mechanisms for denting or crushing the fuel assemblies such that they no longer provide an optimum geometry for criticality. It was concluded that denting of the fuel rods would not occur because there is sufficient void space for expansion of the corroding basket materials, thus preventing them from causing any load on the fuel assemblies. Preliminary structural analyses were also performed which determined that the bottom-most fuel assemblies would be capable of supporting the entire degraded basket structure, and all fuel assemblies above them, without being crushed. Based on this information, the assumption of intact fuel assemblies for criticality analyses is appropriate and conservative until significant corrosion of the fuel rods and spacer grids has occured. Efforts to estimate the amount of corrosion required for such failures are currently under way.

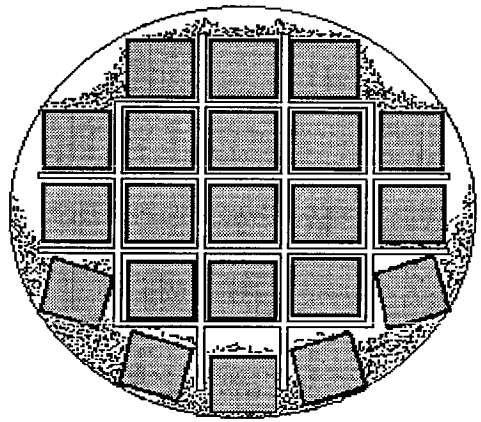
Figure 7.1.1-1 shows the initial and degraded waste package internal configurations. As will be discussed in the following sections the final stage, where complete degradation of the basket components has occured, will be the primary configuration of concern for postclosure internal AUCF WP criticality.



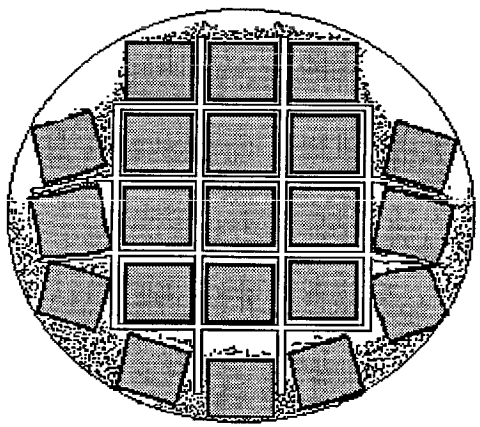
Initial Configuration



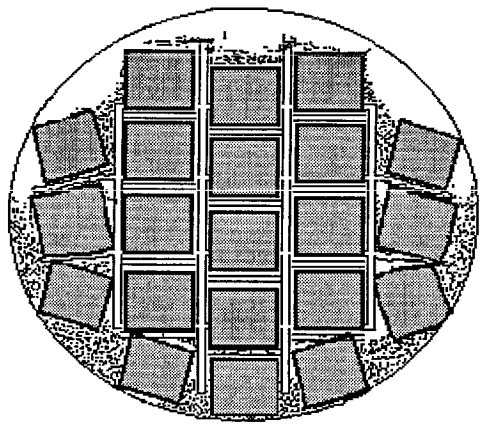
Side Guide Failure
60 to 340 years after WP breach



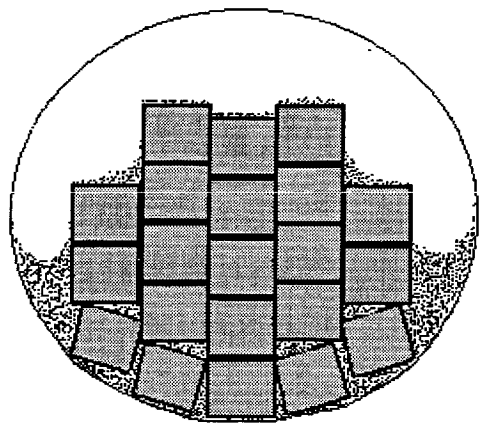
Corner Guide Failure
100 to 500 years after WP breach



Long Criticality Control Plates
Bend at Ends
2000 to 8500 years after WP breach



Complete Basket Collapse
2000 to 18000 years after WP breach
(remainder of plates still between assemblies)



Complete Basket Degradation
5700 to 24000 years
after WP breach

Figure 7.1.1-1. Initial and Degraded Waste Package Internal Configurations

7.1.1.2 Neutron Absorber Loss

As discussed above in Section 7.1.1.1, the degradation and collapse of the basket will leave behind a significant amount of iron, nickel, and chromium oxide corrosion products. In addition, the boron in borated stainless steel is in the form of a boride of iron (or one of the other metal components of stainless steel). Since such borides are generally found to be very stable (as described in Reference 5.25), the borides can be assumed to oxidize much more slowly than the iron, and some fraction will be trapped in the solid iron/chromium/nickel oxide matrix of the corroding stainless steel. Oxide corrosion products from the carbon steel components will also contribute to this trapping process.

Reference 5.54 performed an evaluation of the times required to remove specific amounts of the oxide corrosion products and the trapped boron from a WP which is assumed to be penetrated only on top and filled with water. A scenario which could lead to this configuration is based on the assumption that there will be very little probability of penetration of the lower portion of the waste package barriers before penetration of the upper portion, because such an "outside-in" process would require pit growth to a depth of 12 centimeters against gravity. The scenario begins with penetration of the upper portion of the barrier in 3000 to 5000 years; during much of the time before 3000 years the barrier temperature is above 90°C, and the aqueous corrosion rate of corrosion resistant inner barrier is modeled as being relatively high (Ref. 5.18), which is the reason why the penetration time is so short. After penetration of the upper portion of the barrier, penetration of the lower portion can begin from the inside out. By this time, however, the temperature is likely to have dropped below 50°C, where the TSPA-95 inner barrier corrosion models predict very small corrosion rates (Ref. 5.18). Because of the present uncertainty in the corrosion model, the probability for achieving a water-filled configuration as a result of this scenario has not yet been estimated. It is expected to be small.

Under such a flooded "bath tub" scenario (which is a required precondition for any internal WP criticality), removal of the oxides is accomplished by dissolution and removal via flushing through the upper portion of the WP. Reference 5.54 assumed that by the time oxides are dissolved, the trapped boride will have oxidized and will also dissolve, in which case it will be quickly flushed out of the package. The alternative is that the boron would still be solid boride, in which case it could remain in place (clinging to the remaining solid iron oxide, or fuel rods) or it could fall to the bottom of the package. The preliminary analysis in Reference 5.54 found that a flooded WP did not exceed a k_{eff} of 0.91 (used as the delimiter for criticality in that reference) until only 90% of the iron, nickel, and chromium oxides (uniformly occupying approximately 26% of the interior void space), and 5% of the initial boron remained. By this time, all internal plates, guides, and tubes had completely degraded. Thus, the first four degraded configurations identified in Figure 7.1.1-1 are of no concern from a postclosure criticality standpoint. Flushing times required to remove this material ranged from 12,000 years to greater than 100,000 years, depending on a number of assumptions such as the fraction of trapped boron, the inflow rate, the solubility of the oxides, the efficiency of the flushing process, and the drip rate of water onto the package.

7.1.2 Determination of Power, Temperature, and Duration

The internal criticality scenarios evaluated thus far simulate a flooded waste package that is gradually approaching a critical condition (k_{eff}=1) as a result of positive reactivity insertions caused by a slow loss of boron and iron from the package interior. Once a waste package reaches a k_{eff} of 1, continued small positive reactivity insertions will cause the power output of the waste package to begin to slowly rise (i.e., a long reactor period). If the power exceeds a certain limit, the rate at which water is consequentially removed from the waste package will exceed the rate of input, and the resulting water level drop will provide a negative reactivity insertion driving the waste package back towards a subcritical condition. Conversely, if insufficient power is produced, the water level will be maintained and the exchange process discussed previously will continue to remove dissolved boron, thus providing a continued source of positive reactivity insertions until the point of equilibrium is achieved. The maximum steady state power can then be estimated by determining the power required to maintain the bulk waste package water temperature at the point where water is removed at the same rate that it drips into the waste package. The waste package must produce sufficient power to raise the temperature of the incoming water to this equilibrium value, as well as account for the heat of vaporization and heat losses to the environment by radiation and/or conduction. Preliminary calculations, which are provided in detail in Reference 5.54, have shown that at a water temperature of 57.4°C, the evaporation rate will match the maximum TSPA-95 rate at which water drips into a WP located beneath a flowing fracture (191 liters/yr, Ref. 5.18, Sect. 7). The thermal power required to raise the water temperature to 57.4°C, while at the same time compensating for heat losses to the environment is 2.18 kW.

7.2 Internal Criticality, Neutronic Evaluation

The neutronic evaluation procedure for the far-field criticality involves three tasks as indicated below:

1) SAS2H burn calculations for intact fuel assemblies were run in a separate analysis (Ref. 5.53) and the results are displayed and utilized in this analysis,
2) Spreadsheet calculations of compositions from various duration criticality events using information from step 1, and
3) MCNP calculations of k_{eff} based on compositions from a 15,000 year decay case and the various duration criticality events.

7.2.1 Radionuclide Increase Resulting From an Internal Criticality

To evaluate the effects of a criticality on the radionuclide inventory of a waste package, the computer code ORIGEN-S was run using the PWR criticality design basis fuel, and the steady state power of 2.18 kW discussed above. The criticality was assumed in References 5.53 and 5.54 to occur after the fuel had aged/decayed for 15,000 years and was maintained at the above mentioned power for three durations: 1000, 5000 and 10,000 years. The maximum duration of 10,000 years is based on the assumption that it is the upper bound for the conditions supporting criticality (high infiltration, integrity of the lower part of the barrier, sufficient fissile material and

void space remaining). The output of these runs was the radionuclide inventory, in curies, at the times corresponding to the end of each criticality, and at fuel ages (time since reactor discharge) of 45,000 and 65,000 years (Ref. 5.53, Atts. VII-XI). In addition a fourth, decay-only case was run to determine the radionuclide inventories at the above times for fuel which did not experience a criticality event (Ref. 5.53, Att. VI). The percentage increase in the inventories of 36 of the isotopes examined in TSPA-95 is provided in Reference 5.54. The overall effect of the criticality on the radionuclide inventory can be summarized by the percentage increase in the total curies, over that of the decay-only case, for the 36 TSPA-95 isotopes. Table 7.2.1-1 shows this comparison. The explicitly stated times are measured from emplacement. Figure 7.2.1-1 graphically shows that even the 10,000 year duration criticality does not increase the inventory of the 36 isotopes above that at the time the criticality began. In addition, the criticality appears to have no significant long-term effect on the inventory of these isotopes. Within 25,000 years the total inventory of these 36 isotopes in fuel assemblies which experienced a criticality can barely be distinguished (<10%) from the inventory in fuel assemblies which did not experience a criticality. Furthermore, Table 7.2.1-2 indicates that the increase in the total inventory of the 36 TSPA-95 isotopes in a fuel assembly which experiences a criticality at 15,000 years does not exceed that of the worst decay only fuel, which is represented by the PWR thermal/shielding DBF.

Table 7.2.1-3 shows that the total increase in the inventory of the 36 TSPA-95 isotopes per unit burnup for the PWR criticality DBF is comparible to the in-reactor burn with ≈400 years of decay. Note that Table 7.2.1-3 gives the increment in Curies due to the specified burn, while Table 7.2.1-2 gives the toal Curies after the specified burn. These results are consistent based on the fact that the short lived isotopes present from the in-reactor burn have decayed by 400 years. It is just these short lived isotopes which are not present after the long post-closure criticality burns. It should be noted that the comparison of the 10,000 year burn increment in totoal Curies with the meaningful 400 year initial decay shows only a 2% increase. All calculations are performed in Attachment VIII. Tables 7.2.1-4 through 7.2.1-6 provide detailed inventories of the 36 isotopes, and the percentage change from the decay-only case, for the 1000, 5000, and 10,000 year criticalities.

Table 7.2.1-1. Percentage Increase in Total Curies of the 36 TSPA-95 Isotopes

Duration of Criticality (years)	Percent Increase at End of Criticality	Percent Increase at 45,000 years	Percent Increase at 65,000 years
1000	8.5% (16k years)	0.73%	0.73%
5000	15% (20k years)	4.2%	3.7%
10,000	24% (25k years)	9.9%	8.5%

Table 7.2.1-2. Total Curies of 36 TSPA-95 Isotopes Per Assembly

Fuel Age (years since)	16,000	20,000	25,000	45,000	65,000
PWR Thermal/Shielding DBF, Decay Only*	-	1.7e+02	-	-	-
PWR Criticality DBF, Decay Only	1.4e+02	1.2e+02	9.8e+01	5.3e+01	3.2e+01
PWR Criticality DBF, 1000 yr Criticality	1.5e+02	-	-	5.4e+01	3.3e+01
PWR Criticality DBF, 5000 yr Criticality	-	1.4e+02	-	5.5e+01	3.3e+01
PWR Criticality DBF, 10,000 yr Criticality	-	-	1.2e+02	5.8e+01	3.5e+01

* - Information for this fuel obtained from the CDB-R (Ref. 5.13).

