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Intact and Degraded Mode Criticality Calculations for the Codisposal of ATR Spent Nuclear Fuel in a Waste Package

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This document does not impact any other organization outside Criticality, therefore an AP-2.14Q review is not required.

THIS DOCUMENT IS IMPACTED BY THE FOLLOWING "ERROR RESOLUTION DOCUMENTS", WHICH SHOULD BE REVIEWED PRIOR TO USING THIS DOCUMENT:

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Attachment	Total Number of Pages
Attachment I. CD	1 CD-ROM
Attachment II	1

RECORD OF REVISIONS

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1. PURPOSE

The objective of this calculation is to perform intact and degraded mode criticality evaluations of the U.S. Department of Energy's (DOE) Advanced Test Reactor (ATR) Spent Nuclear Fuel (SNF) placed in the DOE standardized SNF canister. This analysis evaluates the codisposal of the DOE SNF canister containing the ATR SNF in a 5-Defense High-Level Waste (5-DHLW) Short Waste Package (WP) (Bechtel SAIC Company, LLC [BSC] 2004a), which is to be placed in a monitored geologic repository (MGR). The scope of this calculation is limited to the determination of the effective neutron multiplication factor (k_{eff}) for both intact and degraded mode internal configurations of the waste package.

These calculations will support the analysis that will be performed to demonstrate the technical viability of the design solution adopted for disposing of ATR spent nuclear fuel in the potential repository.

This calculation addresses the codisposal viability of ATR SNF at Yucca Mountain repository and is subject to the Quality Assurance Requirements and Description (QARD) (DOE 2004a) per the activity evaluation for activity identifier 2.1.2.3, Section 8 in the *Technical Work Plan for: Criticality Department Work Packages ACRM01 and NSN002* (BSC 2004e). This document is prepared in accordance with AP-3.12Q, *Design Calculations and Analyses*, and AP-3.15Q, *Managing Technical Product Inputs.*

2. METHOD

The method to perform the criticality calculations consists of using MCNP Version 4B2 (CRWMS M&O 1998a, CRWMS M&O 1998b) to calculate the effective neutron multiplication factor of the waste package. The calculations are performed using the continuous-energy cross section libraries, which are part of the qualified code system MCNP 4B2 (CRWMS M&O 1998a, CRWMS M&O 1998b). All calculations are performed with the most reactive fissile concentration that bounds the beginning-of-life (BOL) and end-of-life (EOL) ATR fuel.

Control of the electronic management of data was evaluated in accordance with AP-SV.1Q, *Control of the Electronic Management of Information.*

3. ASSUMPTIONS

3.1 DEGRADATION OF MATERIALS CONTAINING ALUMINUM

Assumption: For the degraded mode criticality calculations, it is assumed that the aluminum in the fuel meat and cladding degrades to gibbsite - $Al(OH)_3$ rather than diaspore - AlOOH.

Rationale: It is conservative to consider gibbsite rather than diaspore since more hydrogen (a moderator) is available in gibbsite. All other impurities in aluminum are neglected since they are neutron absorbers, and hence their absence provides a conservative (higher) value for the k_{eff} of the system.

Confirmation Status: This assumption does not require further confirmation by testing, design, or analysis.

Use in the Calculation: This assumption is used throughout Sections 5 and 6.2.1.

3.2 NEUTRON INTERACTION CROSS SECTIONS FOR ^{137}BA

Assumption: ^{138}Ba cross sections are used instead of ^{137}Ba cross sections in the MCNP input since the cross sections of ^{137}Ba are not available in either ENDF/B-V or ENDF/B-VI cross section libraries.

Rationale: This assumption is conservative since the thermal neutron capture cross section and the resonance integral of ^{137}Ba (5.1 and 4 barn, respectively [Parrington et al. 1996, p. 34]) are greater than the thermal neutron capture cross section and the resonance integral of ^{138}Ba (0.43 and 0.3 barn, respectively [Parrington et al. 1996, p. 34]).

Confirmation Status: This assumption does not require further confirmation by testing, design, or analysis.

Use in the Calculation: This assumption is used throughout Section 5.

3.3 ATR SNF COMPOSITION

Assumption: Beginning of life (BOL) composition of the ATR SNF fuel is considered in the present calculation and no credit is taken for the initial boron neutron absorber present in the fuel.

Rationale: The rationale for this assumption is that it is conservative because it results in a higher k_{eff} of the system.

Confirmation Status: This assumption does not require further confirmation by testing, design, or analysis.

Use in the Calculation: This assumption is used throughout Sections 5, 6, and Attachment I.

3.4 BOUNDING FISSILE CONTENT OF ATR FUEL

Assumption: The most reactive fissile content of 94 wt% ^{235}U is used for the ATR fuel to bound the enrichment of any ATR fuel assembly.

Rationale: The basis for this assumption is that the selected enrichment is conservative since it maximizes the fissile isotope (^{235}U) content while minimizing the effect of neutron absorption (^{238}U).

Confirmation Status: This assumption does not require further confirmation by testing, design, or analysis.

Use in the Calculation: This assumption is used throughout Sections 5 and 6.

3.5 DEGRADATION PRODUCTS CHARACTERISTICS

Assumption: For the degraded configurations, the degradation products (gibbsite, schoepite) are assumed to form with void occupying 30% or more of their volume. The void can be filled with water and/or remain as void.

Rationale: The basis for this assumption is the corroborative information given in Coelho et al. (1997).

Confirmation Status: This assumption does not require further confirmation by testing, design, or analysis.

Use in the Calculation: This assumption is used throughout Sections 5 and 6.2.1.

3.6 NEUTRON INTERACTION CROSS SECTIONS FOR ZN

Assumption: Al cross sections are used instead of Zn cross sections in the MCNP input since the cross sections of Zn are not available in the MCNP 4B2LV cross-section libraries.

Rationale: It is a conservative assumption since the thermal neutron capture cross section and the resonance integral of Zn (Parrington et al., 1996, p.24) are greater than the thermal neutron capture cross section and the resonance integral of Al (Parrington et al., 1996, p.21).

Confirmation Status: This assumption does not require further confirmation by testing, design, or analysis.

Use in the Calculation: This assumption is used throughout Section 5.

3.7 VOID FRACTION OF AL FILL MATERIAL

Assumption: A void fraction of 0.4667 is assumed for the Al fill material (Al shot mixed with gadolinium phosphate).

Rationale: This value is within the range of porosities for random packings of particles of various shapes presented in Coelho et al. (1997). The value was also assumed in a similar analysis (CRWMS M&O 2000, p.11) using Al fill material.

Confirmation Status: This assumption does not require further confirmation by testing, design, or analysis.

Use in the Calculation: This assumption is used throughout Section 5 and Attachment I.

3.8 VOLUME CONSERVATION FOR THE MIXING OF ALUMINUM AND GADOLINIUM PHOSPHATE

Assumption: It is assumed that the volume of the aluminum and gadolinium phosphate is conserved when mixed.

Rationale: This assumption is used in calculating the density of the Al fill mixture and is based on engineering judgment. The gadolinium content of the fill material is expressed as a weight percentage of the Al-$GdPO_4$ mix.

Confirmation Status: This assumption does not require further confirmation by testing, design, or analysis.

Use in the Calculation: This assumption is used throughout Sections 5, 6, and Attachment I.

4. USE OF COMPUTER SOFTWARE

4.1 SOFTWARE

The commercial off-the-shelf software MS EXCEL Version 2000 SP-2 installed on a personal computer (PC) Dell Optiplex GX270 operating under MS Windows XP operating system, was used for performing graphical representations and arithmetical manipulations in a spreadsheet type environment. Microsoft EXCEL Version 2000 SP-2 is an exempt software application in accordance with LP-SI-11Q-BSC, Sections 2.1.1 and 2.1.6. The developed spreadsheet files are included in Attachment I. The spreadsheets contain sufficient information to allow an independent check to reproduce or verify the results.

4.1.1 MCNP

The MCNP code (CRWMS M&O [1998b]) is used to calculate the k_{eff} of the waste package. The software specifications are as follow:

- Status: Qualified
- Software name: MCNP
- Software version/revision number: Version 4B2
- Software tracking number (computer software configuration item [CSCI]): 30033 V4B2LV
- Computer type: Hewlett Packard (HP) 9000 Series Workstations
- Operating system: HP-UX 10.20
- Computer processing unit number: Software is installed on the Framatome ANP workstation "gr1" whose CPU number is E 9000/785 2008515632 and "gr0" whose CPU number is E 9000/782 2002611431.

The input and output files for the various MCNP calculations are documented in Attachment I. The calculation files described in Sections 5 and 6 are such that an independent repetition of the software use may be performed.

The MCNP software used is: (a) appropriate for the application of k_{eff} calculations, (b) used only within the range of validation as documented in CRWMS M&O (1998a) and Briesmeister (1997), (c) obtained from the Software Configuration Management in accordance with LP-SI.11Q-BSC, *Software Management*.

5. CALCULATION

This section describes the calculations performed to evaluate the k_{eff} of a waste package containing degraded high-level waste material and ATR spent nuclear fuel. Section 5.1 describes the waste package and its contents. Section 5.2 gives the composition of the materials used in this calculation. The basic formulas used in this calculation are listed in Section 5.3. The investigated intact configurations of the waste package are outlined in Section 5.4. Section 5.5 describes calculations performed to characterize the degraded configurations of a waste package. The MCNP input and output files developed for this section are presented in Attachment I. The spreadsheets used to prepare the MCNP input files are given also in Attachment I. The results of the calculations are presented in Section 6.

The description of the ATR spent nuclear fuel is from Paige (1969), Idaho National Engineering and Environmental Laboratory (INEEL, 2003) and Reed et al. (1992). All fuel-related information is taken from these references unless otherwise noted.

The Savannah River Site defense high-level waste (DHLW) glass composition and density are from CRWMS M&O (1999b) and Stout and Leider (1991), respectively. The Savannah River Site DHLW glass degraded composition (pre-breach clay) is from BSC (2001).

The tuff composition and the tuff density are taken from DTN: GS000308313211.001 and DTN: MO0109HYMPROP.001, respectively.

Avogadro's number and atomic weights are from Parrington et al. (1996).

The number of digits in the values cited herein may be the result of a calculation or may reflect the input from another source; consequently, the number of digits should not be interpreted as an indication of accuracy.

The metric units used in this document are calculated using the English units as given in the cited references. The differences that might exist between the metric units calculated and the metric units cited in references have no effect on the calculation and should not be interpreted as an indication of accuracy.

5.1 WASTE PACKAGE COMPONENTS DESCRIPTION

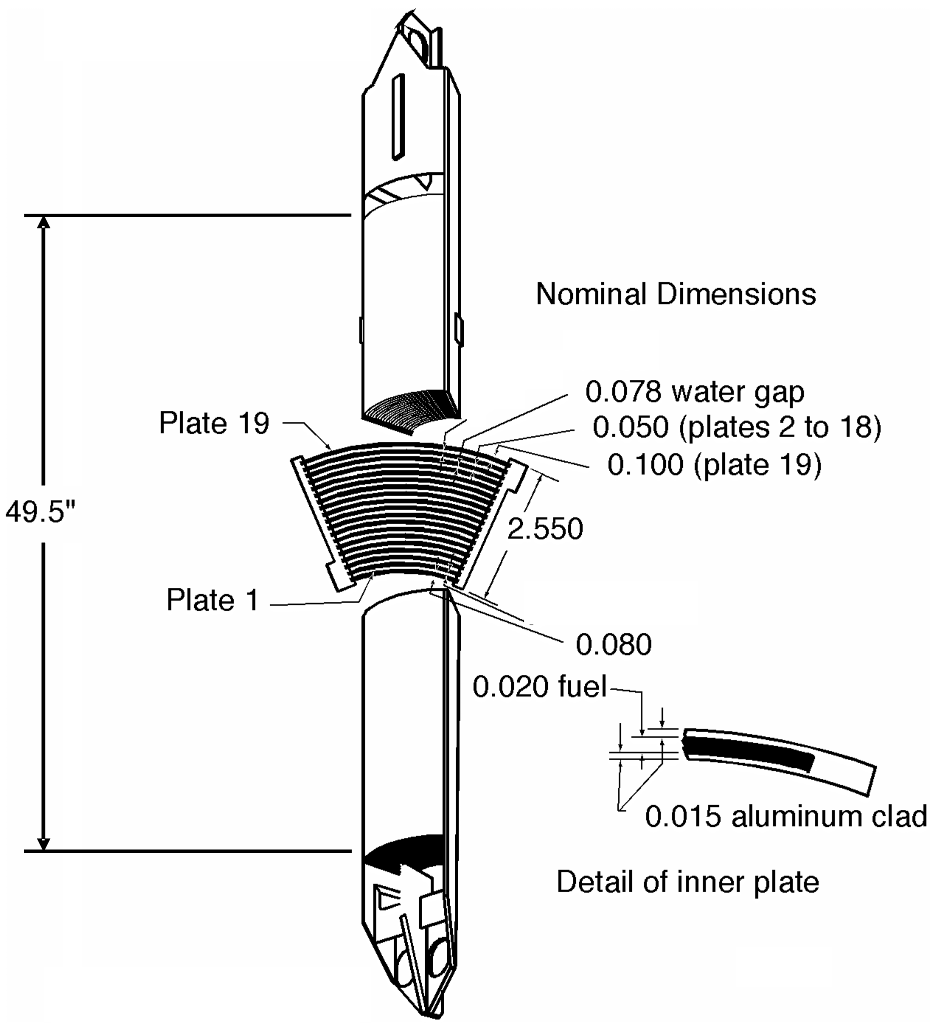
5.1.1 ATR Spent Nuclear Fuel

The following dimensions and information are from Paige (1969), INEEL (2003) and Reed et al. (1992).

A typical ATR fuel element consists of 19 curved aluminum clad uranium aluminide (UAl_x) plates containing highly enriched (93±1 wt% ^{235}U) uranium (Reed et al. 1992). The highest nominal fissile loading (^{235}U) of the fresh fuel element is 1075 g (ATR 7F fuel element, [Paige, 1969]). The allowable uncertainty in the fuel loading is 1 percent or 10.75g (INEEL 2003). The highest fissile loading of 1085.75 g was considered in the present analysis.

Figure 1 presents a simplified view of a typical ATR fuel element. For the purpose of disposal, the fuel elements are cropped to a length of 49.5 in. (length of the fuel plates) by removing the upper and lower end boxes. The fuel plates are 49.5 in. (1257.3 mm) long with a fuel zone that is 48.76 in. (1238.504 mm) long.

The following data are characteristics for the ATR 7F fuel elements (Paige 1969). The thickness of each plate is 0.05 in. (1.27 mm) except plates 1 and 19, which are 0.08 in. (2.032 mm) and 0.1 in. (2.54 mm), respectively. The fuel matrix section in each plate is 0.02 in. (0.508 mm) thick. The cladding is made of aluminum (T-6061). The plates are held in place by aluminum side plates that are 2.55 in. (64.77 mm) wide (thickness of the fuel assembly), 0.187 in. (4.7498 mm) thick, and 49.5 in. (1257.3 mm) long. When assembled, the angle of curvature of the fuel elements is 45 degrees with an inner radius of 2.964 in. (75.2856 mm) and an outer radius of 5.513 in. (140.03 mm). The detailed dimensions of each fuel plate and fuel meat are presented in Table 1.



NOTE: Figure not to scale. All dimensions are in inches.

Figure 11. Simplified View of the ATR Fuel Element

Table 1~~1~~. Dimensions and Fissile Loading for Individual Plates in ATR Fuel Element

Plate Number	Inner Radius (mm)	Outer Radius (mm)	Plate Arc Length (mm)	Fuel Meat Arc Length (mm)	^{235}U content (max) (g)
1	76.5810	78.6130	54.1020	41.3258	24.543
2	80.5942	81.8642	55.4228	49.2506	29.391
3	83.8454	85.1154	57.9882	51.8160	39.087
4	87.0966	88.3666	60.5028	54.3306	40.804
5	90.3478	91.6178	63.0936	56.9214	52.621
6	93.5990	94.8690	65.6336	59.4614	55.146
7	96.8502	98.1202	68.1990	62.0268	57.570
8	100.1014	101.3714	70.7390	64.5668	59.994
9	103.3526	104.6226	73.3044	67.1322	62.418
10	106.6038	107.8738	75.8444	69.6722	64.842
11	109.8550	111.1250	78.4098	72.2376	67.266
12	113.1062	114.3762	80.9752	74.8030	69.690
13	116.3574	117.6274	83.5152	77.3430	72.114
14	119.6086	120.8786	86.0806	79.9084	74.538
15	122.8598	124.1298	88.6206	82.4484	77.063
16	126.1110	127.3810	91.1860	85.0138	64.640
17	129.3622	130.6322	93.7260	87.5538	66.559
18	132.6134	133.8834	96.2914	88.8492	54.338
19	135.8646	138.4046	100.8634	88.0872	53.126

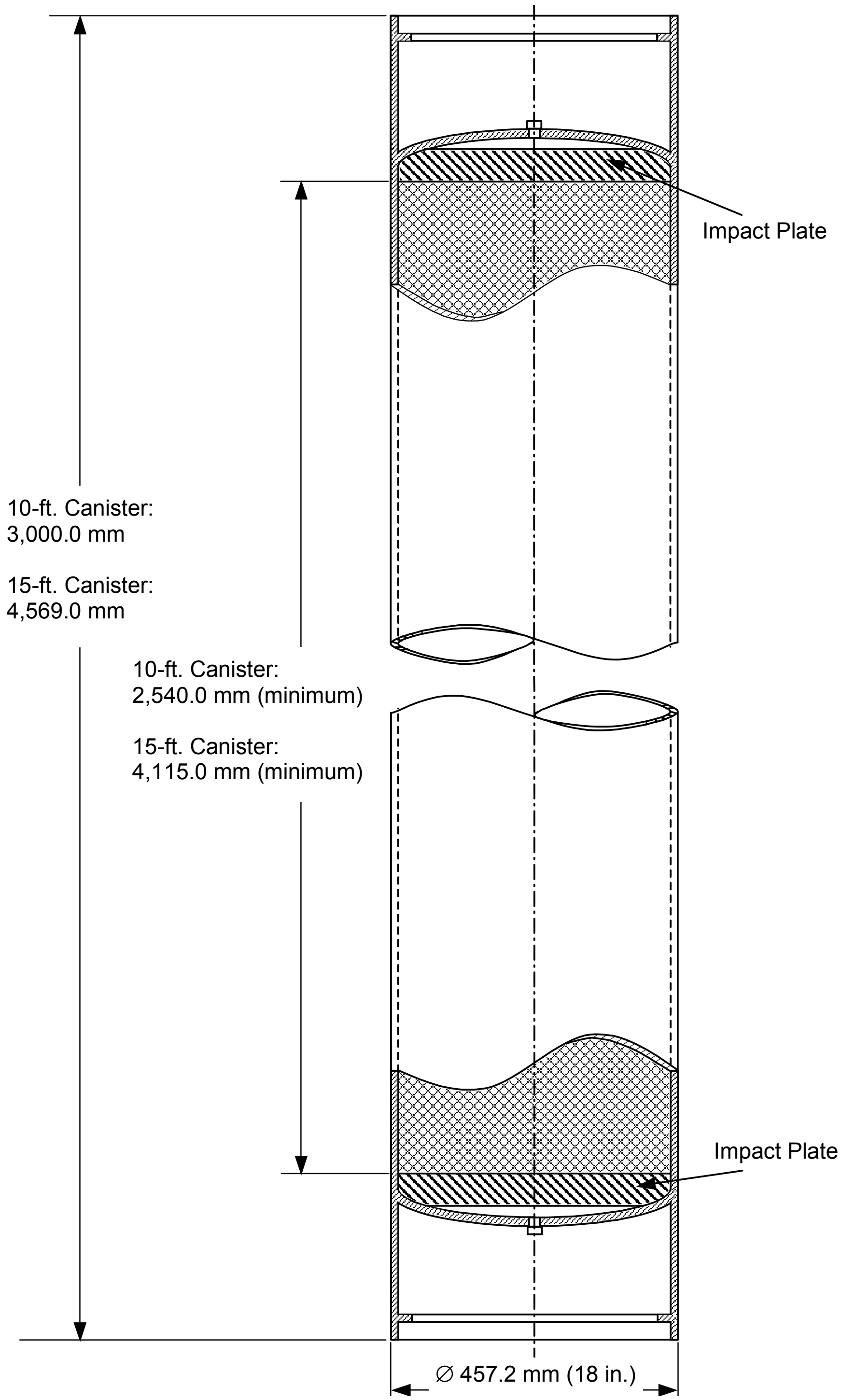
Source: Paige (1969), ATR 7F fuel element.

5.1.2 Description of DOE SNF Canister

The conceptual design for the standardized DOE SNF canister (also referred to as the 18-in.-diameter DOE SNF canister) is taken from DOE (1999, p. 5 and A-2). The DOE SNF canister is a right circular cylinder pipe made of stainless steel (Type 316L or Unified Numbering System [UNS] S31603) with an outside diameter of 457.2 mm (18 in.) and a wall thickness of 9.525 mm (0.375 in.). The minimum internal length of the short canister is 2,540.0 mm and the nominal overall length is 3,000.0 mm (approximately 10 ft). There is a curved carbon steel (American Society for Testing and Materials [ASTM] A 516 Grade 70) impact plate, 50.8-mm (2.0-in.) thick, at the top and bottom boundaries of the canister. Dished heads seal the ends of the DOE SNF canister. The maximum loaded mass is 2,270 kg for the short canister (DOE 1999, Table 3.2). A sketch of the canister is shown in Figure 2.