Table 7.2.1-3. Total Curies of 36 TSPA-95 Isotopes Per Unit Burnup (Ci/GWd) Per Assembly

	Incremental Burnup (GWd)	Fuel Age (years since discharge)							
		30	400	15,000	16,000	20,000	25,000	45,000	65,000
PWR Criticality DBF, Decay Only	9.3e+00	1.3e+03	1.2e+02	1.6e+01	1.5e+01	1.3e+01	1.1e+01	5.7e+00	3.5e+00
PWR Criticality DBF, 1000 yr Criticality	3.8e-02	-	-	-	3.0e+02	-	-	2.6e+01	2.6e+01
PWR Criticality DBF, 5000 yr Criticality	1.9e-01	-	-	-	-	1.1e+02	-	1.1e+01	5.3e+00
PWR Criticality DBF, 10,000 yr Criticality	3.8e-01	-	-	-	-	-	5.8e+01	1.3e+01	7.9e+00

Inventory of 36 TSPA 95 Nuclides as a Function of Time for a PWR SNF Assembly After A 10,000 Year Criticality Starting at 15,000 Years

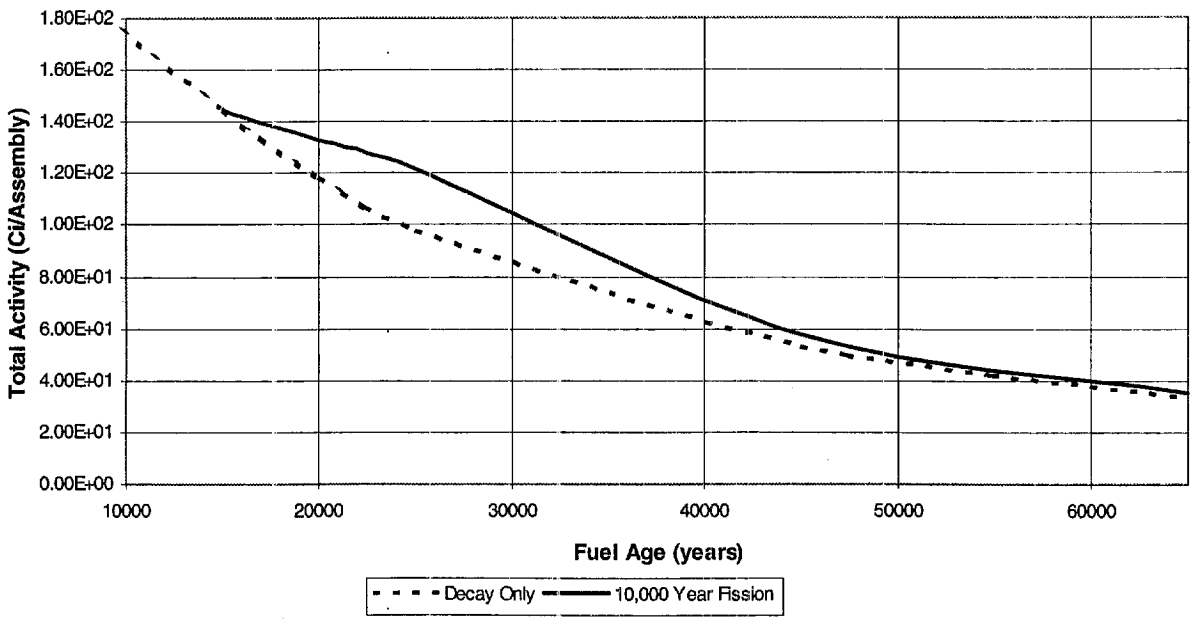


Figure 7.2.1-1

Table 7.2.1-4. Effects of 1000 Year Criticality on the Radionuclide Inventory of a PWR Fuel Assembly (Ref. 5.54)

	16,000 yr Act. (Ci) Critical	Act. (Ci) Decay Only	% Diff. Isotope	% Diff. Total	45,000 yr Act. (Ci) Critical	Act. (Ci) Decay Only	% Diff. Isotope	% Diff. Total	65,000 yr Act. (Ci) Critical	Act. (Ci) Decay Only	% Diff. Isotope	% Diff. Total
ac227	4.9e-003	4.3e-003	1.6e+001	4.9e-004	1.0e-002	1.0e-002	3.0e+000	5.6e-004	1.3e-002	1.3e-002	2.3e+000	9.3e-004
am241	2.6e+000	2.2e-003	1.2e+005	1.9e+000	2.0e-004	2.0e-004	-1.5e+000	-5.6e-006	3.9e-005	3.9e-005	-1.5e+000	-1.9e-006
am242m	2.0e-003	0.0e+000	N/A	1.4e-003	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000
am243	4.8e-001	4.5e-001	7.2e+000	2.3e-002	3.1e-002	2.9e-002	7.2e+000	3.9e-003	4.8e-003	4.5e-003	7.2e+000	9.9e-004
c 14	4.9e-006	4.8e-006	2.5e+000	8.7e-008	1.5e-007	1.4e-007	2.8e+000	7.5e-009	1.3e-008	1.3e-008	2.3e+000	9.3e-010
cm244	1.7e-002	0.0e+000	N/A	1.2e-002	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000
cm245	2.1e-003	2.1e-003	-1.4e+000	-2.2e-005	2.0e-004	2.0e-004	-1.5e+000	-5.6e-006	3.9e-005	3.9e-005	-1.5e+000	-1.9e-006
cm246	9.6e-005	8.8e-005	9.2e+000	5.8e-006	1.4e-006	1.3e-006	9.5e+000	2.3e-007	7.3e-008	6.7e-008	9.2e+000	1.9e-008
cs135	2.0e-001	2.0e-001	9.9e-001	1.4e-003	2.0e-001	2.0e-001	1.0e+000	3.8e-003	2.0e-001	2.0e-001	1.0e+000	6.2e-003
i129	8.8e-003	8.8e-003	4.5e-001	2.9e-005	8.8e-003	8.8e-003	4.5e-001	7.5e-005	8.8e-003	8.8e-003	3.4e-001	9.3e-005
nb 93m	3.5e-001	3.5e-001	5.8e-001	1.4e-003	3.4e-001	3.4e-001	2.9e-001	1.9e-003	3.4e-001	3.4e-001	2.9e-001	3.1e-003
nb 94	1.9e-005	1.4e-005	4.0e+001	4.0e-006	7.1e-006	5.0e-006	4.1e+001	3.9e-006	3.6e-006	2.5e-006	4.1e+001	3.2e-006
np237	3.8e-001	3.8e-001	2.6e-001	7.2e-004	3.8e-001	3.8e-001	2.6e-001	1.9e-003	3.8e-001	3.8e-001	2.7e-001	3.1e-003
pa231	4.9e-003	4.3e-003	1.6e+001	4.9e-004	1.0e-002	1.0e-002	3.0e+000	5.6e-004	1.3e-002	1.3e-002	1.6e+000	6.2e-004
pb210	8.0e-002	8.0e-002	0.0e+000	0.0e+000	2.1e-001	2.1e-001	4.7e-001	1.9e-003	2.8e-001	2.8e-001	7.1e-001	6.2e-003
pd107	2.6e-002	2.6e-002	3.8e-001	7.2e-005	2.6e-002	2.6e-002	3.8e-001	1.9e-004	2.6e-002	2.6e-002	7.7e-001	6.2e-004
pu238	2.9e+000	0.0e+000	N/A	2.1e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000
pu239	1.0e+002	1.0e+002	9.7e-001	7.2e-001	4.5e+001	4.5e+001	6.7e-001	5.6e-001	2.6e+001	2.5e+001	7.9e-001	6.2e-001
pu240	2.9e+001	2.8e+001	4.3e+000	8.7e-001	1.4e+000	1.3e+000	3.8e+000	9.4e-002	1.7e-001	1.6e-001	4.4e+000	2.2e-002
pu241	3.2e+000	2.1e-003	1.5e+005	2.3e+000	2.0e-004	2.0e-004	-1.5e+000	-5.6e-006	3.9e-005	3.9e-005	-1.5e+000	-1.9e-006
pu242	2.7e-001	2.7e-001	-3.7e-001	-7.2e-004	2.6e-001	2.6e-001	-3.9e-001	-1.9e-003	2.5e-001	2.5e-001	-4.0e-001	-3.1e-003
ra226	8.0e-002	8.0e-002	-1.3e-001	-7.2e-005	2.1e-001	2.1e-001	4.7e-001	1.9e-003	2.8e-001	2.8e-001	7.1e-001	6.2e-003
ra228	9.0e-008	9.0e-008	0.0e+000	0.0e+000	2.8e-007	2.8e-007	3.6e-001	1.9e-009	4.1e-007	4.1e-007	4.9e-001	6.2e-009
se 79	1.4e-001	1.4e-001	7.3e-001	7.2e-004	7.5e-002	7.5e-002	6.7e-001	9.4e-004	4.9e-002	4.9e-002	6.1e-001	9.3e-004
sm151	7.9e-001	0.0e+000	N/A	5.7e-001	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000
sn126	1.3e-001	1.2e-001	8.1e-001	7.2e-004	1.0e-001	1.0e-001	0.0e+000	0.0e+000	8.9e-002	8.8e-002	4.5e-001	1.2e-003
tc 99	3.8e+000	3.7e+000	5.3e-001	1.4e-002	3.4e+000	3.4e+000	5.9e-001	3.8e-002	3.2e+000	3.2e+000	3.1e-001	3.1e-002
th229	1.1e-002	1.2e-002	-8.7e-001	-7.2e-005	5.1e-002	5.1e-002	0.0e+000	0.0e+000	7.8e-002	7.8e-002	0.0e+000	0.0e+000
th230	9.2e-002	9.2e-002	-2.2e-001	-1.4e-004	2.2e-001	2.2e-001	4.5e-001	1.9e-003	2.9e-001	2.9e-001	7.0e-001	6.2e-003
th232	9.0e-008	9.0e-008	0.0e+000	0.0e+000	2.8e-007	2.8e-007	3.6e-001	1.9e-009	4.1e-007	4.1e-007	4.9e-001	6.2e-009
u233	2.5e-002	2.5e-002	-8.0e-001	-1.4e-004	6.7e-002	6.7e-002	0.0e+000	0.0e+000	9.3e-002	9.3e-002	1.1e-001	3.1e-004
u234	6.7e-001	6.7e-001	9.0e-001	4.3e-003	6.3e-001	6.3e-001	9.6e-001	1.1e-002	6.1e-001	6.0e-001	1.0e+000	1.9e-002
u235	1.6e-002	1.6e-002	-6.4e-001	-7.2e-005	1.8e-002	1.8e-002	-5.6e-001	-1.9e-004	1.8e-002	1.8e-002	-5.4e-001	-3.1e-004
u236	1.3e-001	1.3e-001	7.9e-001	7.2e-004	1.3e-001	1.3e-001	0.0e+000	0.0e+000	1.4e-001	1.3e-001	7.5e-001	3.1e-003
u238	1.5e-001	1.5e-001	0.0e+000	0.0e+000	1.5e-001	1.5e-001	0.0e+000	0.0e+000	1.5e-001	1.5e-001	0.0e+000	0.0e+000
zr 93	3.5e-001	3.5e-001	5.8e-001	1.4e-003	3.4e-001	3.4e-001	2.9e-001	1.9e-003	3.4e-001	3.4e-001	2.9e-001	3.1e-003
36 Iso. Totals	1.5e+002	1.4e+002	8.5e+000	0.0e+000	5.4e+001	5.3e+001	7.3e-001	0.0e+000	3.3e+001	3.2e+001	7.3e-001	0.0e+000

Table 7.2.1-5. Effects of 5000 Year Criticality on the Radionuclide Inventory of a PWR Fuel Assembly (Ref. 5.54)