The DOE SNF canister typically contains a basket structure to hold the spent fuel. The basket is not a standard part of the DOE SNF canister. The basket design is modified for each specific spent fuel type and the basket structure provides material for controlling criticality, provides structural support, and acts as a guide for assemblies during loading. For disposing ATR SNF a basket structure made of low-carbon nickel-chromium-molybdenum-gadolinium alloy (UNS N06464) with a Gd content of 2.0 wt% has been proposed for the conceptual design (DOE 2004b, pp. 53-55). The basket structure contains two axial identical sections (layers) separated by a circular plate with a thickness of 9.525 mm made from 304L stainless steel. The length of each section was considered to be 1260.475 mm (49.625 in). All Gd alloy plates (including the separation plate) have been assumed to have a thickness of 9.525 mm (0.375 in.). A cross sectional view is shown in Figure 3 (DOE 2004b, p.53). The basket is surrounded by a type

304L stainless steel sleeve with an outer diameter of 429.25 mm and a thickness of 1.557 mm (0.1875 in.).

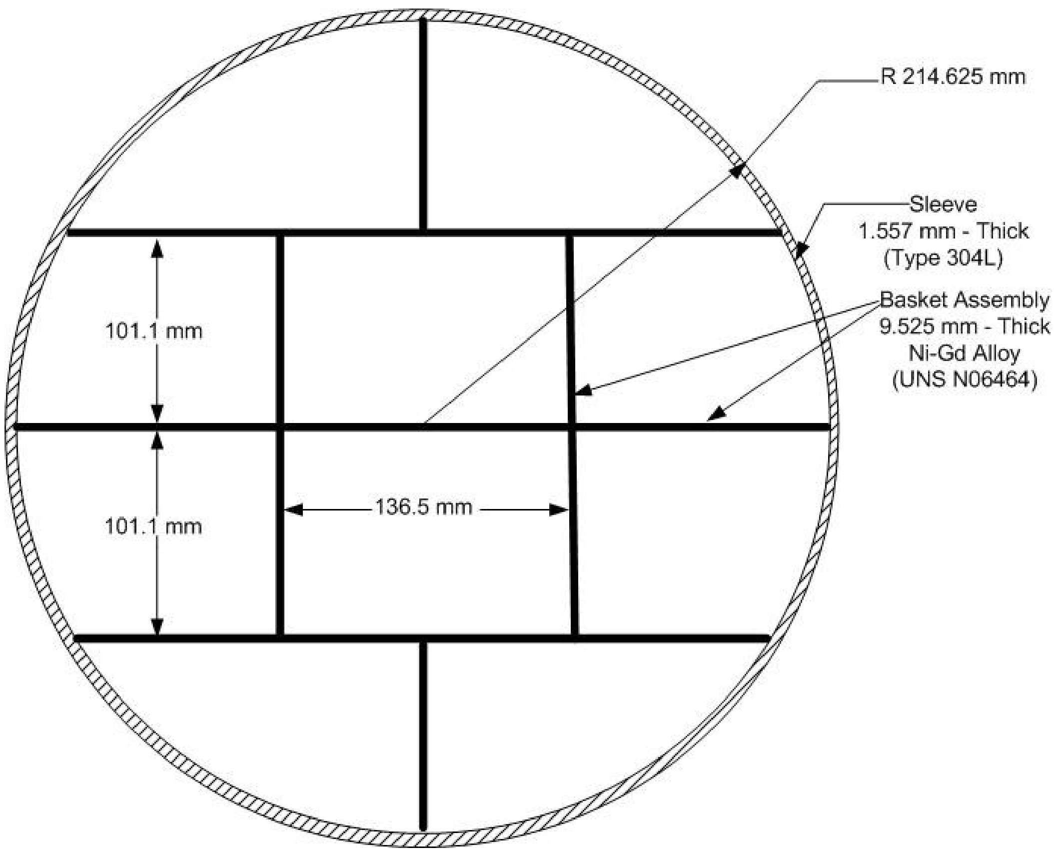


Source: DOE 1999, p. A-2.

NOTE: Figure not to scale.

Figure 22. Plan View of the 18-in-outer Diameter DOE Standardized SNF Canister

The DOE SNF canister for the ATR SNF contains ten basket locations for each axial section. As shown in Figure 3, the basket compartments are delimited by horizontal and vertical plates. Three horizontal plates are placed symmetrically around the center of the stainless steel sleeve (separation distance between plates is 101.1 mm. The structure also contains three vertical plates: one extending outside the upper and bottom horizontal plates (centered on the vertical diameter of the sleeve) and two plates placed symmetrically between the horizontal plates (separation distance between plates is 136.5 mm).



NOTE: Figure not to scale.

Figure 3~~3~~. Cross-sectional Schematic of the Basket Structure and Sleeve

5.1.3 DHLW Glass Pour Canister

The SRS Defense Waste Processing Facility (DWPF) high-level radioactive waste canister, as shown in Figure 4, is a cylindrical Stainless Steel Type 304L shell. The outer diameter of the cylindrical shell is 61 cm and the nominal length is 3.00 m (BSC 2004g, Table 3-1). The nominal dimensions of the canister are used for the analyses and are summarized in Table 2.

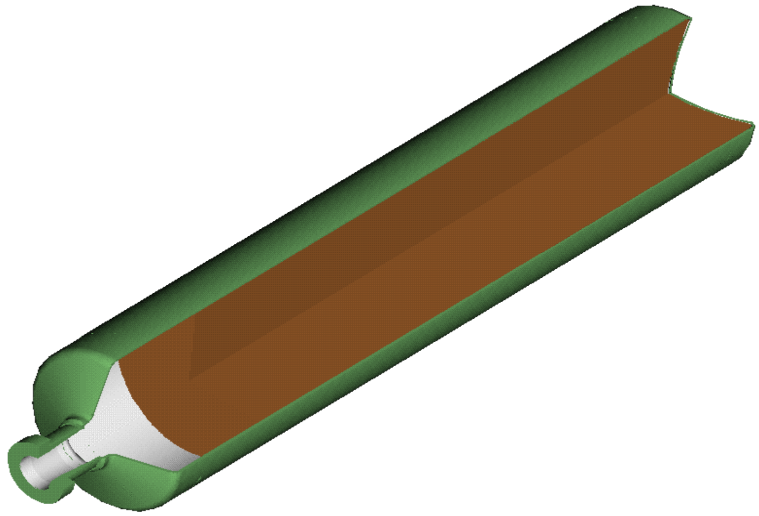


Figure 44. DHLW Glass Pour Canister

Table 22. Geometry and Material Specifications for DHLW Glass Pour Canisters

Material/Parameter	SRS 3-m (10-ft) Canister
Material	Stainless Steel Type 304L
Outer diameter	61.0 cm[a]
Wall thickness	9.525 mm[b]
Length	3.00m[a]

Sources: [a] BSC 2004g, Table 3-1.
[b] BSC 2001, Table 1.

5.1.4 Waste Package Description

The 5-DHLW/DOE SNF-short waste package contains five DHLW glass pour canisters spaced radially around an 18 in. DOE SNF canister. The waste package description used to generate the calculated results in this report is based on recent design changes (BSC 2004a, BSC 2004b, BSC 2004c and BSC 2004d) of the 5-DHLW/DOE SNF-short waste package LA design. The waste package barrier materials are typical of those used for commercial spent nuclear fuel waste containers. The inner vessel is composed of 50.8 mm (2 in.) of Stainless Steel Type 316 (also identified as SA-240) and serves for structural support and as a corrosion resistant material. The outer corrosion barrier is composed of 25.4 mm (1 in.) high-nickel alloy ASTM B 575 (Alloy 22) and serves as a corrosion resistant material. The outside diameter of the waste container is 2044.7 mm (80.5 in.) and the length of the inner cavity is 3013.202 mm (118.63 in.). The inner vessel lids are 50.8 mm (2 in.) thick, the middle lid is 12.7 mm (1/2 in.) thick, and the outer lid is 25.4 mm (1 in.) thick. There is a 30.2-mm (1.19 in.) thick closure lid gap between the inner vessel lid and middle lid and a 49.467 mm (1.9475 in.) gap between the middle lid and the outer lid.

The DOE SNF canister is placed in a 31.75-mm (1.25-in.) -thick carbon steel (ASTM A 516 Grade 70 or UNS K02700) support tube with a 565 mm (22.244 in.) nominal outer diameter. The support tube is connected to the inside wall of the waste package by web-like carbon steel (ASTM A 516 Grade 70 or UNS K02700) support plates that form five emplacement positions for the DHLW glass pour canisters equally spaced in angle about the center support tube. The support tube and plates are 3000.5 mm (118.13 in.) long, respectively. A summary of pertinent dimensions and materials is provided in Table 3.

Table 3~~3~~. 5-DHLW/DOE SNF-Short Waste Package Dimensions and Material Specifications

Component	Material	Parameter	Dimension (mm)
Outer corrosion barrier	High-Nickel Alloy (ASTM B 575)	Thickness	25.4
		Outer diameter	2,044.7
		Inner Diameter	1,993.9
Inner vessel	Stainless Steel Type 316 (SA-240)	Thickness	50.8
		Outer diameter	1,984.5
		Inner Diameter	1,882.9
		Inner length	3,013.2
Outer lid	High-Nickel Alloy (ASTM B 575)	Thickness	25.4
Middle lid	High-Nickel Alloy (ASTM B 575)	Thickness	12.7
Inner vessel lid	Stainless Steel Type 316 (SA-240)	Thickness	50.8
Gap between the middle lid and outer lid	Air	Thickness	30.2
Gap between the inner vessel lid and middle lid	Air	Thickness	49.467
Support tube	Carbon Steel (ASTM A 516 Grade 70)	Outer diameter	565.0
		Inner diameter	501.5
		Length	3,000.5
Inner bracket	Carbon Steel (ASTM A 516 Grade 70)	Thickness	25.4
		Length	3,000.5
Outer bracket	Carbon Steel (ASTM A 516 Grade 70)	Thickness	12.7
		Length	3,000.5

Sources: BSC 2004a, BSC 2004b, BSC 2004c, BSC 2004d, and BSC 2004g.

5.2 MATERIALS DESCRIPTION

Material nomenclature for the materials used throughout this document includes: UNS S31603 stainless steel (referred to as 316L stainless steel); UNS S31600 stainless steel (referred to as 316 stainless steel); UNS S30403 stainless steel (referred to as 304L stainless steel); UNS N06022 (referred to as Alloy 22); UNS K02700 carbon steel (referred to as A516 Grade 70 carbon steel), UNS N06464 low-carbon nickel-chromium-molybdenum-gadolinium alloy (referred to as Ni-Gd alloy), and UNS A96061 aluminum (referred to as Aluminum 6061).