	20,000 yr Act. (Ci) Critical	Act. (Ci) Decay Only	% Diff. Isotope	% Diff. Total	45,000 yr Act. (Ci) Critical	Act. (Ci) Decay Only	% Diff. Isotope	% Diff. Total	65,000 yr Act. (Ci) Critical	Act. (Ci) Decay Only	% Diff. Isotope	% Diff. Total
Ac227	8.8e-003	5.2e-003	7.0e+001	3.1e-003	1.2e-002	1.0e-002	2.0e+001	3.8e-003	1.4e-002	1.3e-002	1.0e+001	4.0e-003
Am241	2.7e+000	1.6e-003	1.7e+005	2.3e+000	1.9e-004	2.0e-004	-7.5e+000	-2.8e-005	3.6e-005	3.9e-005	-7.4e+000	-9.0e-006
Am242m	2.4e-003	0.0e+000	N/A	2.0e-003	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000
Am243	4.4e-001	3.1e-001	4.4e+001	1.1e-001	4.2e-002	2.9e-002	4.4e+001	2.4e-002	6.4e-003	4.5e-003	4.3e+001	6.0e-003
C 14	3.5e-006	3.0e-006	1.7e+001	4.3e-007	1.7e-007	1.4e-007	1.7e+001	4.5e-008	1.5e-008	1.3e-008	1.7e+001	6.8e-009
Cm244	1.6e-002	0.0e+000	N/A	1.3e-002	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000
Cm245	1.4e-003	1.5e-003	-7.1e+000	-9.3e-005	1.9e-004	2.0e-004	-7.0e+000	-2.6e-005	3.6e-005	3.9e-005	-7.4e+000	-9.0e-006
Cm246	7.4e-005	4.9e-005	5.1e+001	2.1e-005	1.9e-006	1.3e-006	5.2e+001	1.2e-006	1.0e-007	6.7e-008	5.2e+001	1.1e-007
Cs135	2.1e-001	2.0e-001	4.4e+000	7.6e-003	2.1e-001	2.0e-001	4.5e+000	1.7e-002	2.1e-001	2.0e-001	4.5e+000	2.8e-002
I129	9.0e-003	8.8e-003	2.0e+000	1.5e-004	9.0e-003	8.8e-003	2.0e+000	3.4e-004	9.0e-003	8.8e-003	2.0e+000	5.6e-004
Nb 93m	3.5e-001	3.5e-001	2.0e+000	5.9e-003	3.5e-001	3.4e-001	2.0e+000	1.3e-002	3.5e-001	3.4e-001	2.1e+000	2.2e-002
Nb 94	4.1e-005	1.2e-005	2.5e+002	2.5e-005	1.8e-005	5.0e-006	2.5e+002	2.4e-005	8.9e-006	2.5e-006	2.5e+002	2.0e-005
Np237	3.8e-001	3.8e-001	1.0e+000	3.4e-003	3.8e-001	3.8e-001	1.1e+000	7.5e-003	3.8e-001	3.8e-001	1.3e+000	1.5e-002
Pa231	8.8e-003	5.2e-003	7.0e+001	3.1e-003	1.2e-002	1.0e-002	2.0e+001	3.8e-003	1.4e-002	1.3e-002	1.0e+001	4.0e-003
Pb210	1.0e-001	1.0e-001	-9.9e-001	-8.5e-004	2.2e-001	2.1e-001	2.3e+000	9.4e-003	2.9e-001	2.8e-001	3.6e+000	3.1e-002
Pd107	2.7e-002	2.6e-002	1.9e+000	4.2e-004	2.7e-002	2.6e-002	1.9e+000	9.4e-004	2.7e-002	2.6e-002	2.3e+000	1.9e-003
Pu238	3.0e+000	0.0e+000	N/A	2.5e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000
Pu239	9.6e+001	9.2e+001	3.6e+000	2.8e+000	4.7e+001	4.5e+001	3.8e+000	3.2e+000	2.6e+001	2.5e+001	4.0e+000	3.1e+000
Pu240	2.3e+001	1.9e+001	2.6e+001	4.1e+000	1.7e+000	1.3e+000	2.6e+001	6.4e-001	2.0e-001	1.6e-001	2.6e+001	1.3e-001
Pu241	2.6e+000	1.5e-003	1.7e+005	2.2e+000	1.9e-004	2.0e-004	-7.5e+000	-2.8e-005	3.6e-005	3.9e-005	-7.4e+000	-9.0e-006
Pu242	2.7e-001	2.7e-001	-1.1e+000	-2.5e-003	2.5e-001	2.6e-001	-1.2e+000	-5.6e-003	2.5e-001	2.5e-001	-1.6e+000	-1.2e-002
Ra226	1.0e-001	1.0e-001	-9.9e-001	-8.5e-004	2.2e-001	2.1e-001	2.8e+000	1.1e-002	2.9e-001	2.8e-001	3.9e+000	3.4e-002
Ra228	1.1e-007	1.1e-007	0.0e+000	0.0e+000	2.8e-007	2.8e-007	1.4e+000	7.5e-009	4.2e-007	4.1e-007	1.7e+000	2.2e-008
Se 79	1.3e-001	1.3e-001	3.2e+000	3.4e-003	7.7e-002	7.5e-002	3.1e+000	4.3e-003	5.1e-002	4.9e-002	3.1e+000	4.6e-003
Sm151	8.0e-001	0.0e+000	N/A	6.8e-001	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000
Sn126	1.2e-001	1.2e-001	2.5e+000	2.5e-003	1.0e-001	1.0e-001	2.0e+000	3.8e-003	9.1e-002	8.8e-002	2.5e+000	6.8e-003
Tc 99	3.8e+000	3.7e+000	2.2e+000	6.8e-002	3.5e+000	3.4e+000	2.1e+000	1.3e-001	3.3e+000	3.2e+000	1.9e+000	1.9e-001
Th229	1.6e-002	1.6e-002	-6.1e-001	-8.5e-005	5.1e-002	5.1e-002	-3.9e-001	-3.8e-004	7.8e-002	7.8e-002	1.3e-001	3.1e-004
Th230	1.1e-001	1.1e-001	-8.8e-001	-8.5e-004	2.3e-001	2.2e-001	2.7e+000	1.1e-002	3.0e-001	2.9e-001	3.8e+000	3.4e-002
Th232	1.1e-007	1.1e-007	0.0e+000	0.0e+000	2.8e-007	2.8e-007	1.4e+000	7.5e-009	4.2e-007	4.1e-007	1.7e+000	2.2e-008
U233	3.1e-002	3.1e-002	-1.9e+000	-5.1e-004	6.7e-002	6.7e-002	-1.5e-001	-1.9e-004	9.3e-002	9.3e-002	3.2e-001	9.3e-004
U234	6.9e-001	6.6e-001	5.3e+000	3.0e-002	6.6e-001	6.3e-001	5.3e+000	6.2e-002	6.3e-001	6.0e-001	5.2e+000	9.6e-002
U235	1.6e-002	1.6e-002	-1.9e+000	-2.5e-004	1.8e-002	1.8e-002	-1.1e+000	-3.8e-004	1.8e-002	1.8e-002	-1.6e+000	-9.3e-004
U236	1.3e-001	1.3e-001	1.6e+000	1.7e-003	1.4e-001	1.3e-001	2.2e+000	5.6e-003	1.4e-001	1.3e-001	2.2e+000	9.3e-003
U238	1.5e-001	1.5e-001	0.0e+000	0.0e+000	1.5e-001	1.5e-001	0.0e+000	0.0e+000	1.5e-001	1.5e-001	0.0e+000	0.0e+000
Zr 93	3.5e-001	3.5e-001	2.0e+000	5.9e-003	3.5e-001	3.4e-001	2.0e+000	1.3e-002	3.5e-001	3.4e-001	2.1e+000	2.2e-002
36 Iso. Totals	1.4e+002	1.2e+002	1.5e+001	0.0e+000	5.5e+001	5.3e+001	4.2e+000	0.0e+000	3.3e+001	3.2e+001	3.7e+000	0.0e+000

Table 7.2.1-6. Effects of 10,000 Year Criticality on the Radionuclide Inventory of a PWR Fuel Assembly (Ref. 5.54)

	25,000 yr Act. (Ci) Critical	Act. (Ci) Decay Only	% Diff. Isotope	% Diff. Total	45,000 yr Act. (Ci) Critical	Act. (Ci) Decay Only	% Diff. Isotope	% Diff. Total	65,000 yr Act. (Ci) Critical	Act. (Ci) Decay Only	% Diff. Isotope	% Diff. Total
Ac227	1.4e-002	6.3e-003	1.2e+002	8.0e-003	1.5e-002	1.0e-002	4.9e+001	9.2e-003	1.6e-002	1.3e-002	2.4e+001	9.6e-003
Am241	2.1e+000	1.1e-003	2.0e+005	2.2e+000	1.7e-004	2.0e-004	-1.4e+001	-5.5e-005	3.4e-005	3.9e-005	-1.5e+001	-1.8e-005
Am242m	1.9e-003	0.0e+000	N/A	2.0e-003	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000
Am243	4.1e-001	1.9e-001	1.1e+002	2.2e-001	6.3e-002	2.9e-002	1.1e+002	6.3e-002	9.5e-003	4.5e-003	1.1e+002	1.6e-002
C14	2.4e-006	1.6e-006	4.8e+001	8.0e-007	2.1e-007	1.4e-007	4.9e+001	1.3e-007	1.9e-008	1.3e-008	4.8e+001	1.9e-008
Cm244	1.5e-002	0.0e+000	N/A	1.6e-002	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000
Cm245	8.8e-004	1.0e-003	-1.4e+001	-1.5e-004	1.7e-004	2.0e-004	-1.4e+001	-5.5e-005	3.4e-005	3.9e-005	-1.5e+001	-1.8e-005
Cm246	5.2e-005	2.4e-005	1.2e+002	2.9e-005	2.8e-006	1.3e-006	1.2e+002	2.8e-006	1.5e-007	6.7e-008	1.2e+002	2.5e-007
Cs135	2.2e-001	2.0e-001	8.4e+000	1.7e-002	2.2e-001	2.0e-001	9.0e+000	3.4e-002	2.2e-001	2.0e-001	8.5e+000	5.3e-002
I129	9.2e-003	8.8e-003	4.1e+000	3.7e-004	9.2e-003	8.8e-003	4.1e+000	6.8e-004	9.2e-003	8.8e-003	4.0e+000	1.1e-003
Nb 93m	3.6e-001	3.4e-001	4.1e+000	1.4e-002	3.6e-001	3.4e-001	4.1e+000	2.6e-002	3.5e-001	3.4e-001	3.8e+000	4.0e-002
Nb 94	7.4e-005	1.0e-005	6.4e+002	6.5e-005	3.7e-005	5.0e-006	6.4e+002	6.1e-005	1.9e-005	2.5e-006	6.4e+002	5.0e-005
Np237	3.9e-001	3.8e-001	2.1e+000	8.2e-003	3.9e-001	3.8e-001	2.1e+000	1.5e-002	3.8e-001	3.8e-001	2.4e+000	2.8e-002
Pa231	1.4e-002	6.3e-003	1.2e+002	8.0e-003	1.5e-002	1.0e-002	4.9e+001	9.2e-003	1.6e-002	1.3e-002	2.4e+001	9.6e-003
Pb210	1.3e-001	1.3e-001	-7.9e-001	-1.0e-003	2.2e-001	2.1e-001	4.7e+000	1.9e-002	3.1e-001	2.8e-001	1.1e+001	9.9e-002
Pd107	2.7e-002	2.6e-002	3.8e+000	1.0e-003	2.7e-002	2.6e-002	3.8e+000	1.9e-003	2.7e-002	2.6e-002	4.2e+000	3.4e-003
Pu238	3.1e+000	0.0e+000	N/A	3.1e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000
Pu239	8.7e+001	8.0e+001	8.6e+000	7.0e+000	4.9e+001	4.5e+001	8.9e+000	7.5e+000	2.8e+001	2.5e+001	9.1e+000	7.1e+000
Pu240	1.8e+001	1.1e+001	6.9e+001	7.7e+000	2.2e+000	1.3e+000	6.8e+001	1.7e+000	2.7e-001	1.6e-001	6.9e+001	3.4e-001
Pu241	2.1e+000	1.0e-003	2.1e+005	2.2e+000	1.7e-004	2.0e-004	-1.4e+001	-5.5e-005	3.4e-005	3.9e-005	-1.5e+001	-1.8e-005
Pu242	2.6e-001	2.7e-001	-2.6e+000	-7.1e-003	2.5e-001	2.6e-001	-2.7e+000	-1.3e-002	2.4e-001	2.5e-001	-2.8e+000	-2.2e-002
Ra226	1.3e-001	1.3e-001	-7.9e-001	-1.0e-003	2.2e-001	2.1e-001	4.7e+000	1.9e-002	3.1e-001	2.8e-001	1.1e+001	9.9e-002
Ra228	1.5e-007	1.5e-007	6.8e-001	1.0e-009	2.8e-007	2.8e-007	2.2e+000	1.1e-008	4.2e-007	4.1e-007	2.9e+000	3.7e-008
Se 79	1.2e-001	1.1e-001	6.1e+000	7.1e-003	7.9e-002	7.5e-002	6.3e+000	8.8e-003	5.2e-002	4.9e-002	6.3e+000	9.6e-003
Sm151	8.1e-001	0.0e+000	N/A	8.2e-001	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000	0.0e+000
Sn126	1.2e-001	1.2e-001	5.1e+000	6.1e-003	1.1e-001	1.0e-001	4.9e+000	9.4e-003	9.3e-002	8.8e-002	5.0e+000	1.4e-002
Tc 99	3.8e+000	3.6e+000	4.1e+000	1.5e-001	3.5e+000	3.4e+000	4.1e+000	2.6e-001	3.3e+000	3.2e+000	3.8e+000	3.7e-001
Th229	2.3e-002	2.3e-002	-1.7e+000	-4.1e-004	5.1e-002	5.1e-002	-1.2e+000	-1.1e-003	7.8e-002	7.8e-002	-1.3e-001	-3.1e-004
Th230	1.4e-001	1.4e-001	0.0e+000	0.0e+000	2.3e-001	2.2e-001	5.0e+000	2.1e-002	3.1e-001	2.9e-001	7.3e+000	6.5e-002
Th232	1.5e-007	1.5e-007	6.8e-001	1.0e-009	2.8e-007	2.8e-007	2.2e+000	1.1e-008	4.2e-007	4.1e-007	2.9e+000	3.7e-008
U233	3.7e-002	3.9e-002	-3.1e+000	-1.2e-003	6.7e-002	6.7e-002	-6.0e-001	-7.5e-004	9.3e-002	9.3e-002	3.2e-001	9.3e-004
U234	7.2e-001	6.5e-001	1.1e+001	7.4e-002	6.9e-001	6.3e-001	1.1e+001	1.3e-001	6.6e-001	6.0e-001	1.1e+001	2.0e-001
U235	1.6e-002	1.6e-002	-3.6e+000	-6.1e-004	1.7e-002	1.8e-002	-2.8e+000	-9.4e-004	1.8e-002	1.8e-002	-2.7e+000	-1.5e-003
U236	1.4e-001	1.3e-001	3.1e+000	4.1e-003	1.4e-001	1.3e-001	4.5e+000	1.1e-002	1.4e-001	1.3e-001	4.5e+000	1.9e-002
U238	1.5e-001	1.5e-001	0.0e+000	0.0e+000	1.5e-001	1.5e-001	0.0e+000	0.0e+000	1.5e-001	1.5e-001	0.0e+000	0.0e+000
Zr 93	3.6e-001	3.4e-001	4.1e+000	1.4e-002	3.6e-001	3.4e-001	4.1e+000	2.6e-002	3.5e-001	3.4e-001	3.8e+000	4.0e-002
36 Iso. Total	1.2e+002	9.8e+001	2.4e+001	0.0e+000	5.8e+001	5.3e+001	9.9e+000	0.0e+000	3.5e+001	3.2e+001	8.5e+000	0.0e+000