Table 44. Composition and Density of Stainless Steel 304L

Element	Composition [a] (wt %)	Value Used (wt %)
C	0.030 (max)	0.030
Mn	2.000 (max)	2.000
P	0.045 (max)	0.045
S	0.030 (max)	0.030
Si	0.750 (max)	0.750
Cr	18-20	19.000
Ni	8-12	10.000
N	0.100 (max)	0.100
Fe	Balance	68.045
Density[b] = 7.94 g/cm^3		

Sources: [a] American Society of Mechanical Engineers (ASME) 2001 Section II, Part A, SA-240, Table 1.
[b] ASTM G 1-90, Table X1.1.

Table 55. Composition and Density of Stainless Steel 316L

Element	Composition [a] (wt %)	Value Used (wt %)
C	0.03 (max)	0.030
N	0.10 (max)	0.100
Si[b]	0.75 (max)	1.000
P	0.045 (max)	0.045
S	0.03 (max)	0.030
Cr	16-18	17.000
Mn	2.00 (max)	2.000
Ni	10-14	12.000
Mo	2-3	2.500
Fe	Balance	65.295
Density[c] = 7.98 g/cm^3		

Sources: [a] ASME 2001 Section II, Part A, SA-240, Table 1.
[b] Value used for Si is taken from ASTM A-276-03, Table 1.
[c] ASTM G 1-90, Table X1.1.

Table 66. Composition and Density of Stainless Steel 316

Element	Composition [a] (wt %)	Value Used (wt %)
C[b]	0.02 (max)	0.020
N[b]	0.08 (max)	0.080
Si	0.75 (max)	0.75
P	0.045 (max)	0.045
S	0.03 (max)	0.030
Cr	16-18	17.000
Mn	2.00 (max)	2.000
Ni	10-14	12.000
Mo	2-3	2.500
Fe	Balance	65.575
Density[c] = 7.98 g/cm^3		

Sources: [a] ASME 2001 Section II, Part A, SA-240, Table 1.
[b] Values for carbon and nitrogen taken from American Society of Metals (ASM) International (1987, p.931).
[c] ASTM G 1-90, Table X1.1.

Table 7~~7~~. Composition and Density of Alloy 22

Element	Composition (wt %)	Value Used (wt%)
C	0.015 (max)	0.015
Mn	0.50 (max)	0.500
Si	0.08 (max)	0.080
Cr	20-22.5	21.250
Mo	12.5-14.5	13.500
Co	2.50 (max)	2.500
W	2.5-3.5	3.000
V	0.35 (max)	0.350
Fe	2.0-6.0	4.000
P	0.02 (max)	0.020
S	0.02 (max)	0.020
Ni	Balance	54.765
Density = 8.69 g/cm^3		

DTN: MO0003RIB00071.000.

Table 8~~8~~. Composition and Density of Carbon Steel A516 Grade 70

Element	Composition[a] (wt %)	Value Used (wt %)
C	0.28	0.28
Mn	0.79-1.30	1.045
P	0.035 (max)	0.035
S	0.035 (max)	0.035
Si	0.13-0.45	0.29
Fe	Balance	98.315
Density[b] = 7.85 g/cm^3		

Sources: [a] ASTM A516/A 516M-01, Table 1.
[b] ASTM A20/ A 20M-99a, p.9.

Table 9~~9~~. Composition and Density of Ni-Gd Alloy

Element	Composition (wt %)	Value Used (wt%)
C	0.01 (max)	0.01
N	0.010 (max)	0.01
Si	0.08 (max)	0.08
P	0.005 (max)	0.005
S	0.005 (max)	0.005
Cr	14.5 - 17.1	15.8
Mn	0.5 (max)	0.5
Mo	13.1 - 16.0	14.55
Fe	1.00 (max)	1
Ni	Balance	64.035
Co	2.0 (max)	2
O	5.0000E-03	0.005
Gd	1.9 - 2.1	2
Density = 8.76 g/cm^3		

Source: ASTM B 932-04, pp. 1-2.

Table 10~~10~~. Composition and Density of Aluminum 6061

Element	Composition[a] (wt %)	Value Used (wt%)
Mg	0.8-1.2	1
Si	0.4 - 0.8	0.6
Fe	0.7 (max)	0.7
Cu	0.15-0.4	0.275
Cr	0.04-0.35	0.195
Mn	0.15 (max)	0.15
Zn[a]	0.25 (max)	0.25
Ti	0.15 (max)	0.15
Al	Balance	96.68
Density[b] = 2.7065 g/cm^3		

Source: [a] ASM International 1990, p. 102.
[b] ASTM G 1-90, Table X1 indicates 2.7 g/cm^3; ASME 2001, Section II, Table NF-2 indicates a converted value from 0.098 lb/in^3 of 2.713 g/cm^3; there fore the midpoint was used.

NOTE: [a] See Assumption 3.6.

Table 11~~11~~. Composition and Density of Savannah River Site DHLW Glass

Element / Isotope	Composition[a] (wt %)	Element / Isotope	Composition[a] (wt %)
O	4.4770E+01	Ni	7.3490E-01
U-234	3.2794E-04	Pb	6.0961E-02
U-235	4.3514E-03	Si	2.1888E+01
U-236	1.0415E-03	Th	1.8559E-01
U-238	1.8666E+00	Ti	5.9676E-01
Pu-238	5.1819E-03	Zn[d]	6.4636E-02
Pu-239	1.2412E-02	B-10	5.9176E-01
Pu-240	2.2773E-03	B-11	2.6189E+00
Pu-241	9.6857E-04	Li-6	9.5955E-02
Pu-242	1.9168E-04	Li-7	1.3804E+00
Cs-133	4.0948E-02	F	3.1852E-02
Cs-135	5.1615E-03	Cu	1.5264E-01
Ba-137[c]	1.1267E-01	Fe	7.3907E+00
Al	2.3318E+00	K	2.9887E+00
S	1.2945E-01	Mg	8.2475E-01
Ca	6.6188E-01	Mn	1.5577E+00
P	1.4059E-02	Na	8.6284E+00
Cr	8.2567E-02	Cl	1.1591E-01
Ag	5.0282E-02		
Density[b] at 25 °C = 2.85 g/cm^3			

Sources: [a] CRWMS M&O 1999b, Attachment I, p. I-7.
[b] Stout and Leider 1991, p. 2.2.1.1-4.

NOTES: [c] See Assumption 3.2.
[d] See Assumption 3.6.

Table 12~~12~~. Pre-Breach Clay Composition

Element	Mass of Element after 15072 Years of Emplacement (kg)
O	5.374E+03
Al	2.084E+02
Ba	1.354E+01
Ca	8.573E+01
F	7.425E-02
Fe	5.292E+03
H	4.020E+01
C	3.183E+01
P	2.186E+00
K	8.778E+01
Mg	7.589E+01
Mn	6.030E+01
Na	1.120E+02
Ni	1.103E+02
Si	2.030E+03
Density (g/cm^3)	3.68E+00

Source: BSC (2003, Table 26).

Table 13~~13~~. Composition and Density of Dry Tuff

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

Sources: [a] DTN: GS000308313211.001, file 'zz_sep_254139.txt', row 41.
[b] The average of rock grain densities of three samples in Tpt flow unit (subzones 'pmn', 'pll', and 'pln') given in DTN: MO0109HYMXPROP.001, file 'DATAQ.xls', rows 1333, 1345, and 1739.

The tuff rock porosity used in this calculation is 0.11766667. Porosity is the arithmetic average of 3 values that come from DTN: LB990501233129.001, Table 1, 'MAT PROP R00A.XLS,' rows for geologic layers TMN, TLL, and TM2. An alternate tuff composition calculated in BSC (2001, Table 8) was also used in some cases to investigate the effect of varying the boundary conditions.

Table 1414. Post-Breach Clay Composition

Element	Mass of Element after 20,400 Years of Emplacement (kg)
O	2.583E+03
Al	1.401E+02
Ba	5.816E-02
Cr	3.251E-07
Fe	5.217E+03
Gd	1.893E-01
H	1.472E+01
P	1.939E+00
K	3.079E-02
Mn	8.256E+01
Mo	2.278E+00
S	6.4087E-02
Si	3.796E+01
Ti	1.571E-01
U	2.165E+01
Total	8.101E+03
Density (g/cm^3)	4.97

Source: BSC (2004f, Table 6-2).

NOTE: Calculated in spreadsheet “clay-composition.xls”, Attachment I.

For the calculations involving degradation of Aluminum to gibbsite and Uranium to schoepite, the following values for the density of minerals have been used: gibbsite – 2.441 g/cm^3 (DTN: MO0009THRMODYN.001) and schoepite – 4.8738 g/cm^3 (DTN: MO0009THRMODYN.001). The density of anhydrous gadolinium phosphate used in this calculation was estimated to be 5 g/cm^3, which is the average density reported in Roberts et al. (1974, p.413) for monazite (anhydrous rare earth phosphate).

5.3 FORMULAS

The basic equation used to calculate the number density values for materials composed of one or more elements/isotopes is shown below. It is used in the spreadsheet included in Attachment I, and used in the cases described throughout Section 5:

$$N_i = (m_i / m) * \rho * N_a / M_i = (V_i / V) * \rho_i * N_a / M_i$$

where: N_i is the number density in atoms/cm^3 of the i^{th} element/isotope (note that the values of the number densities are expressed in the spreadsheets from Attachment I in atoms/(barn*cm) by multiplying N_i with 10^{-24} cm^2/barn)

m_i is the mass in grams of the i^{th} element/isotope in the material

m is the mass in grams of the material; note that $m = \sum m_i$

N_a is the Avogadro’s number ($6.022*10^{23}$ atoms/mole [Parrington et al. 1996, p. 59])

M_i is the atomic mass in g/mole of the i^{th} element/isotope
M is the atomic mass in g/mole of the material
V_i is the volume in cm^3 of the of the i^{th} element/isotope in the material
V is the volume in cm^3; note that $V = \sum V_i$
ρ_i is the density of the i^{th} element/isotope (g/cm^3)
ρ is the density of the material (g/cm^3); note that $\rho = \sum \rho_i * (V_i / V)$

Volumes of cylinder segments (volume = area of circle segment × length of the cylinder) are also calculated throughout Attachment I. These calculations are based on the equation for the area of a segment of a circle shown below (Beyer 1987, p.125):

$$\text{Area of a segment of a circle} = \left(R^2 \cos^{-1}\left(\frac{R-h}{R}\right) - (R-h)\sqrt{2Rh - h^2} \right)$$

where: R is the cylinder radius,
h is the height of the segment.

5.4 DESCRIPTION OF THE INTACT MODE CONFIGURATIONS

The intact mode configurations of the waste package containing ATR SNF include configurations that represent the waste package as being breached allowing inflow of water. The internal components of the waste package are considered non-degraded (intact). Modeling of the end structure of the DOE SNF canister treats both the impact plate and the dished head (see Figure 2) as a single piece that serves as an end reflector. The curved gap between the two end pieces is conservatively modeled as filled with carbon steel. Unless noted otherwise, the unoccupied spaces inside the DOE SNF canister and waste package are modeled as filled with water. Variations of the intact configurations are examined to identify the configuration that results in the highest calculated k_{eff} value within the range of possible conditions.

Figure 5 presents a cross sectional view of the baseline intact configuration modeled with MCNP. The fuel is settled in gravitationally stable positions in each compartment. Since the ATR fuel assemblies can be loaded with different orientations relative to each compartment, a study of the influence of the fuel elements positions on k_{eff} has been performed.

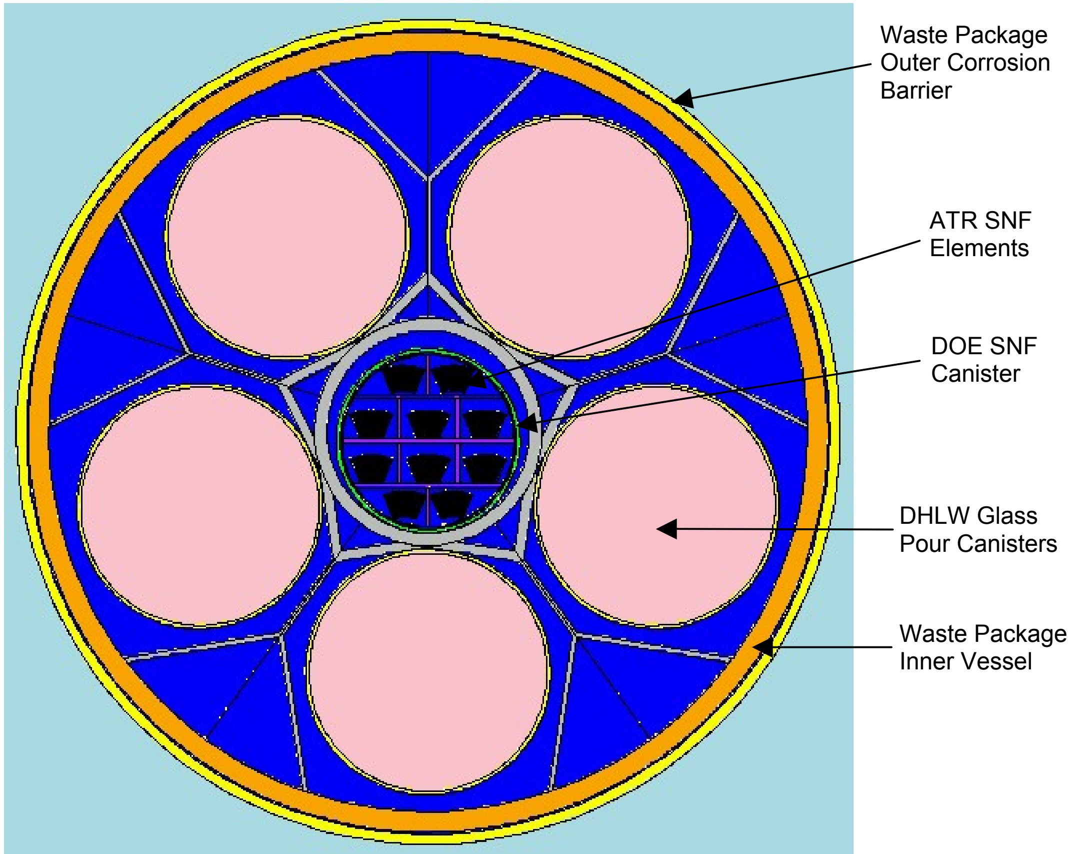
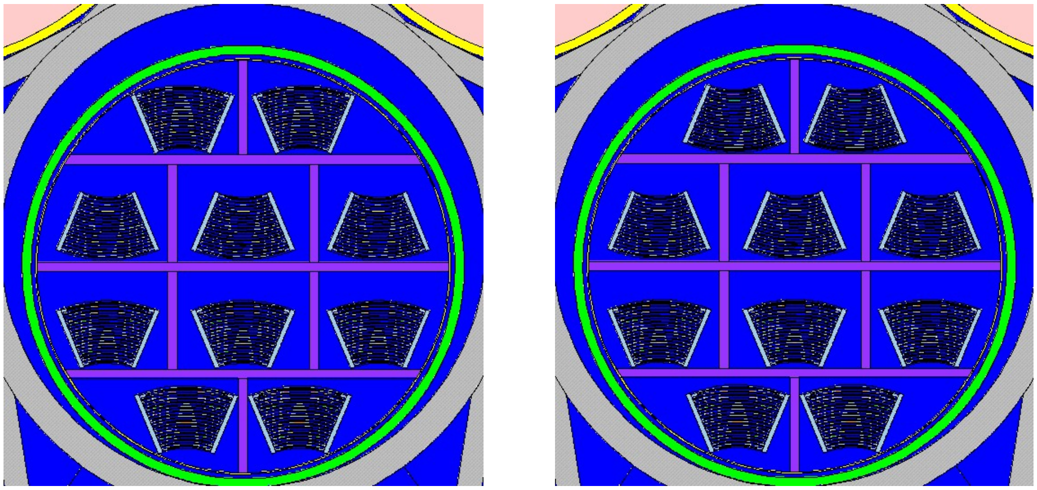


Figure 5~~5~~. Cross-sectional View of the Baseline Intact Configuration

Additional cases have evaluated the influence of varying various geometrical and material parameters from a base case configuration. The most important parameters investigated are: moderation (variation of water density, filling with water the porosity inside fuel meat), reflection and absorption of neutrons (partial flooding of the waste package, gravitationally stable arrangements of fuel elements, rotations of fuel elements, rotation of the DOE SNF canister, waste package boundary conditions). Finally, the effect of coupling of the most important variations is investigated to identify the bounding cases for the intact configurations. Figure 6 presents two possible arrangements of the ATR fuel elements inside the DOE SNF canister that have been investigated in the present calculation.



a) case: "atr_int_1b-s" b) case: "atr_int_1c-s"

Figure 66. Various Possible Arrangements of ATR SNF Elements inside DOE SNF Canister

A separate case was also run to analyze the effectiveness of the design solution regarding introduction of additional Gd as a neutron absorber distributed with a moderator displacer (Al shot).

5.5 DESCRIPTION OF THE DEGRADED MODE CONFIGURATIONS

The criticality calculations conducted for the degraded cases are discussed in this section. The configurations have been obtained by applying the general degradation scenarios postulated in Yucca Mountain Site Characterization Project (YMP) 2003 (Section 3). General descriptions of some of the postulated generic degraded configurations for the waste package are presented in CRWMS M&O 1999a (pp.27-37). The degradation scenarios postulate water breaching the waste package and pooling inside. The configurations resulting from water flowing through the waste package have a higher potential to leach the fissile material (flushed out of the waste package) than the configurations with water pooled inside the waste packages. Loss of fissile material results in a lower potential for internal criticality. The configurations presented below are considered to conservatively encompass the possible configurations resulting from the flow-through scenarios described in YMP 2003 by retaining all fissile material in the waste package.

The degraded configurations are analyzed as a sequence of progressing degradation rather than an immediate transition from intact to completely degraded. These degraded configurations are expected to be more reactive than the intact configurations. Water is always considered present and is responsible for the degradation analyzed here. The details of this process depend on degradation rates and how the water enters the waste package and interacts with its contents.

A particular aspect that is characteristic for the Al clad fuel is the fact that the fuel elements will degrade in a short period of time once the water penetrates the DOE SNF canister due to the higher rates of corrosion (BSC 2004f, Table 5-2). This makes the generic degradation scenarios in which the fuel elements degrade after the internal components of the waste package not directly applicable to the waste package containing ATR SNF. The only scenario that allows preservation of relatively intact fuel for a longer period of time is a late breaching of the DOE SNF canister. After the DOE SNF canister is breached, the degradation of the spent fuel is postulated to occur quickly and was considered in defining the configurations investigated in the present calculation.

By analyzing the description of the general degradation scenarios given in YMP 2003 (Section 3), the most appropriate degradation scenario for the waste package containing ATR SNF is IP-1 (spent fuel degrades before the internal components of the waste package). Two different branches for this scenario can be postulated, based on the timing of the DOE SNF canister breach. They include a) breaching of the DOE SNF canister occurs immediately after breaching of the waste package; and b) breaching of the DOE SNF canister occurs after the degradation of the internals of the waste package.

5.5.1 Contents of the DOE SNF Canister Degrades

If the DOE SNF canister is breached shortly after the breach and flooding of the waste package, the ATR SNF fuel will start to degrade in place. The configurations can include partially degraded to completely degraded fuel placed in the basket compartments of the DOE SNF canister. The Al was assumed (Assumption 3.1) to degraded to gibbsite [$Al(OH)_3$] and uranium to schoepite [$(UO_2)_8O_2(OH)_{12} \cdot 12(H_2O)$]. The degraded materials expand and quickly fill the available space inside the canister. The basket material containing Gd does not degrade and stays in place. Figure 7 presents a configuration with partial degradation of the fuel (only Al clad degrades to gibbsite) and the spacing between fuel sectors are increased due to expansion. The results are presented in Section 6.1.

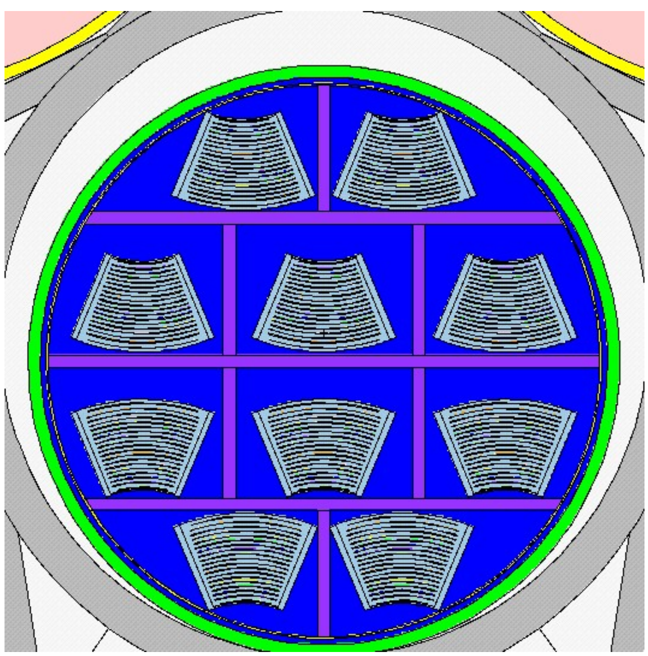


Figure 77. Cross-sectional View of the Partially Degraded Fuel inside Intact DOE SNF Canister

Figure 8 below presents a subsequent stage of degradation that includes complete degradation of the fuel element in each compartment. The degradation products are considered homogeneously mixed and formed with various values for internal porosity. The expansion of the degradation products is limited by the space available in each compartment. A separate configuration allow expansion of the degradation material in all space available in the DOE SNF canister, including the space occupied by the inner sleeve and the gap between the sleeve and DOE SNF canister.