7.2.2 Compositions as a Function of Duration for Internal Criticality

Number densities for the fuel accounting for burnup and production of isotopes were calculated for a base case with decay out to 15,000 years and for the criticalities lasting 1000, 5000 and 10,000 years. The SAS2H and ORIGEN-S case descriptions which support these number density calculations are provided in Sections 7.5.1 and 7.5.2 of Reference 5.53. The grams/assembly compositions are taken from Attachments XI and XII of Reference 5.53. The grams/assembly output per appropriate time step ("initial" decay column for criticality cases) in conjunction with the assembly volume was used to calculate the number density of each of the required isotopes using a LOTUS 1-2-3 spreadsheet. The equation for number density is shown below (Ref. 5.20, p. 34):

$$N = \rho N_A / M$$

where,
- ρ is the physical density in g/cm^3, calculated as grams/assembly ÷ assembly volume (51575.24 cm^3, Ref. 5.54 Att. VIII),
- N_A is Avagadro's Number - 0.602252E+24 atoms/mole (Ref. 5.43), and
- M is the gram atomic weight.

The units of the resulting number density is in atoms/cm^3. The required units for subsequent use are atoms/barn-cm where 1 barn equals 10^{-24} cm^2. The calculations in the spreadsheet drops the E+24 from Avagadro's Number to account for the conversion. As a conservatism in the criticality calculations which will use these number densities, the values are adjusted up to a 96% theoretical density.

The Principal Isotopes previously established (Ref. 5.46, p. 4-4) were used with the addition of Cd, Gd-157, Xe-131, and Cs-133. These four additional isotopes were identified in the top 15 fission product absorber list for 1000 and 5000 year criticalities as described in Section 7.4.4. These four isotopes were added to provide a indication of realistic reactivity changes due to burnup in the long term low power criticality being analyzed.

The grams/assembly (Ref. 5.53, Attachments XI and XII) for each isotope and the results of the number density calculations are shown in Attachment II which is the LOTUS 1-2-3 spreadsheet used to generate the values.

The burnup associated with each of the criticality durations is shown in the Table 7.2.2-1 along with the masses of the major fissile isotopes (U-235 and Pu-239), Pu-240 (actinide absorber) and fission products absorbers. Note that while the mass of Pu-239 decreased by 19% (partially offset by U-235 mass increase), the mass of major absorbers such as Pu-240, Sm-149, and Eu-151 decreased by 41%, 51%, and 10%, respectively. The mass of the Pu isotopes decreased due to absorption and decay, while the mass of these two fission products decreased by absorption.

Table 7.2.2-1. Burnup and Composition Changes Associated with Criticality Duration

Duration of Criticality (years)	0	1000	5000	10,000
Burnup (MWd)	0	37.95	189.76	379.52
Mass of U-235 (g)	7.21E+3	7.23E+3	7.29E+3	7.35E+3
Mass of Pu-239 (g)	1.72E+3	1.68E+3	1.54E+3	1.40E+3
Mass of Pu-240 (g)	1.38E+2	1.30E+2	1.03E+2	8.09E+1
Mass of Sm-149 (g)	1.42E+0	1.18E+0	7.88E-1	6.96E-1
Mass of Nd-143 (g)	2.69E+2	2.70E+2	2.73E+2	2.77E+2
Mass of Eu-151 (g)	6.22E+0	6.12E+0	5.87E+0	5.60E+0
Mass of Rh-103 (g)	1.44E+2	1.44E+2	1.45E+2	1.47E+2
Mass of Xe-131 (g)	1.38E+2	1.38E+2	1.40E+2	1.42E+2

7.2.3 Check of Reactivity Changes With Time Due to Internal Criticality

The AUCF waste package design model in MCNP consists of ½ of the package with a reflective plane along the axis to represent the entire package. The AUCF waste package containment barriers are modeled as separate units in the MCNP model. The composition, thicknesses, radii, and lengths of the containment barriers are modeled explicitly as listed in Table 4.1-2. The outer containment barrier's skirt was not modeled in detail, since the skirt would not effect the criticality results. For this degraded model, no basket structure remains and a uniform mixture of iron oxide, water, and boron surrounds the fuel assemblies. The fuel assemblies are uniformly stacked together, with no separation, at the bottom of the waste package. The fuel assemblies in the AUCF waste package are modeled in a lattice. Each fuel assembly is treated as a heterogeneous system with the fuel pins, control rod guide tubes, and instrument guide tube modeled explicitly. The properties of the design basis B&W 15×15 Mark B5 assembly are used in the analyses as listed in Table 4.1-1. A cross-sectional view from the MCNP model is shown in Figure 7.2.3-1. The non-fuel material compositions were taken from a previous QAP-3-9 analysis on material compositions (Ref. 5.5).

A degraded configuration with 5371.1 kg of Fe and 1.6 kg of B was identified as appropriate for determination of the reactivity effect of burnup because it represented the Fe, B combination at the earliest possible time of criticality (the last case in Table 7.4-2 of Reference 5.54, with the specific Fe, B amounts given in Attachment II, p. II-3 of that document). To be consistent with previous calculations (Ref. 5.54, p. 10), the masses were rounded to whole percentages. The moderator was modeled as 26% Fe_2O_3 (based on the mass conversion equation in Reference 5.54, p. VIII-6: Fe mass=20.94 x void %) displacing water in the void space within the waste package with 5% of the original B-10 (based on total mass of B in Reference 5.54, p. VIII-5: 30.474 kg) also incorporated into the moderator. The calculation for the number densities for the

moderator composition is shown in Attachment II.

The fuel compositions described in Section 7.2.2 were inserted into the MCNP model and the cases were run to generate values of k_{eff} as a function of criticality duration. The results of the cases are shown in Table 7.2.3-1. The corresponding attachments containing the input and relevant output for each case are shown in parentheses.

Table 7.2.3-1. MCNP Case Results to Demonstrate Reactivity Changes Due to an Internal Criticality

Criticality Duration (years)	0	1000	5000	10,000
k_{eff}	0.8967 ± 0.0020 (III)	0.8989 ± 0.0019 (IV)	0.9006 ± 0.0021 (V)	0.9002 ± 0.0022 (VI)

The slight increase in k_{eff} with burnup comparing 0 and 10,000 years can be attributed to the higher relative burnup/decay of absorbers compared to fissile isotopes as discussed in Section 7.2.1.

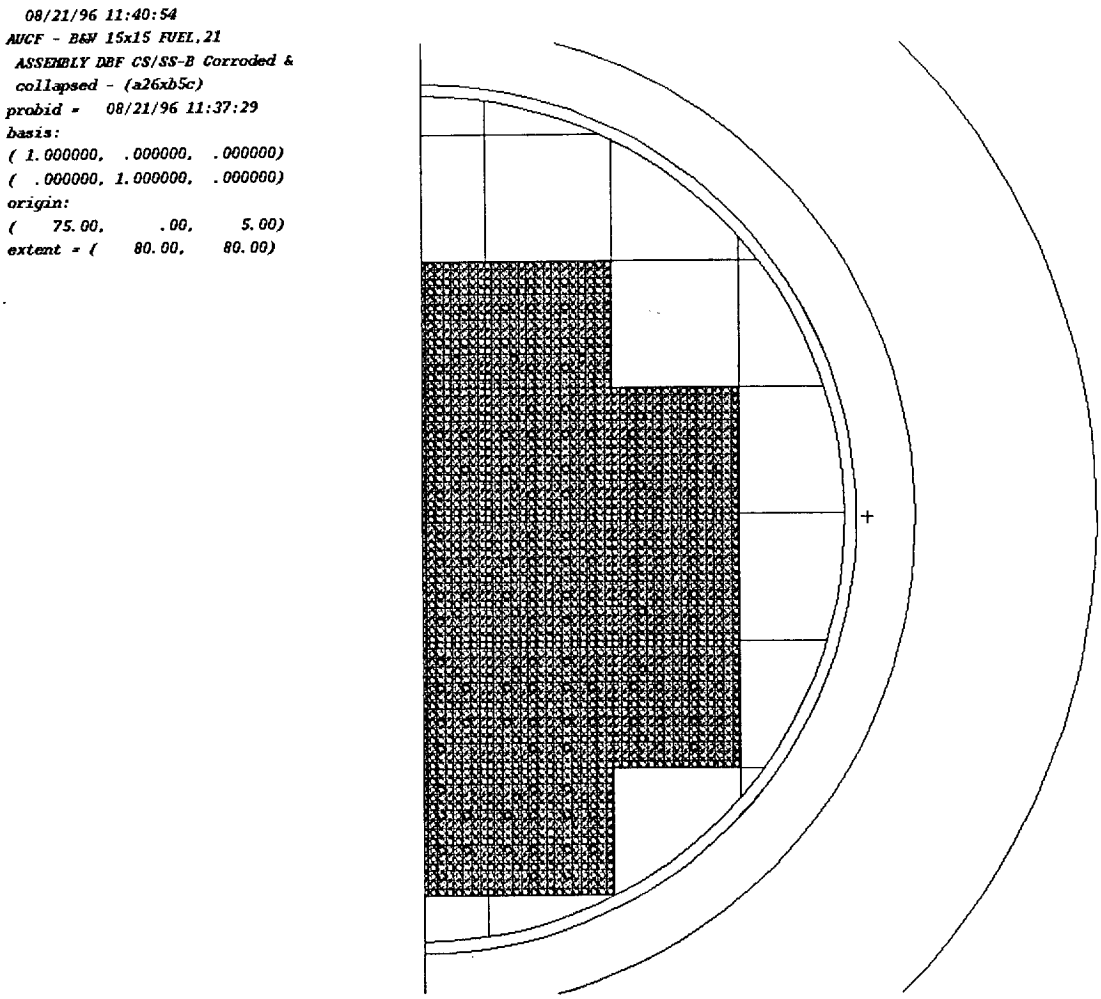


Figure 7.2.3-1. MCNP Model of 21 PWR AUCF WP with Fully Degraded Basket

7.3 External Criticality, Basic Parameters

7.3.1 Geometry and Material Composition

The concentrations of water and UO_2 used for this analysis are chosen with the following considerations:

- The maximum porosity of the rock beneath the repository site, in the saturated zone, is taken to be the sample maximum, 40%, explained in the footnote to Table 4.1-4. Since the sample size was over 100, the probability of some random location exceeding this value is taken to be less than 0.01. (This is conservative, since the probability that 1% of the true population exceed a porosity of 40% is $0.99^{126} = 0.28$. Restated in probability terms, the probability that the 99 percentile of the true population is greater than 40% porosity is 0.28. It should be noted, however, that the sample comes from a limited number of boreholes, so there could be a greater variation than is estimated here.) If a value of porosity larger than 40% were selected, the probability would have to be reduced by a factor smaller than 0.01. Since there are no new probability calculations in this analysis to which to apply such a factor, it is reasonably conservative to take 40% as the porosity.
- The water volume percent plus UO_2 volume percent should equal the porosity.
- The very conservative value of 8% UO_2 by volume with 32% water by volume is equivalent to 32% UO_2 by weight according to the formula in the third footnote to Table 7.5-1 of Reference 5.52; this weight percent is higher than any known natural uranium deposit of 1m radius. There are smaller size regions of well known uranium deposits (e.g., Oklo, Cigar Lake, Pena Blanca) which have higher concentrations (Ref. 5.52, p. 26, and references cited therein).