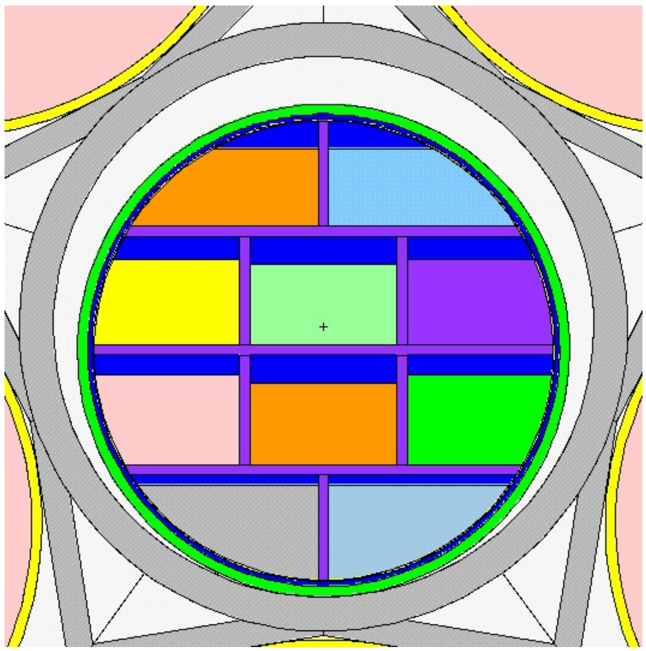


Figure 88. Cross-sectional View of the Intact DOE SNF Canister with Totally Degraded ATR Fuel

Various compositions and arrangements of the degraded materials inside the DOE SNF canister have been analyzed. The rest of the waste package was considered to be intact. The results of the analyzed configurations are presented in Section 6.2.

5.5.2 Internal Components of the Waste Package Outside DOE SNF Canister Degrade

The second branch of the above mentioned scenario postulates that the DOE SNF canister will breach long after the breaching of the waste package. This will allow the waste package internals to degrade and form a clay-like material (named "pre-breach" clay in the present analysis). At some point in time the DOE SNF canister will breach allowing internal fuel to degrade as presented in the previous scenario. The "pre-breach clay" composition is not dependent on the DOE SNF canister content and is obtained by running a 2 stage geochemistry calculation for a short waste package and selecting the results at the end of the first stage (DOE SNF canister internals not exposed to degradation). For the purpose of this calculation the "pre-breach clay" composition is taken from BSC (2001, Table 26).

The configurations analyzed in this report include the DOE SNF canister placed in various positions inside the clayey material (mixed with various fractions of water). The spent nuclear fuel inside the DOE SNF canister can be intact or in various stages of degradation. Typically, the most reactive arrangements of the intact and degraded spent fuel identified in the previous analyses are considered. Figure 9 presents an example of a configuration in this category.

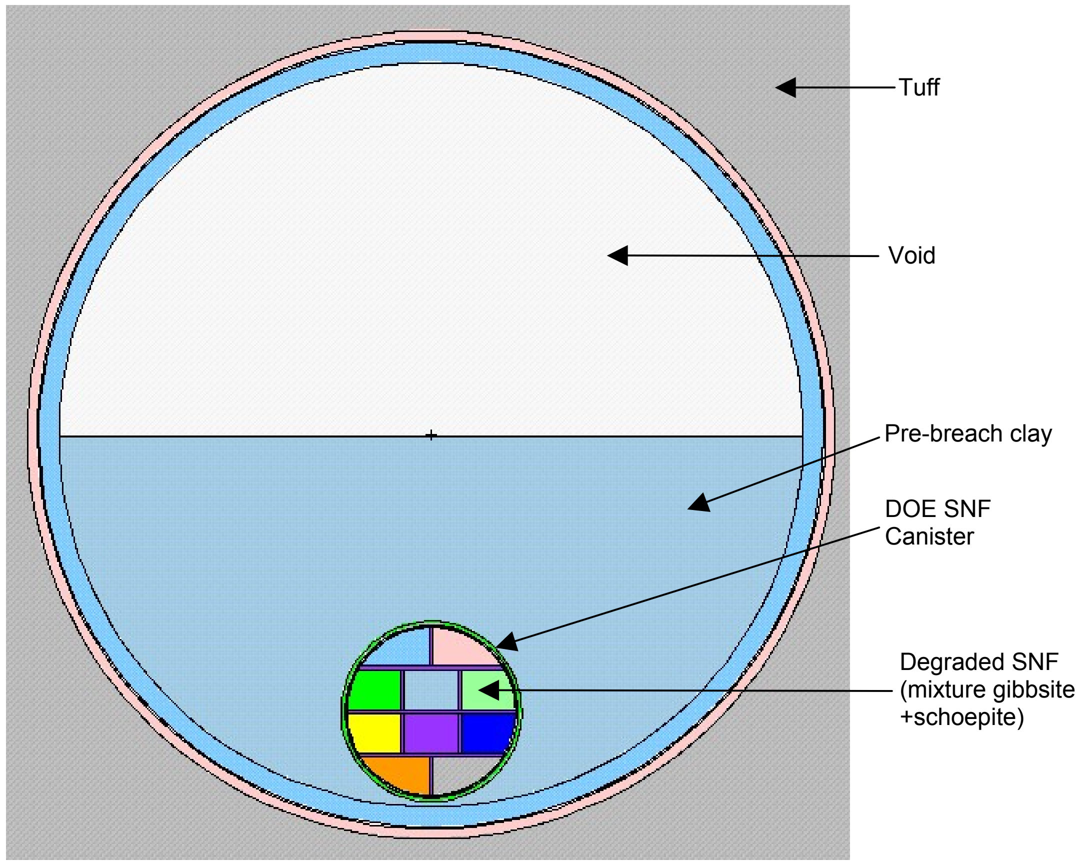


Figure 9~~9~~. Cross-sectional View of the DOE SNF Canister Containing Degraded SNF Surrounded by Pre-breach Clay

5.5.3 All Components of the Waste Package Have Degraded

The next stage of degradation involves configurations in which the content of the DOE SNF canister is mixed with the degradation products obtained from the degradation of the waste package internals. This class of configurations (class 2 in reference YMP [2003, p. 3-14]) can be obtained at the end of IP-1 scenario or by applying any IP-2 scenario (all constituents degrade in the same time). Geochemistry calculations have produced compositions for the clay-like materials that can be obtained by applying both scenarios. For the purpose of the present calculation, a scenario that postulates degradation of the DOE SNF canister after degradation of all other waste package internals has been investigated. This scenario preserves all fissile material that is finally settled in a layer at the bottom of the waste package. The calculation considered a mixture of schoepite, gibbsite and gadolinium phosphate placed in a layer at the bottom of the waste package. The layer is covered with a mixture of pre-breach clay and water. All other components of the DOE SNF canister are neglected (including basket structure containing Gd). This scenario also encompasses configurations that can result when the degraded fuel is displaced from the DOE SNF canister and accumulates at the bottom of the waste package. The composition of the layers is varied considering that various fractions of the degraded materials are leached from the waste package. A typical configuration is presented in Figure 10.

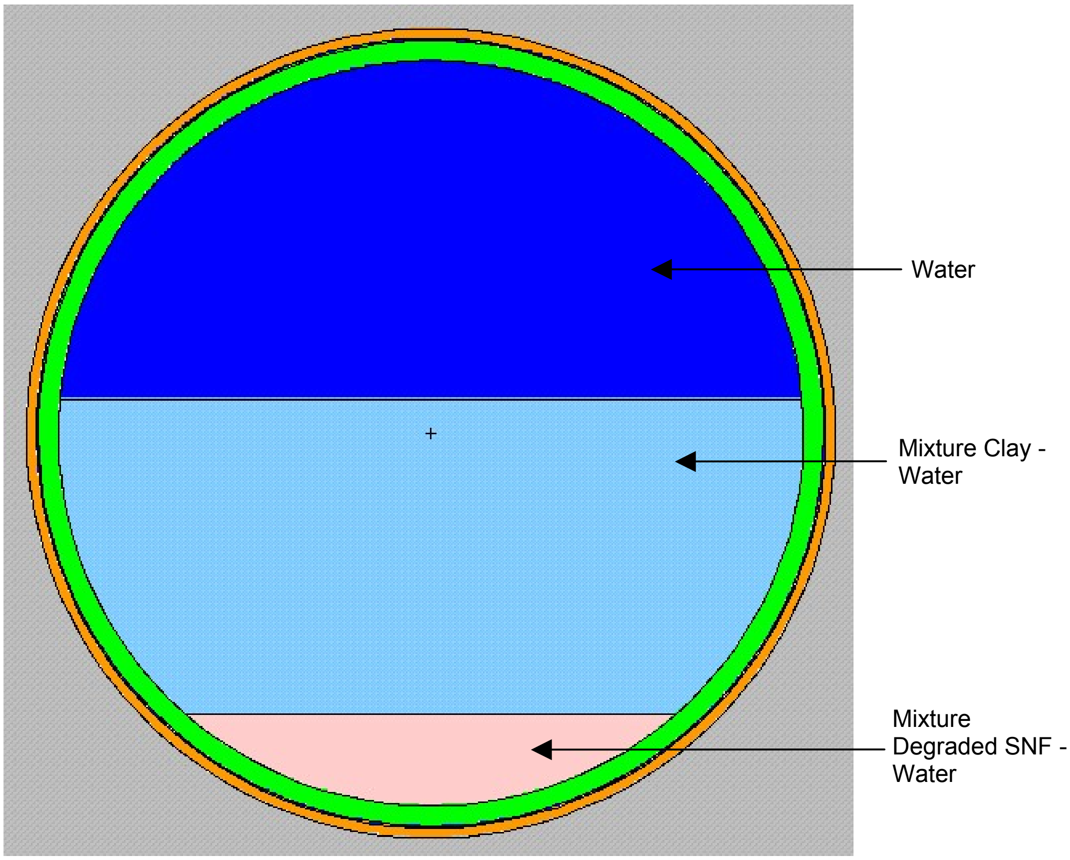


Figure 10~~10~~. Cross-sectional View of the Waste Package Containing All Components Degraded Settled in Layers

6. RESULTS

This section documents the results for the intact and degraded configurations of the ATR SNF waste package evaluated for criticality. The k_{eff} results represent the average collision, absorption, and track length estimator from the MCNP calculations. The standard deviation (σ) represents the standard deviation of k_{eff} about the average combined collision, absorption, and track length estimate due to Monte Carlo calculation statistics. The average energy of a neutron causing fission (AENCF) is the energy per source particle lost to fission divided by the weight per source neutron lost to fission from the "problem summary section" of the MCNP output. The MCNP input and output files developed for this calculation are included in ASCII format in Attachment I. The H/X ratio presented in the following tables is the ratio of mole of hydrogen to mole of fissile materials (^{235}U).