Of the alternative concentrations evaluated in Reference 5.52 (Table 7.5-1), the parameter set falls between the 4th and 7th cases, indicating a critical mass above 10.1 metric tons of U, but less than 18 tons. Such a large mass implies a very small probability of accumulation, according to the methodology of Reference 5.52; in fact, several of the cases in Reference 5.52, Table 7.5-1, have a higher probability, according to the probabilities given in Table 7.6-1 of Reference 5.52. This apparent contradiction, of taking a case which the methodology estimates to have a significantly lower probability, results from the principal inadequacy of the methodology of Reference 5.52, which is the lack of correlation between size of reducing zone and the maximum amount of UO_2 it can extract or concentrate. The cases in Reference 5.52 which appear to have higher probabilities than the one selected here, actually require a porosity higher than is consistent with physical reality; with additional data on the joint distribution of concentration of UO_2 (or grade) and areal extent (or deposit size) these cases with apparently higher probability may be seen to be impossible and not considered any further.

The compositions in the form of number densities for UO_2, 30.6% porosity tuff, and water were taken from Attachment VIII of Reference 5.55 and entered into a LOTUS 1-2-3 spreadsheet which is included as Attachment VII. The 30.6% porosity tuff number densities were converted to those representative of 40% porosity tuff by the ratio (1-0.4)/(1-0.306). The corresponding

weight percents of the components in the UO_2 feed were calculated by multiplying the component atom density by the component atomic weight and dividing by the sum of this product for all the components. The homogeneous mixture number densities for the combination of 40% porosity tuff with 8 volume percent UO_2 and 32 volume percent H_2O occupying the pore/fracture space (porosity) were calculated as shown in the spreadsheet by multiplying the UO_2 number densities by 0.08 and the water number densities by 0.32.

The critical radius for a similar composition in a spherical geometry was found to be 140 cm (Ref. 5.55, p. 35).

7.3.2 Relation Between Power and Temperature

For this analysis the relation between the steady state power output of an external criticality and the resulting temperature is determined primarily by heat conduction from the spherical mass to the distant environment. Since there are no free surfaces in the external far-field, there can be no cooling by radiation. It is further assumed that cooling by convection is small by comparison with conduction, for the reasons given in Assumption 4.3.5. The temperature is then determined by solving the steady state heat conduction equation; the details of this process are given in Attachment I. The results are as follows.

Within a sphere generating total power P, uniformly throughout its volume, at a power density of $3P/(4\pi R^3)$, where R is the radius of the sphere, the solution for temperature given in Attachment I is:

$$T = T_s + P(1-r^2/R^2)/(8k\pi R),$$

where k is the thermal conductivity in W/m·K, r is the distance from the center of the sphere, and T_s is the temperature of the surface of the sphere, assumed to be constant (Assumption 4.3.7). The consequence of this general result is that the temperature at the center of the sphere is:

$$T_c = T_s + P/(8k\pi R),$$

and the average temperature (computed in Attachment I) is:

$$T_{av} = T_s + P/(20k\pi R).$$

If the power, P, is parabolically distributed throughout the sphere, with peak power at the center, the power density will be, $15P(1-r^2/R^2)/(8\pi R^3)$, which is normalized so that multiplying the power density by $4\pi r^2$ and integrating over r from 0 to R gives P. The general solution for temperature within the sphere is derived in Attachment I as:

$$T = T_s + 7P/(32k\pi R) - 15P[r^2/(6R^2) - r^4/(20R^4)]/(8k\pi R),$$

which leads to the center temperature:

$$T_c = T_s + 7P/(32k\pi R),$$

and the average temperature:

$$T_{av} = T_s + P/(14k\pi R).$$

For any spherically symmetric power density inside the sphere, the solution for the temperature outside the sphere can be used to determine the surface temperature in terms of the temperature of the rock far from the sphere, T_∞:

$$T_s = T_\infty + P/(4k\pi R).$$

7.3.3 Maximum Possible Power and Temperature

The maximum possible temperature under isobaric conditions is the boiling temperature of water, at 50 atmospheres (735 psia, 5.07 MPa) pressure (hydrostatic pressure at approximately 500 meters below the water table, Assumption 4.3.6) because bulk boiling will drive the power down based on previous results (Ref. 5.55, p. 40). The saturated temperature and density of liquid water at 50 atm pressure were linearly interpolated from the values in Table 4.1-5 to be 265 °C (508.7 °F) and 0.776 g/cm^3 (48.45 lb/ft^3). The depth from the surface to the saturated zone is taken to be 611 m (approximate, from Ref 5.18, Fig 2.3-7). The temperature of the rock can be determined from the following relation (Ref. 5.44, p. 6-168) assuming that the last thermal gradient extends 500 m below the saturated zone level (total of 1111 m; see Assumption 4.3.6):

$T_\infty =$ 18.7 °C + 0.019 °C/m (0 to 150 m) + 0.018 °C/m (150 to 400 m)
+ 0.030 °C/m (400 to 541 m),

$T_\infty =$ 47.4 °C.

The average thermal conductivity, k, of the rock at a depth of 535.2 m has been estimated to be 1.38 W/m·K (Ref. 5.31, p. 6). This value will be used for the tuff in this analysis.

Based on the temperature equations for a parabolic power density in a sphere in Section 7.3.2, the average temperature can be determined from the following equation:

$$T_{av} = T_\infty + P/(4k\pi R) + P/(14k\pi R).$$

Power corresponding to a given average temperature can be determined by manipulating this equation to the following form:

$$P = (T_{av} - T_\infty) \cdot (1/(4k\pi R) + 1/(14k\pi R))^{-1}.$$

Using the values described above and limiting the power based on an average temperature of 265 °C, a value of 4.1 kW is calculated for the maximum power.

7.3.4 Maximum Sustainable Power, Temperature, and Duration

Maximum mobilization rate of uranium and plutonium in SNF:

It is assumed that mobilization is much slower than dissolution so that removal is solubility limited (Assumption 4.3.20).

WP area (horizontal cross section through the axis) = 6.62 m^2.

Infiltration rate = 10 mm/yr (or 1 mm/yr with 10x concentration) (Ref. 5.18 and Assumption 4.3.16).

Solubility of U and Pu = 2000 ppm (g UO_2/ton water) (conservatively taken to be approximately the maximum of solubility for both U and Pu, Ref. 5.18, p. 6-29).

Mass mobilized/yr = (2000 g UO_2/ton water) x (6.62x0.01 tons/yr) = 132 g/yr, for a single waste package.

For reference: Time to remove 10 tons of U plus Pu: $10^7/132$ = 75,800 years (note: more than 1 waste package of SNF).

Maximum sustainable power:

Approximately 1.23 g/day of U-235 is consumed per megawatt of power if the fissions are induced primarily by thermal neutrons (Ref. 5.20, p. 78) and the production of other fissile isotopes is ignored. The maximum infiltration rate of UO_2 was calculated to be 132 g/year per WP above and the weight fraction of U-235 in the UO_2 was calculated to be 0.017 as shown in the spreadsheet included in Attachment VII. Multiplying these two numbers together provides a U-235 infiltration rate of 2.244 g/year which would support a burnup of 1.824 MWd. Dividing the burnup possible for the maximum infiltration rate by the number of days in the year (365.25) provides a maximum steady state power of 0.004995 MW (4.995 kW) which can be maintained by the criticality. This result indicates that 22% more fissile material could enter the critical volume than could be consumed based on the temperature limited power calculated above.

However, the Oklo experience suggests that a natural reactor can only be burned down to an effective enrichment $^{235}U/(^{238}U+^{235}U)$ of 1.37% (see Assumption 4.3.8) so the sustainable power is limited to:

$$4995*(1.94-1.37)/1.94 = 1468 \text{ W},$$

where 1.94 is the % fissile content in the design basis fuel after discharge (Ref. 5.52, p. 40).

The criticality duration is determined by the 100,000 year hydrologic cycle divided into four subcycles having power levels determined by the cycle average for that 25,000 year time period.

25,000 years at 132 g/yr UO_2 infiltration rate and power of 1468 W (125 °C)
25,000 years at 2/3*(132 g/yr) UO_2 infiltration rate and power of 979 W (99.0 °C)
25,000 years at 1/3*(132 g/yr) UO_2 infiltration rate and power of 489 W (73.0 °C)
25,000 years at 0 g/yr UO_2 infiltration rate and power of 0 W (47.4 °C)

The temperatures indicated above are the average temperatures of the critical spheres as calculated from the equations listed in Section 7.3.2. This cycle requires 6.6 metric tons of UO_2 from a second waste package to sustain the criticality under this scenario.

7.4 External Criticality, Neutronics Evaluation

The neutronic evaluation procedure for the far-field criticality involves five tasks as indicated below:

1) MCNP model and k_{eff} calculation based on initial composition.

2) SAS2H model and burn calculation for 1, 10, 100, 1000, 5000, and 10,000 year events.

3) ORIGEN-S decay calculations for the 1000, 5000, and 10,000 year events.

4) Spreadsheet calculations of compositions from various duration criticality events.

5) MCNP calculations (recomputation of k_{eff}) based on compositions from the various duration criticality events.

The details of each task, along with the results, are provided in the following five subsections.

7.4.1 Reference MCNP Calculation for Initial Composition

A reference MCNP case using the initial homogeneous composition was set up based on a previously developed MCNP model (Ref. 5.55, Sections 7.4.2, 7.4.3). The model is composed of an inner spherical region 140 cm in radius containing the tuff/water/UO_2 mixture and an outer reflector region 60 cm thick containing a 40% porosity tuff/water mixture. This initial case was run based on compositions representative of a temperature of 300 K. A second case was run based on the ambient conditions described in Section 7.3.1 in which water densities were adjusted to a density of 0.990 g/cm^3 corresponding to a temperature of 50 °C (323 K) and a pressure of 5.07 MPa (50 atm). A third case was run based on the average temperature of 538 K (265 °C) in the fuel region which corresponds to the 4 kW power level. Cross sections are not available for exactly the 4 kW power conditions so the closest available were used. Hydrogen thermal cross section data representative of 400 K (lwtr.02t) was used for the reflector and of 500 K (lwtr.03t) for the inner region. Cross sections for H, O, U-235, and U-238 representative of 600 K were used in the inner region. The k_{eff} results are shown in Table 7.4.1-1. The input and pertinent output are included in Attachments IX, X, and XI. These results indicate that the temperature calculated for a 4 kW power level would drive the criticality on a negative transient

(reduce power). Determination of actual powers would require dynamic analysis which is beyond the scope of the present report and the capability of MCNP with the limited temperature dependance of the current library. These results do indicate that operation at this temperature (power) will provide conservative overestimates of any radioisotopes which may be produced.

Table 7.4.1-1. Variation of k_{eff} with Temperature for an External Criticality

Temperature (K)	300	323	538
$k_{eff} \pm 2\sigma$	0.9776 ± 0.0016	0.9772 ± 0.0015	0.9424 ± 0.0020

The previous external criticality analysis (Ref. 5.55) used a fresh fuel bias and uncertainty of -0.015 in k_{eff}, because power level and duration of criticalities were not considered. The burnup of fuel and the production of fission products will introduce additional bias and uncertainty. For this analysis, an additional bias and uncertainty of -0.005 in k_{eff} is applied to account for burnup effects. This bias and uncertainty is applied uniformly to all results, fresh and burned, in order to provide a consistent comparison base between results. As will be shown in Section 7.4.5, the additional bias and uncertainty of -0.005 in k_{eff} bounds the worth of fission products at 1000 years. With the application of a total bias and uncertainty of -0.020 in k_{eff}, the 300 K and the 323 K cases would be slightly supercritical.