For all the cases, no credit is taken for the fuel burnup, i.e., fuel is considered to be fresh (non-irradiated) and also no credit is taken for the initial content of neutron absorber (boron) in the fresh fuel elements (Assumption 3.3).

6.1 RESULTS FOR INTACT MODE CONFIGURATIONS

Table 15 presents the results of the MCNP calculations for the configurations described in Section 5.4. Table 15 gives the k_{eff} of the configurations containing intact ATR fuel elements placed in various positions inside the basket structure (Figures 5 and 6).

Table 15~~15~~. Calculated Results for Intact Cases

Case (MCNP Input File)	Description	k_{eff}	σ	$k_{eff}+2\sigma$	AENCF (MeV)	H/X[a]
atr-int-1a-s	Initial base case. Fuel elements placed in gravitationally stable positions in each compartment. DOE SNF canister is settled in the support tube. Fuel meat has 11 vol% inner porosity (void). All other available spaces in the waste package are filled with full density water. Waste package is surrounded by dry tuff (BSC 2001, Table 8). See Figure 5.	0.6243	0.0008	0.6259	0.0271	85.6
Effect of fuel porosity						
atr-int-2a-s	Similar to base case, but inner porosity in fuel meat is only 3 vol% (void)	0.6243	0.0008	0.6259	0.0272	85.6
Effect of DOE SNF canister position in the support tube						
atr-int-3a-s	Similar to base case, but DOE SNF canister is centered in the support tube of the waste package	0.6176	0.0008	0.6192	0.0277	85.6
Effect of fuel element position within the basket compartments						
atr_int_1b-s	Similar to base case, but fuel elements in middle row are rotated with 180 degrees (see Figure 6)	0.6250	0.0008	0.6266	0.0275	85.6
atr_int_1c-s	Similar to base case, but upper half of the basket has all fuel elements rotated with 180 degrees (see Figure 6)	0.6250	0.0008	0.6266	0.0274	85.6
atr_int_1a-s-rot	Similar to base case, but basket rotated with 90 degrees	0.6215	0.0008	0.6231	0.0273	85.6
atr_int_1a-s-rot-s	Similar to above case, but fuel elements are settled in each compartment in gravitationally stable positions	0.6240	0.0008	0.6256	0.0279	85.6
Effect of partial flooding in the waste package						
atr_int_1a-s-dry	Similar to base case, but no water in the waste package	0.0696	0.0001	0.0698	0.5773	0

Case (MCNP Input File)	Description	k_{eff}	σ	k_{eff}+2σ	AENCF (MeV)	H/X[a]
atr_int_1a-s-pf	Similar to base case, but only DOE SNF canister is flooded	0.6421	0.0008	0.6437	0.0266	85.6
atr_int_1a-s-pf-chlw	Similar to above case, but DHLW canister are repositioned in a gravitationally stable geometry	0.6368	0.0008	0.6384	0.0266	85.6
Effect of reflection outside waste package						
atr_int_1a-s-refl	Similar to base case, but the waste package has reflective boundary conditions	0.6243	0.0008	0.6259	0.0271	85.6
atr_int_1a-s-tf	Similar to base case, but the waste package is surrounded by dry tuff with composition given in Table 13	0.6243	0.0008	0.6259	0.0271	85.6
Effect of water density						
atr_int_1a-s-w070	Similar to base case, but water density is 0.75 g/cm^3	0.5493	0.0008	0.5509	0.0352	59.9
atr_int_1a-s-w080	Similar to base case, but water density is 0.80 g/cm^3	0.5788	0.0008	0.5804	0.0317	68.5
atr_int_1a-s-w090	Similar to base case, but water density is 0.90 g/cm^3	0.6028	0.0008	0.6044	0.0286	77.0
atr_int_1a-s-w095	Similar to base case, but water density is 0.95 g/cm^3	0.6139	0.0008	0.6155	0.0278	81.3
Effect of water filling the void space inside fuel meat						
atr_int_1a-s-04vfw	Similar to base case, but water fills partially the porosity inside the fuel meat (36% of the porosity is filled with full density water)	0.6261	0.0008	0.6277	0.0264	86.4
atr_int_1a-s-11vfw	Similar to base, but all inner porosity is filled with full density water	0.6306	0.0009	0.6324	0.0260	87.8
Combined effects						
atr_int_1a-s-comb	Similar to case "atr_int_1a-s" with partial flooding (only DOE SNF canister) and fuel porosity filled with water	0.6474	0.0008	0.6490	0.0259	87.8
atr_int_1a-s-comb-tf	Similar to above case, but the waste package is surrounded by dry tuff with composition given in Table 13	0.6458	0.0009	0.6476	0.0261	87.8
atr_int_1a-s-comb-r	Similar to above case, but the waste package has reflective boundary conditions at outer surfaces	0.6484	0.0008	0.6500	0.0259	87.8
Effect of neutron absorber						
atr_int_1a-s-ngd	Similar to base case, but no Gd in basket plates	0.7150	0.0008	0.7166	0.0240	85.6
atr_int_1a-s-comb-Algd01shot	Similar to case "atr_int_1a-s-comb," but additional Gd is introduced with Al fill material that occupies all spaces around fuel elements in each compartment. Gd content is 0.1 wt% in Al fill material (mixture of Al shot and gadolinium phosphate).	0.4394	0.0007	0.4408	0.0433	87.8
atr_int_1a-s-comb-Algd01shot-tf	Similar to above case, but the waste package is surrounded by dry tuff with composition given in Table 13	0.4386	0.0007	0.4408	0.0440	87.8

NOTE: [a] Calculated based on volumes in the fuel element.

The results show that the parameters investigated have small influences on the k_{eff} of the intact system. Repositioning of various components in gravitationally stable positions, positioning of the fuel inside the canister or rotation of the DOE SNF canister have almost insignificant effects.

The flooded configurations are undermoderated as can be seen from the results presenting the influence of the moderator density. The completely dry configuration has a very low k_{eff}, so there is no potential for fast criticality.

The most significant effect on the reactivity of the system is given by changing the boundary conditions outside the DOE SNF canister (partial flooding) and by removing or adding neutron absorber (Gd). The system in its intact state has the values of k_{eff} for all investigated configurations well below the interim criticality limit of 0.93.

6.2 RESULTS FOR DEGRADED MODE CONFIGURATIONS

6.2.1 Results for Configurations Containing Partially/Totally Degraded Fuel Inside DOE SNF Canister

This section gives the results of the calculations described in Section 5.5.1. The water enters the DOE SNF canister and contributes first to the degradation of the Al cladding. The Al clad degrades to gibbsite (Assumption 3.1) producing a volume expansion of approx. 3.2 (spreadsheet “atr_degraded-1.xls”, Attachment I) that has the potential to increase the distance between the fuel plates. This aspect was investigated by running a number of cases with increased spacing between the sectors containing fuel meat. The space between sectors was filled with gibbsite formed with various void fractions. Water of full density fills all available space (including void in gibbsite). The Aluminum not degraded is conservatively neglected in these calculations. The fuel meat is considered non-degraded and preserves the initial geometry. The DOE SNF canister outer shell is considered intact and filled with water and the rest of the waste package is considered intact and dry (Figure 7). The input files have been constructed starting from the intact case “atr_int_1a-s-comb” presented in Table 15 in which the upper five assemblies are rotated with 180 degrees (Figure 6 and 7) to allow more space for volumetric expansion. The results are summarized in the following table (Table 16).

Table 1616. Results for Configurations with Partial Degradation of ATR SNF Inside DOE SNF Canister

Case (MCNP Input File)	Description	Void fraction in gibbsite	k_{eff}	σ	$k_{eff}+2\sigma$	AENCF (MeV)	H/X[a]
atr_pdeg-n30	Similar to case “atr_int-1a-s-comb,” but Al cladding and the space between fuel plates is replaced with gibbsite containing 30 vol% porosity filled with water; the five upper assemblies have been rotated with 180 degrees (see Figure 7)	0.3	0.7041	0.0009	0.7059	0.0223	110
atr_pdeg-n40	Similar to above case, but void fraction in gibbsite is 0.4 (filled with water)	0.4	0.7069	0.0009	0.7087	0.0214	111
atr_pdeg-n50	Similar to above case, but void fraction in gibbsite is 0.5 (filled with water)	0.5	0.7112	0.0009	0.7130	0.0222	113
atr_pdeg-n30-ext01	Similar to case “atr_pdeg-n30” above, but distance between fuel sectors is increased by 0.1 mm	0.3	0.7181	0.0008	0.7197	0.0216	114
atr_pdeg-n40-ext01	Similar to case “atr_pdeg-n40,” but distance between fuel sectors is increased by 0.1 mm	0.4	0.7183	0.0008	0.7196	0.0216	116
atr_pdeg-n50-ext01	Similar to case “atr_pdeg-n50,” but distance between fuel sectors is increased by 0.1 mm	0.5	0.7231	0.0008	0.7247	0.0213	118
atr_pdeg-n30-ext03	Similar to case “atr_pdeg-n30,” but distance between fuel sectors is increased by 0.3 mm	0.3	0.7328	0.0009	0.7346	0.0205	123

Case (MCNP Input File)	Description	Void fraction in gibbsite	k_{eff}	σ	$k_{eff}+2\sigma$	AENCF (MeV)	H/X[a]
atr_pdeg-n40-ext03	Similar to case “atr_pdeg-n40,” but distance between fuel sectors is increased by 0.3 mm	0.4	0.7358	0.0008	0.7374	0.0205	126
atr_pdeg-n50-ext03	Similar to case “atr_pdeg-n50,” but distance between fuel sectors is increased by 0.3 mm	0.5	0.7374	0.0009	0.7392	0.0204	128

NOTE: [a] Calculated based on the volume of fuel element.

The tendency that can be observed in the above results is that k_{eff} of the system is slowly increasing with degradation of the cladding and expansion of the degraded materials. It is expected that this tendency will continue once the fuel meat starts to degrade. For the purpose of this calculation, uranium is considered to degrade to schoepite (Assumption 3.1), which is accompanied by a volumetric expansion of approximately 5.35 (spreadsheet “atr_degraded-1.xls”, Attachment I). Since the expansion of the degraded fuel as modeled in the above cases is limited by the dimensions of the compartments, the complete degradation of the fuel is treated below considering a homogeneous mixing of the degraded components and uniform filling of the basket compartments (Figure 8).

The results of the MCNP cases describing the next stage of degradation (complete degradation of the fuel elements) are presented in Table 17. As mentioned in Assumption 3.5, the degradation products are assumed to form with void that is typically filled with water. The atomic densities of the mixtures and the geometry calculations supporting these cases are included in spreadsheet “atr_degraded-1.xls” from Attachment I. The rest of the waste package is considered intact. An example of the configuration analyzed is shown in Figure 8.