7.4.2 SAS2H Burnup Calculations

SAS2H cases were set up for critical events lasting 1, 10, 100, 1000, 5000 and 10,000 years at a power level which was rounded to 4 kW corresponding to the scenario described in Section 7.3.4 where power is limited by the boiling point of water. The material descriptions in weight fractions and densities were taken directly from print table 40 in the MCNP case output included in Attachment XI. The isotopes and corresponding weight fractions from Attachment XI are listed in Table 7.4.2-1. The density of the tuff/water/UO_2 region is 2.6344 g/cm^3 and the density of the reflector region is 1.9053 g/cm^3. The temperatures for materials are entered in Kelvin and are 538 K (265 °C) for the fuel region and 323 K (50 °C) for the reflector region. SAS2H does not have a spherical geometry option. The most suitable cell geometry option available in SAS2H for the burnup calculation is an infinite slab (symmslabcell option). The fuel region is modeled as a 280 cm thick slab and a 60 cm thick reflector region is added on each side. Because three regions are required in the model, the reflector is broken into two regions. The volume of the fuel region is calculated as $4/3\pi(140\text{ cm})^3$ and is entered as "volfueltot=1.1494E7." All grams and curies tables for the isotopes in the output are normalized to this volume.

Table 7.4.2-1. Isotopic/Elemental Weight Fractions for External Criticality SAS2H Cases

Material ID	Weight Fraction	Material ID	Weight Fraction	Material ID	Weight Fraction	Material ID	Weight Fraction
Tuff/Water/UO_2 Region							
1001	0.01055	8016	0.40755	11023	0.00570	12000	0.00354
13027	0.04434	14000	0.20193	19000	0.01370	20000	0.01439
26000	0.00494	92234	0.00007	92235	0.00567	92236	0.00136
92238	0.28593	93237	0.00033	-	-	-	-
Tuff/Water Reflector Region							
1001	0.02326	8016	0.57779	11023	0.00789	12000	0.00490
13027	0.06130	14000	0.27919	19000	0.01894	20000	0.01989
26000	0.00683	-	-	-	-	-	-

The operating time was adjusted for each of the burn cases. A five year (1826.25 day) down time was added to the end of each case to provide decay compositions for comparison with those from the follow-on ORIGEN-S cases described in Section 7.4.3. Note that the infiltration of UO_2 during the criticality cannot be modeled in SAS2H and is accounted for in the number density calculations described in Section 7.4.4.

The input and relevant output from each of the six SAS2H cases are listed in Attachments XIII through XVIII.

As a check of the effect of burn step size, the 1000 year case with a step size of 100 years was compared with the 1000 year print of the 10,000 year case with a step size of 1000 years. The order of ranking per absorption rate of the top 15 fission products listed in the "fraction of total absorption rate" tables in the outputs for the 1000 year time print included in Attachments XVI and XVIII are the same and the absorption rates vary between cases less than 3%. The actinides "nuclide concentrations" in gram atoms for the same times also indicate that the major nuclides U-233, U-234, U-235, U-236, U-238, and Np-237 match. The Pu isotopes are overpredicted by 4% or less in the 10,000 year case (1000 year timesteps). These results are acceptable and conservative.

The burnup associated with each of the criticality durations is shown in the Table 7.4.2-2 along with the masses of the major fissile isotopes (U-235 and Pu-239).

Table 7.4.2-2. Burnup and Fissile Composition Changes Associated with Criticality Duration

Duration of Criticality (Years)	1	10	100	1000	5000	10,000
Burnup (MWd)	1.461E00	1.461E01	1.461E02	1.461E03	7.305E03	1.461E04
Mass of U-235 (kg)	1.72E02	1.72E02	1.71E02	1.70E02	1.63E02	1.56E02
Mass of Pu-239 (kg)	1.18E-3	1.21E-2	1.19E-1	1.15E00	5.18E00	9.03E00

A SAS2H case was set up for critical event corresponding to the 100,000 year hydrologic cycle described in Section 7.3.4 where power is limited by a time dependent UO_2 infiltration rate. The case models three 25,000 year periods of decreasing power as described in Section 7.3.4 followed by a 25,000 year decay period. The base material description was the same as described above. The average temperature for each period was set with the temkcyc variable for the corresponding power level. The total burnup for this case is 2.681E4 MWd. At the end of the 75,000 years at power the U-235 and Pu-239 masses are 154 and 5.81 kg, respectively. The input and summarized output for this case is included in Attachment XIX.

7.4.3 ORIGEN-S Decay Calculations

Simple, decay only, ORIGEN-S cases were set up with decay times out to 999,999 years for the 1000, 5000, and 10,000 year duration criticality cases. The input was the same for each case except for titles which include the criticality duration for the 1000 and 5000 year cases. The entire output (including echo of input) is included in Attachments XX through XXII for the 1000, 5000, and 10,000 year duration criticalities, respectively. The ORIGEN-S case was run immediately after the corresponding SAS2H case and utilized the final binary cross section file on unit 21 from the SAS2H case. The case correspondence by attachment number is XVI/XX, XVII/XXI, and XVIII/XXII. The fact that the correct library is used (unit 21) is verified by comparing the final downtime print of concentrations in the SAS2H output with the concentrations in the corresponding decay times in the ORIGEN-S output (compositions will match). The library contains only the final cycle step (1 position in library). The library unit number and data position are entered in the input (3$$ card).

The decay times are grouped in 10 steps with the units changing from days to years as appropriate. The activity of isotopes of concern are shown in Tables 7.4.3-1, -2, and -3. The activities are listed for 0, 10,000, 20,000, 50,000, 100,000, and 250,000 year decay times. Data for additional decay times and isotopes can be found in the outputs included in Attachments XX through XXII. Because the SAS2H case was set up on the appropriate volume, the activities and masses listed in the output are per critical volume.

The same ORIGEN decay case was run in conjunction with the 100,000 year geologic cycle and the activity of isotopes of concern are shown in Table 7.4.3-4. Data for additional decay times and isotopes can be found in the output included in Attachment XXIII. The input and output for the case is included in Attachment XXIII and was run in conjunction with the SAS2H case

included in Attachment XIX.

7.4.4 Burnup Compositions

Number densities for the homogeneous mixtures accounting for burnup and production of isotopes were calculated for each criticality from 1 to 10,000 years duration as well as the 100,000 year geologic cycle criticality. The tuff composition portion of the mixture remained constant. The component densities for UO_2 with burnup and fission products were calculated from the grams/assembly output for the "initial" decay column of data from the SAS2H outputs included in Attachments XIII through XIX by dividing by the volume of the criticality. The component density was incorporated into the equation for number density as shown below (Ref. 5.20, p. 34):

$$N = \rho N_A / M$$

where, ρ is the physical density in g/cm^3, N_A is Avagadro's Number - 0.602252E+24 atoms/mole (Ref. 5.43), and M is the gram atomic weight.

The units of the resulting number density is in atoms/cm^3. The required units for subsequent use are atoms/barn-cm where 1 barn equals 10^{-24} cm^2. The calculations in the spreadsheet (Attachment VII) drop the E+24 from Avagadro's Number to account for the conversion.

The top 15 fission products from the standpoint of absorption were identified from the "fraction of total absorption rate" tables for the last burn step of each case which can be found in the SAS2H outputs included in Attachments XIII through XIX. Two exceptions to this were made in the 1 and 10 year duration criticality cases. Pm-147 and Eu-155 show up in the top 15 absorbers for these cases but no cross sections exist in the MCNP library. Sm-147 and Gd-155, which are the daughter products of Pm-147 and Eu-155, respectively, were substituted. An isotopic cross section for Cd-113 is not available in the MCNP cross sections, so the Cd isotopes from 110 to 116 were summed and the Cd elemental cross section was used in all cases. In addition, the mass of Xe-135 was not printed in the SAS2H outputs because it falls below a threshold for listing, even though its absorption rate is significant and it shows up in the absorption rate tables. The Xe-135 mass used in the 1 year and 10 year compositions was taken from the first "nuclide concentrations, grams" for fission products in the charge column in the 1000 year duration criticality ORIGEN-S case (Attachment XX), which has a significantly lower print threshold. Because of its short half-life (~ 9 hours) the mass of Xe-135 will remain relatively constant through all the cases. The value was rounded to 8.7E-5 grams of X-135.

Two variations of the number density calculations were run to account for the extreme UO_2 infiltration cases of 132 g/year and 0 g/year after initiation of the criticality. In the maximum infiltration rate case, the number densities for the UO_2 feed isotopes U-234, U-235, U-236, U-238, and Np-237 were multiplied by the quantity (132 g/fuel region volume (cm^3)/10.96 g/cm^3)

Table 7.4.3-1. Additional TSPA-95 Radionuclide Inventory (in Ci) Generated by a 1000 Year External Criticality (initial inventory at the end of criticality with subsequent decay)

Isotope	Initial	10,000yr	20,000yr	50,000yr	100,000yr	250,000yr
ac227	7.62E-03	7.65E-02	1.32E-01	2.44E-01	3.26E-01	3.68E-01
am241	8.40E-02	1.01E-08	1.14E-15	3.53E-18	5.97E-20	2.90E-25
am242m	7.96E-05	3.56E-26	0.00E+00	0.00E+00	0.00E+00	0.00E+00
am243	1.19E-08	4.66E-09	1.82E-09	1.08E-10	9.83E-13	7.34E-19
c 14	5.01E-06	1.49E-06	4.46E-07	1.18E-08	2.79E-11	3.66E-19
cm244	5.20E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
cm245	2.08E-16	9.20E-17	4.07E-17	3.52E-18	5.96E-20	2.90E-25
cm246	3.19E-19	7.37E-20	1.70E-20	2.10E-22	1.38E-25	0.00E+00
cs135	6.67E-02	6.65E-02	6.63E-02	6.57E-02	6.48E-02	6.19E-02
i129	1.14E-03	1.14E-03	1.14E-03	1.14E-03	1.14E-03	1.13E-03
nb 93m	6.26E-02	6.38E-02	6.35E-02	6.27E-02	6.13E-02	5.72E-02
nb 94	1.92E-06	1.36E-06	9.68E-07	3.47E-07	6.30E-08	3.76E-10
np237	7.03E+00	7.01E+00	6.99E+00	6.92E+00	6.81E+00	6.48E+00
pa231	7.87E-03	7.65E-02	1.32E-01	2.43E-01	3.26E-01	3.68E-01
pb210	2.15E-02	1.02E+00	2.07E+00	4.57E+00	7.27E+00	8.69E+00
pd107	7.17E-04	7.16E-04	7.16E-04	7.13E-04	7.10E-04	6.98E-04
pu238	9.54E+01	7.82E-26	0.00E+00	0.00E+00	0.00E+00	0.00E+00
pu239	7.15E+01	5.36E+01	4.02E+01	1.70E+01	4.03E+00	5.40E-02
pu240	1.25E+00	4.33E-01	1.51E-01	6.34E-03	3.22E-05	4.24E-12
pu241	2.25E-01	9.21E-17	4.07E-17	3.53E-18	5.97E-20	2.90E-25
pu242	8.70E-08	9.05E-08	8.88E-08	8.40E-08	7.66E-08	5.80E-08
ra226	2.28E-02	1.02E+00	2.07E+00	4.57E+00	7.27E+00	8.70E+00
ra228	1.31E-07	1.45E-06	2.78E-06	6.74E-06	1.33E-05	3.31E-05
se 79	3.12E-03	3.06E-03	2.99E-03	2.81E-03	2.53E-03	1.85E-03
sm151	1.44E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
sn126	1.03E-02	9.66E-03	9.01E-03	7.32E-03	5.17E-03	1.83E-03
tc 99	6.76E-01	6.54E-01	6.33E-01	5.74E-01	4.87E-01	2.98E-01
th229	1.30E-03	1.19E-01	3.37E-01	1.10E+00	2.23E+00	4.35E+00
th230	1.21E-01	1.27E+00	2.30E+00	4.73E+00	7.17E+00	8.58E+00
th232	1.32E-07	1.45E-06	2.78E-06	6.74E-06	1.33E-05	3.31E-05
u233	3.04E-02	3.28E-01	6.12E-01	1.39E+00	2.46E+00	4.46E+00
u234	1.34E+01	1.31E+01	1.28E+01	1.20E+01	1.08E+01	8.09E+00
u235	3.67E-01	3.68E-01	3.68E-01	3.69E-01	3.70E-01	3.70E-01
u236	2.68E+00	2.68E+00	2.68E+00	2.68E+00	2.67E+00	2.66E+00
u238	2.91E+00	2.91E+00	2.91E+00	2.91E+00	2.91E+00	2.91E+00
zr 93	6.41E-02	6.38E-02	6.35E-02	6.27E-02	6.13E-02	5.72E-02
Total	2.10E+02	8.50E+01	7.50E+01	6.00E+01	5.50E+01	5.70E+01

Table 7.4.3-2. Additional TSPA-95 Radionuclide Inventory (in Ci) Generated By a 5000 Year External Criticality (initial inventory at the end of criticality with subsequent decay)

Isotope	Initial	10,000yr	20,000yr	50,000yr	100,000yr	250,000yr
ac227	3.97E-02	9.99E-02	1.49E-01	2.48E-01	3.23E-01	3.63E-01
am241	3.62E+00	4.14E-07	1.94E-13	1.24E-14	2.09E-16	1.02E-21
am242m	5.17E-03	2.31E-24	0.00E+00	0.00E+00	0.00E+00	0.00E+00
am243	6.76E-06	2.64E-06	1.03E-06	6.13E-08	5.56E-10	4.16E-16
c 14	1.99E-05	5.94E-06	1.77E-06	4.70E-08	1.11E-10	1.45E-18
cm244	3.28E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
cm245	7.28E-13	3.22E-13	1.43E-13	1.23E-14	2.09E-16	1.02E-21
cm246	6.12E-15	1.41E-15	3.27E-16	4.03E-18	2.65E-21	7.53E-31
cs135	3.34E-01	3.33E-01	3.32E-01	3.29E-01	3.24E-01	3.10E-01
i129	5.83E-03	5.83E-03	5.83E-03	5.82E-03	5.81E-03	5.77E-03
nb 93m	3.17E-01	3.15E-01	3.14E-01	3.09E-01	3.03E-01	2.83E-01
nb 94	1.08E-05	7.70E-06	5.47E-06	1.96E-06	3.56E-07	2.12E-09
np237	6.98E+00	6.96E+00	6.94E+00	6.87E+00	6.76E+00	6.44E+00
pa231	3.97E-02	9.98E-02	1.49E-01	2.48E-01	3.23E-01	3.63E-01
pb210	3.61E-01	1.53E+00	2.61E+00	5.15E+00	7.89E+00	9.21E+00
pd107	5.05E-03	5.04E-03	5.04E-03	5.02E-03	4.99E-03	4.91E-03
pu238	9.40E+01	5.08E-24	0.00E+00	0.00E+00	0.00E+00	0.00E+00
pu239	3.22E+02	2.41E+02	1.81E+02	7.64E+01	1.81E+01	2.43E-01
pu240	2.45E+01	8.53E+00	2.97E+00	1.25E-01	6.34E-04	8.34E-11
pu241	4.61E+00	3.23E-13	1.43E-13	1.24E-14	2.09E-16	1.02E-21
pu242	2.07E-05	2.06E-05	2.02E-05	1.91E-05	1.74E-05	1.32E-05
ra226	3.61E-01	1.53E+00	2.61E+00	5.16E+00	7.89E+00	9.21E+00
ra228	6.67E-07	2.02E-06	3.38E-06	7.45E-06	1.42E-05	3.45E-05
se 79	1.55E-02	1.52E-02	1.49E-02	1.40E-02	1.26E-02	9.19E-03
sm151	1.53E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
sn126	5.69E-02	5.31E-02	4.95E-02	4.02E-02	2.84E-02	1.01E-02
tc 99	3.35E+00	3.24E+00	3.14E+00	2.84E+00	2.41E+00	1.47E+00
th229	2.85E-02	1.96E-01	4.31E-01	1.19E+00	2.30E+00	4.36E+00
th230	6.12E-01	1.79E+00	2.84E+00	5.32E+00	7.78E+00	9.09E+00
th232	6.67E-07	2.02E-06	3.38E-06	7.45E-06	1.42E-05	3.45E-05
u233	1.48E-01	4.38E-01	7.16E-01	1.47E+00	2.52E+00	4.47E+00
u234	1.42E+01	1.39E+01	1.36E+01	1.27E+01	1.14E+01	8.48E+00
u235	3.53E-01	3.56E-01	3.58E-01	3.62E-01	3.64E-01	3.64E-01
u236	2.75E+00	2.75E+00	2.75E+00	2.75E+00	2.75E+00	2.73E+00
u238	2.91E+00	2.91E+00	2.91E+00	2.91E+00	2.91E+00	2.91E+00
zr 93	3.17E-01	3.15E-01	3.14E-01	3.09E-01	3.03E-01	2.83E-01
Total	5.00E+02	2.90E+02	2.20E+02	1.20E+02	7.50E+01	6.10E+01

Table 7.4.3-3. Additional TSPA-95 Radionuclide Inventory (in Ci) Generated By a 10,000 Year External Criticality (initial inventory at the end of criticality with subsequent decay)

Isotope	Initial	10,000yr	20,000yr	50,000yr	100,000yr	250,000yr
ac227	8.05E-02	1.30E-01	1.71E-01	2.55E-01	3.21E-01	3.56E-01
am241	1.21E+01	1.38E-06	3.08E-12	2.43E-13	4.11E-15	2.00E-20
am242m	1.79E-02	8.02E-24	0.00E+00	0.00E+00	0.00E+00	0.00E+00
am243	6.91E-05	2.70E-05	1.05E-05	6.27E-07	5.69E-09	4.25E-15
c 14	3.08E-05	9.18E-06	2.74E-06	7.26E-08	1.71E-10	2.25E-18
cm244	3.35E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
cm245	1.43E-11	6.33E-12	2.80E-12	2.42E-13	4.11E-15	1.99E-20
cm246	2.26E-13	5.22E-14	1.21E-14	1.49E-16	9.79E-20	2.79E-29
cs135	6.70E-01	6.68E-01	6.66E-01	6.60E-01	6.50E-01	6.21E-01
i129	1.19E-02	1.19E-02	1.19E-02	1.19E-02	1.19E-02	1.18E-02
nb 93m	6.25E-01	6.22E-01	6.20E-01	6.11E-01	5.98E-01	5.58E-01
nb 94	2.74E-05	1.95E-05	1.38E-05	4.97E-06	9.01E-07	5.37E-09
np237	6.93E+00	6.91E+00	6.89E+00	6.82E+00	6.71E+00	6.39E+00
pa231	8.04E-02	1.30E-01	1.71E-01	2.55E-01	3.21E-01	3.56E-01
pb210	9.53E-01	2.18E+00	3.28E+00	5.88E+00	8.64E+00	9.83E+00
pd107	1.31E-02	1.30E-02	1.30E-02	1.30E-02	1.29E-02	1.27E-02
pu238	9.30E+01	1.76E-23	0.00E+00	0.00E+00	0.00E+00	0.00E+00
pu239	5.61E+02	4.21E+02	3.16E+02	1.33E+02	3.16E+01	4.24E-01
pu240	7.28E+01	2.53E+01	8.81E+00	3.70E-01	1.88E-03	2.48E-10
pu241	1.36E+01	6.34E-12	2.81E-12	2.43E-13	4.11E-15	2.00E-20
pu242	1.51E-04	1.49E-04	1.47E-04	1.39E-04	1.26E-04	9.57E-05
ra226	9.53E-01	2.18E+00	3.28E+00	5.88E+00	8.65E+00	9.83E+00
ra228	1.35E-06	2.75E-06	4.16E-06	8.37E-06	1.54E-05	3.64E-05
se 79	3.09E-02	3.03E-02	2.97E-02	2.78E-02	2.51E-02	1.83E-02
sm151	1.61E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
sn126	1.24E-01	1.15E-01	1.08E-01	8.75E-02	6.18E-02	2.19E-02
tc 99	6.62E+00	6.41E+00	6.20E+00	5.62E+00	4.77E+00	2.91E+00
th229	9.73E-02	3.02E-01	5.49E-01	1.30E+00	2.37E+00	4.38E+00
th230	1.24E+00	2.45E+00	3.52E+00	6.04E+00	8.53E+00	9.70E+00
th232	1.35E-06	2.75E-06	4.16E-06	8.37E-06	1.54E-05	3.64E-05
u233	2.85E-01	5.68E-01	8.37E-01	1.57E+00	2.59E+00	4.48E+00
u234	1.51E+01	1.48E+01	1.45E+01	1.35E+01	1.21E+01	8.96E+00
u235	3.38E-01	3.43E-01	3.47E-01	3.53E-01	3.56E-01	3.57E-01
u236	2.83E+00	2.84E+00	2.85E+00	2.85E+00	2.84E+00	2.83E+00
u238	2.91E+00	2.91E+00	2.91E+00	2.91E+00	2.91E+00	2.91E+00
zr 93	6.25E-01	6.22E-01	6.20E-01	6.11E-01	5.98E-01	5.58E-01
Total	8.10E+02	4.90E+02	3.70E+02	1.90E+02	9.50E+01	6.60E+01

Table 7.4.3-4. Additional TSPA-95 Radionuclide Inventory (in Ci) Generated By a 100,000 Year External Criticality (initial inventory at the end of criticality with subsequent decay)

Isotope	Initial	10,000yr	20,000yr	50,000yr	100,000yr	250,000yr
ac227	3.40E-01	3.39E-01	3.38E-01	3.39E-01	3.42E-01	3.44E-01
am241	3.03E-01	3.44E-08	5.18E-14	3.99E-15	6.75E-17	3.28E-22
am242m	5.40E-05	2.41E-26	0.00E+00	0.00E+00	0.00E+00	0.00E+00
am243	8.31E-06	3.24E-06	1.27E-06	7.54E-08	6.84E-10	5.11E-16
c 14	5.62E-06	1.68E-06	5.00E-07	1.33E-08	3.13E-11	4.10E-19
cm244	4.94E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
cm245	2.35E-13	1.04E-13	4.60E-14	3.98E-15	6.74E-17	3.27E-22
cm246	2.84E-15	6.56E-16	1.52E-16	1.87E-18	1.23E-21	3.42E-31
cs135	1.21E+00	1.21E+00	1.21E+00	1.20E+00	1.18E+00	1.13E+00
i129	2.18E-02	2.18E-02	2.18E-02	2.17E-02	2.17E-02	2.15E-02
nb 93m	1.13E+00	1.12E+00	1.12E+00	1.10E+00	1.08E+00	1.01E+00
nb 94	1.03E-04	7.31E-05	5.19E-05	1.86E-05	3.38E-06	2.02E-08
np237	6.72E+00	6.70E+00	6.67E+00	6.61E+00	6.50E+00	6.20E+00
pa231	3.40E-01	3.39E-01	3.38E-01	3.39E-01	3.42E-01	3.44E-01
pb210	7.06E+00	7.73E+00	8.32E+00	9.63E+00	1.09E+01	1.02E+01
pd107	2.33E-02	2.33E-02	2.33E-02	2.32E-02	2.31E-02	2.27E-02
pu238	1.12E+01	5.30E-26	0.00E+00	0.00E+00	0.00E+00	0.00E+00
pu239	3.60E+02	2.70E+02	2.03E+02	8.56E+01	2.03E+01	2.72E-01
pu240	1.33E+01	4.64E+00	1.61E+00	6.78E-02	3.45E-04	4.53E-11
pu241	3.05E-01	1.04E-13	4.60E-14	3.99E-15	6.75E-17	3.28E-22
pu242	4.65E-05	4.56E-05	4.48E-05	4.24E-05	3.86E-05	2.92E-05
ra226	7.06E+00	7.73E+00	8.32E+00	9.63E+00	1.09E+01	1.03E+01
ra228	1.06E-05	1.21E-05	1.35E-05	1.80E-05	2.53E-05	4.74E-05
se 79	5.22E-02	5.11E-02	5.01E-02	4.70E-02	4.23E-02	3.09E-02
sm151	2.02E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
sn126	1.73E-01	1.61E-01	1.50E-01	1.22E-01	8.63E-02	3.05E-02
tc 99	1.06E+01	1.03E+01	9.94E+00	9.01E+00	7.65E+00	4.67E+00
th229	1.57E+00	1.77E+00	1.98E+00	2.55E+00	3.34E+00	4.79E+00
th230	7.23E+00	7.88E+00	8.44E+00	9.71E+00	1.07E+01	1.01E+01
th232	1.06E-05	1.21E-05	1.35E-05	1.80E-05	2.53E-05	4.74E-05
u233	1.80E+00	2.01E+00	2.21E+00	2.75E+00	3.50E+00	4.86E+00
u234	1.48E+01	1.45E+01	1.42E+01	1.33E+01	1.19E+01	8.79E+00
u235	3.32E-01	3.35E-01	3.37E-01	3.41E-01	3.44E-01	3.44E-01
u236	2.99E+00	2.99E+00	2.99E+00	2.99E+00	2.98E+00	2.97E+00
u238	2.90E+00	2.90E+00	2.90E+00	2.90E+00	2.90E+00	2.90E+00
zr 93	1.13E+00	1.12E+00	1.12E+00	1.10E+00	1.08E+00	1.01E+00
Total	4.50E+02	3.40E+02	2.80E+02	1.60E+02	9.60E+01	7.00E+01

and the resulting product was added to the number density calculated from the mass entered from the SAS2H output shown in the spreadsheet. Oxygen was adjusted for the additional material while also being adjusted down for the displaced water. Hydrogen was adjusted down to account for the displaced water by the volume fraction of UO_2 added (quantity described above). In the 0 g/yr infiltration rate case, number densities were calculated directly from the SAS2H masses for actinides and fission products and the water number densities were maintained constant.

The calculations and results are shown in the LOTUS 1-2-3 spreadsheet included in Attachment VII.

7.4.5 Check of Reactivity Changes With Time Due to Criticality

The MCNP base case for 538 K described in Section 7.4.1 was used with the number densities calculated in the previous section for the 3 criticality durations from 1000 to 10,000 years. The results of the MCNP cases are shown in Table 7.4.5-1 (Attachment numbers shown in parentheses). These cases demonstrate that the system reactivity is not significantly affected by the continued infiltration of material or by the burnup of fissile material and generation of fission products. The burnup is only 1.45 GWd/MTU (1.461E4 GWd/ 10.1 MTU) even after 10,000 years and at the maximum infiltration rate only adds 1.3 metric tons of UO_2. As indicated by the results in Reference 5.55, very large changes in the characteristics of these very large thermal systems are required to significantly change the k_{eff} value.

Table 7.4.5-1. MCNP Case Results to Demonstrate Reactivity Changes with Time

Time (years)	132 g/yr UO_2 Infiltration	0 g/yr UO_2 Infiltration
0.00	0.9424 ± 0.0020 (XI)	-
1000	0.9395 ± 0.0019 (XXV)	0.9373 ± 0.0018 (XXVIII)
5000	0.9417 ± 0.0016 (XXVI)	0.9348 ± 0.0016 (XXIX)
10,000	0.9453 ± 0.0019 (XXVII)	0.9336 ± 0.0016 (XXX)

Two additional cases were run for the 1000 year duration criticality with high UO_2 infiltration. In one case the fission products were removed providing a k_{eff} of 0.9440 ± 0.0018 (XXXI). In the other case Pu-238, Pu-239, and U-233 were removed providing a k_{eff} of 0.9349 ± 0.0016 (XXXII). This represents a nominal worth compared to the reference case above (XXV) of -0.48% and 0.49% for fission products and Pu, respectively at 1000 years. These same two cases were also run for the 10,000 year duration criticality with high UO_2 infiltration. For the case with fission products removed, a k_{eff} of 0.9556 ± 0.0019 (XXXIII) was calculated and for the case with Pu-238, Pu-239, and U-233 removed, a k_{eff} of 0.9090 ± 0.0018 (XXXIV) was calculated. This represents a nominal worth compared to the reference case above (XXVII) of -1.09% and +3.84% for fission products and Pu, respectively at 10,000 years.

In order to demonstrate that the top 15 fission product absorbers were sufficient to cover fission

product effects, the next 16 highest fission product absorbers were reviewed for inclusion in an additional case based on the 10,000 year duration criticality with high UO_2 infiltration. The "fraction of total absorption rate" table for the last burn step of the 10,000 year duration case which can be found in the SAS2H output included in Attachments XVIII provides the absorption data. Five of these next highest fission product absorbers do not have cross sections available for MCNP and were discarded. The other eleven of these absorbers were added to the 10,000 year composition in the MCNP case providing a k_{eff} of 0.9448 ± 0.0018 (XXXV). Comparison of this result with that which included only 15 fission products demonstrates that the 15 fission products are sufficient.

The MCNP base case for 323 K (50 °C) described in Section 7.4.1 was used with the number densities calculated in the previous section for the 100,000 year hydrologic cycle. The results of the MCNP cases are a k_{eff} of 0.9994 ± 0.0019 (XXXVI) for the UO_2 infiltration case and 0.9477 ± 0.0017 (XXXVII) for no UO_2 infiltration. Note that these calculations are performed at 323 K while those reported above were performed at 538 K, representative of the respective power levels. At the variable infiltration rate, 6.6 metric tons of UO_2 are added displacing water over the 75,000 years of operation.

7.5 Probability Estimates

7.5.1 Summary of Prior Probability Estimates

The principal contribution to the probability of internal criticality (Refs. 5.8 and 5.9) came from a combination of the following events or processes:

- A given waste package has sufficiently reactive fuel.
- Hydraulically conductive fracture, or focusing, over the waste package.
- Increased infiltration rate (at least 10 times present value) within some time, T_1.
- Given the increased flow, the waste package barriers are breached within some time, T_2, after T_1.
- Given the barrier breach, a sufficient quantity of neutron absorber is removed from the waste package within some time, T_3, after $T_1 + T_2$.
- Water which has filled the waste package does not corrode through the inner barrier at the bottom of the waste package lying on its side.

The result, for the uncanistered fuel waste package was an expectation of less than 1 criticality in 80,000 years (Ref. 5.8, p. 55).

The principal contribution to the probability of external criticality (Ref. 5.52) came from a combination of the following events or processes:

- The number of waste packages having sufficient fissile content to provide a critical mass for a reducing zone in the repository far-field.
- The probability that a fissile bearing stream from a waste package having sufficient fissile content will encounter a single reducing zone, based on the distribution of

organic/carbonaceous deposits on the Colorado Plateau.
- The probability of the reducing zone being of sufficient size (based on the random juxtaposition of individual organic/carbonaceous deposits) to trap a critical mass.

The result is that the expected number of external criticalities from commercial SNF, over an arbitrarily long time period, is less than 2×10^{-7} (Ref. 5.52, p. 41, which was the highest value found in that analysis, although it was for a configuration different from the principal case in this analysis).

7.5.2 Data Needs for Future Probability Estimates

The following paragraphs identify the items of information which are expected to become available within the next year and will enable improvement of the accuracy of the probability estimates.

Internal criticality:

- Actual fracture density data from the Yucca Mountain tunnel at the repository horizon to more realistically estimate the probability of dripping on a given waste package and the associated concentration factor.
- Improved model of aqueous corrosion rate of the corrosion resistant inner barrier of the waste package, particularly as a function of temperature. This will facilitate the calculation of a probability density function for the criticality duration which is based on the length of time water can be contained in the WP to a depth sufficient to provide moderator for a critical mass of assemblies, including consideration of the increased temperature caused by the criticality (e.g., a peak temperature of 57 °C versus the drift wall temperature of less than 50 °C beyond 10,000 years given in the TSPA-95 data (Ref 5.18).
- Improved model for corrosion of borated stainless steel and the metal borides contained in the stainless steel matrix.

External criticality:

- Fissile mobilization rate, which consists of the waste form dissolution rate and the solubility of the fissile species (since the solution is the medium for the removal of the fissile material from the waste package).
- Systematic identification of organic (carbonaceous) deposits and other reducing zones in tuff, characterizing their size and density. These parameters could replace the hypothetical log combination methodology used in Reference 5.52, particularly at the base of tuff layers.
- Identification of exceptionally high permeability formations below the water table which could focus the fissile bearing water from more than one waste package at a time (assuming that it could reach the water table without any lateral spreading).
- More data on the areal extent of highest grade ores at Oklo, to be used to generate a joint probability distribution for the occurrence of possible values of concentration and size, which will, in turn be used for an alternative estimate of the maximum possible size and concentration of any individual reducing zone. This may also serve to eliminate the

possibility of the high uranium, high water cases which were considered in Reference 5.52, but were rejected for the nominal case in this analysis for the reasons given in Section 7.3.1, above.

8. Conclusions

In compliance with the M&O Quality Administrative Procedures, the design results presented in this document should not be used for procurement, fabrication, or construction unless properly identified, tracked as TBV, and controlled by the appropriate procedures.

The purpose of this probabilistic evaluation was to estimate the consequences of a criticality event, both internal and external to a waste package. As a result of the calculations performed in this analysis, it can be concluded that:

- Maximum power determined by the boiling temperature of water is less than 5 kW.
- Duration is nominally less than 10,000 years, but can be cycled up to 100,000 years.
- Maximum sustainable power, as determined by the inflow of the worst case high concentration of fissile bearing water, is less than 1.5 kW.
- Change in k_{eff} over the duration of the criticality is small, for nominal 10,000 year duration and even for 100,000 year cycling due to temperature and UO_2 infiltration limited power.
- Increase in radionuclide inventory is small (both for a single package and for the number of packages which are likely to go critical).

9. Attachments -

List of Attachments

Attachment	Description	Date	Number of Pages
I	Derivation of Power-Temperature Relationship	8/28/96	2
II	LOTUS 1-2-3 Spreadsheet - Number Densities for Internal Criticality (ucfcalcs.wk4 sheet F)	8/30/96	4
III	MCNP Case - Internal Criticality 0 Year Duration (a26xb5cO.sum)	8/22/96	10
IV	MCNP Case - Internal Criticality 1000 Year Duration (a26xb5dO.sum)	8/23/96	10
V	MCNP Case - Internal Criticality 5000 Year Duration (a26xb5eO.sum)	8/22/96	10
VI	MCNP Case - Internal Criticality 10,000 Year Duration (a26xb5fO.sum)	8/22/96	10
VII	LOTUS 1-2-3 Spreadsheet - Tuff/Water/UO2 Mixture Number Densities (leshpher2.wk4 Sheet C)	8/29/96	10
VIII	LOTUS 1-2-3 Spreadsheet - Internal Criticality Radionuclide Inventory Comparisons	9/4/96	3
IX	MCNP Case - External Criticality 0 Year Duration, 300K (sp40aO.sum)	8/22/96	4
X	MCNP Case - External Criticality 0 Year Duration, 323K (sp40a2O.sum)	8/23/96	4
XI	MCNP Case - External Criticality 0 Year Duration, 538K (sp40a1O.sum)	8/22/96	4
XII	Not Used	n/a	n/a
XIII	SAS2H Case - External Criticality 1 Year Duration (tuff7.sum)	8/29/96	54
XIV	SAS2H Case - External Criticality 10 Year Duration (tuff6.sum)	8/29/96	56
XV	SAS2H Case - External Criticality 100 Year Duration (tuff5.sum)	8/29/96	59
XVI	SAS2H Case - External Criticality 1000 Year Duration (tuff3.sum)	8/29/96	100

Attachment	Description	Date	Number of Pages
XVII	SAS2H Case - External Criticality 5000 Year Duration (tuff2.sum)	8/29/96	64
XVIII	SAS2H Case - External Criticality 10,000 Year Duration (tuff1.sum)	8/29/96	102
XIX	SAS2H Case - External Criticality 100,000 Year Hydrologic Cycle (tuff9.sum)	9/3/96	231
XX	ORIGEN-S Case - Decay of 1000 Year Criticality (origen3.output)	8/28/96	231
XXI	ORIGEN-S Case - Decay of 5000 Year Criticality (origen2.output)	8/28/96	231
XXII	ORIGEN-S Case - Decay of 10,000 Year Criticality (origen1.output)	8/28/96	231
XXIII	ORIGEN-S Case - Decay of 100,000 Year Hydrologic Cycle Criticality (origen9.output)	8/29/96	231
XXIV	Not Used	n/a	n/a
XXV	MCNP Case - External Criticality 1000 Year Duration, 538K, UO_2 infiltration (sp40e1O.sum)	8/30/96	4
XXVI	MCNP Case - External Criticality 5000 Year Duration, 538K, UO_2 infiltration (sp40f1P.sum)	8/22/96	4
XXVII	MCNP Case - External Criticality 10,000 Year Duration, 538K, UO_2 infiltration (sp40g1O.sum)	8/30/96	4
XXVIII	MCNP Case - External Criticality 1000 Year Duration, 538K, No UO_2 infiltration (sp40e1nO.sum)	8/30/96	4
XXIX	MCNP Case - External Criticality 5000 Year Duration, 538K, No UO_2 infiltration (sp40f1nP.sum)	8/22/96	4
XXX	MCNP Case - External Criticality 10,000 Year Duration, 538K, No UO_2 infiltration (sp40g1nO.sum)	8/30/96	4
XXXI	MCNP Case - External Criticality 1000 Year Duration, 538K, UO_2 infiltration, No FP (sp40e1yO.sum)	8/30/96	4
XXXII	MCNP Case - External Criticality 1000 Year Duration, 538K, UO_2 infiltration, No U-233, Pu-238, Pu-239 (sp40e1zO.sum)	8/30/96	4
XXXIII	MCNP Case - External Criticality 10,000 Year Duration, 538K, UO_2 infiltration, No FP (sp40g1yO.sum)	8/30/96	4

Attachment	Description	Date	Number of Pages
XXXIV	MCNP Case - External Criticality 10,000 Year Duration, 538K, UO_2 infiltration, No U-233, Pu-238, Pu-239 (sp40g1zO.sum)	8/30/96	4
XXXV	MCNP Case - External Criticality 10,000 Year Duration, 538K, UO_2 infiltration, Extended FP (sp40g1xO.sum)	8/30/96	4
XXXVI	MCNP Case - External Criticality 100,000 Year Duration, 323K, UO_2 infiltration (sp40lO.sum)	8/30/96	4
XXXVII	MCNP Case - External Criticality 100,000 Year Duration, 323K, No UO_2 infiltration (sp40lnO.sum)	8/30/96	4