Table 17~~17~~. Results for Configurations with Complete Degradation of ATR SNF Inside DOE SNF Canister

Case (MCNP Input File)	Description	Void fraction in mixtures	k_{eff}	σ	$k_{eff}+2\sigma$	AENCF (MeV)	H/X
atr_pdeg_tot00	Fuel elements completely degraded to mixture of schoepite and gibbsite; mixture with no voids; water above fuel in each compartment and in DOE SNF canister; rest of the waste package is dry	0.0	0.8242	0.0008	0.8258	0.0133	182
atr_pdeg_tot00-nw	Similar to above case, but no water in DOE canister	0	0.8422	0.0008	0.8438	0.0160	182
atr_pdeg_tot00-f	Similar to above case, but waste package and DOE SNF canister are fully flooded	0	0.8064	0.0008	0.8080	0.0133	182
atr_pdeg_tot_30void	Similar to case “atr_pdeg_tot00,” but void fraction is 0.3 in mixture; water present above fuel mixture and in DOE SNF canister only	0.3	0.8270	0.0008	0.8286	0.0139	182
atr_pdeg_tot_30void-nw	Similar to above case, but no water above mixture and in DOE SNF canister	0.3	0.8049	0.0008	0.8065	0.0161	182
atr_pdeg_tot_30void-f	Similar to above case DOE canister and waste package are fully flooded	0.3	0.7982	0.0008	0.7998	0.0142	182

Case (MCNP Input File)	Description	Void fraction in mixtures	k_{eff}	σ	k_{eff}+2σ	AENCF (MeV)	H/X
atr_pdeg_tot_30wet	Similar with case "atr_deg_tot_30void" but water fills void in mixtures	0.3	0.9521	0.0008	0.9537	0.0097	276
atr_pdeg_tot_30wet-nw	Similar to above case, but the water is removed from all spaces in DOE SNF canister except void in mixture	0.3	0.9534	0.0008	0.9550	0.0107	276
atr_pdeg_tot_30wet-f	Similar to above case, but water fills all available spaces in the waste package	0.3	0.9300	0.0008	0.9316	0.0100	276
atr_pdeg_tot_3040void	Similar to case "atr_pdeg_tot_30void" but mixture in six central compartments forms with 40 vol% void fraction; water in DOE SNF canister only	0.3 and 0.4	0.8207	0.0008	0.8223	0.0147	182
atr_pdeg_tot_3040wet	Similar to above case, but water fills the void in the mixture	0.3 and 0.4	0.9879	0.0008	0.9895	0.0091	276-328
atr_pdeg_tot_fill_wet	Degraded mixtures are filling all available space in each compartment; void and spaces in DOE SNF canister are filled with water; the rest of the waste package is dry	0.40 to 0.48	0.9961	0.0008	0.9977	0.0088	325-384
atr_pdeg_tot_fill_wet-f	Similar to above case, but waste package is completely flooded	0.40 to 0.48	0.9758	0.0008	0.9774	0.0088	325-384
atr_pdeg_tot_all_wet	Similar case "atr_pdeg_tot_fill"_wet" but mixture in compartments bordered by the inner sleeve is allowed to fill all space inside DOE SNF canister. Sleeve is neglected; mixture is homogenized for all these compartments; waste package outside DOE SNF canister is dry	0.46 to 0.48	0.9977	0.0008	0.9993	0.0083	369-384
atr_pdeg_tot_all_wet-f	Similar to above case, but waste package is completely flooded	0.46 to 0.48	0.9747	0.0008	0.9763	0.0082	369-384

The results show that by degrading the fuel elements to a mixture of schoepite, gibbsite and void filled with water, the reactivity of the system is increasing significantly (strongly dependent on the ratio $H/^{235}U$). All configurations investigated of the system are undermoderated and are affected by reflection from the remaining waste package components. The highest k_{eff} +2σ (0.9993) is obtained for a system that has a degraded mixture that completely fills the space inside the DOE canister and is surrounded by a dry intact geometry of the waste package.

Since the value of the highest k_{eff} +2σ is above the interim criticality limit of 0.93, an additional design solution aiming to reduce the potential for criticality of the degraded configurations has been investigated. The design solution consists of utilizing a moderator displacer mixed with a neutron absorber. A mixture of Aluminum shot with gadolinium phosphate is evaluated, solution that has been previously proposed for disposal of other DOE SNF (CRWMS M&O 2000). A special spreadsheet has been created to calculate the corresponding atomic densities for both non-degraded and degraded configurations (spreadsheet "atr_degraded-2.xls" from Attachment I). In the following table (Table 18), the most reactive case from Table 17 has been modified to include the degraded fill material and additional neutron absorber. Variations of this case include complete or partial degradation of the Aluminum shot and fuel. Conservative assumptions regarding the possible loss of the degraded materials have also been investigated.

Table 18~~18~~. Results for Configurations with Additional Neutron Absorber

Case (MCNP Input File)	Description	Void fraction in mixtures	k_{eff}	σ	$k_{eff}+2\sigma$	AENCF (MeV)	H/X
0.1 wt% Gd as GdPO4 in Al fill material (Al shot)							
atr_all_gd01-al	Case with a geometry identical with case "atr_pdeg_tot_all" from Table 17. Degraded materials in compartments contain a homogeneous mixture of degraded fuel and aluminum shot with 0.1 wt% Gd as $GdPO_4$. The Al is degraded to gibbsite that fills all space available. Non–degraded Aluminum is also uniformly distributed in mixture.	0.0	0.5070	0.0005	0.5080	0.0226	199 -211
atr_all_gd01-g100	Similar to above case, but gibbsite is filling all available space (non-degraded Aluminum is neglected)	0	0.5535	0.0005	0.5545	0.0151	340 -353
atr_all_gd01-g90	Similar to above case, but gibbsite is formed with 10 vol% void filled with water	0.1 (in gibbsite only)	0.5545	0.0005	0.5555	0.0147	346 -359
atr_all_gd01-g70	Similar to above case, but gibbsite is formed with 30 vol% void filled with water	0.3	0.5550	0.0005	0.5560	0.0149	359 -371
atr_all_gd01-g60	Similar to above case, but gibbsite is formed with 40 vol% void filled with water	0.4	0.5565	0.0005	0.5575	0.0150	365 -378
atr_all_gd01-g60-tf	Similar to above case, but the waste package is surrounded by dry tuff with composition given in Table 13	0.4	0.5572	0.0005	0.5582	0.0152	365 -378
atr_all_gd01-g50	Similar to above case, but gibbsite is formed with 50 vol% void filled with water	0.5	0.5562	0.0005	0.5572	0.0148	371-384
0.05 wt% Gd as GdPO4 in Al fill material (Al shot)							
atr_all_gd005-g100	Similar to case "atr_all_gd01-g100," but only 0.05 wt% Gd in Al shot	0	0.6902	0.0006	0.6914	0.0122	340 -353
atr_all_gd005-g90	Similar to case "atr_all_gd01-g90," but only 0.05 wt% Gd in Al shot	0.1 (in gibbsite only)	0.6902	0.0006	0.6914	0.0120	346 -359
atr_all_gd005-g70	Similar to case "atr_all_gd01-g70," but only 0.05 wt% Gd in Al shot	0.3	0.6938	0.0006	0.6950	0.0120	359 -372
atr_all_gd005-g60	Similar to case "atr_all_gd01-g60," but only 0.05 wt% Gd in Al shot	0.4	0.6958	0.0006	0.6970	0.0120	365 -378
atr_all_gd005-g60-tf	Similar to above case, but the waste package is surrounded by dry tuff with composition given in Table 13	0.4	0.6957	0.0006	0.6969	0.0121	365 -378

The results in Table 18 show that the presence of the uniform distributed additional neutron absorber (0.1 wt% Gd in Al shot which translates in approximately 0.6 kg of $GdPO_4$ in 377 kg of Al shot) is very effective in reducing the k_{eff} of the system for this class of configurations. By varying the moderation of the system (void fraction of gibbsite filled with water) a maximum of the effective multiplication factor is found at $H/^{235}U$ ratios around 370, which corresponds to a void fraction of 0.4 in gibbsite. Few additional cases have been run with the amount of Gd reduced in half to simulate the hypothetical effect of separation of the neutron absorber. The $k_{eff}+2\sigma$ of the system increase with more than 25% but is still well below the interim criticality limit of 0.93.

6.2.2 Results for Configurations Containing Degraded Components Outside DOE SNF Canister

This section gives the results of the calculations described in Section 5.5.2. The components outside the DOE SNF canister are considered partially/totally degraded. Typically the degradation of materials forms a clay-like material that is deposited around the relatively intact DOE SNF canister. The content of the canister can be as in the initial intact configurations or in one of the degraded arrangements analyzed in the previous section. The "pre-breach clay" was considered homogeneous distributed containing various fractions of void filled with water. The composition of the clay is calculated in spreadsheet "clay-composition.xls" presented in Attachment I. The internal components of the waste package that were not fully degraded were conservatively neglected from the models. The intact DOE SNF canister was placed at various positions inside the clay-like material.

The following table (Table 19) presents configurations of the DOE SNF canister similar to that described by case "atr_int_1a-s-comb" from Table 15 but placed in various positions in pre-breach clay mixed with various fractions of water.

Table 1919. Results for Configurations with Intact DOE SNF Canister and Fuel Surrounded by Pre-breach Clay

Case (MCNP Input File)	Description	k_{eff}	σ	$k_{eff}+2\sigma$	AENCF (MeV)	H/X
Effect of DOE SNF canister position in the waste package						
atr_int_comb-pbc-0wb	DOE SNF canister similar to that from case "atr_int_1a-s-comb" in Table 15. The canister is located at the bottom of the waste package and is surrounded by dry pre-breach clay. No water above clay.	0.6484	0.0008	0.6500	0.0259	87.8
atr_int_comb-pbc-0wb-w	Similar to above case, but water present above clay	0.6464	0.0008	0.6480	0.0253	87.8
atr_int_comb-pbc-0wm	Similar to case "atr_int_comb-pbc-0wb," but canister placed in the middle of the clay	0.6452	0.0008	0.6468	0.0258	87.8
atr_int_comb-pbc-0wbs	Similar to above case, but DOE SNF canister is placed under the surface of the clay	0.6394	0.0008	0.6410	0.0262	87.8
Effect of water content in clay						
atr_int_comb-pbc-20%wb-w	Similar to case "atr_int_comb-pbc-0wb" above, but pre-breach clay has 20 vol% void filled with water	0.6362	0.0009	0.6381	0.0261	87.8
atr_int_comb-pbc-40%wb-w	Similar with above case, but pre-breach clay has 40 vol% void filled with water	0.6304	0.0008	0.6320	0.0260	87.8
atr_int_comb-pbc-50%wb-w	Similar with above case, but pre-breach clay has 50 vol% void filled with water	0.6278	0.0008	0.6294	0.0263	87.8

The results indicate that the presence of dry clay does not significantly change the reflecting conditions outside the DOE SNF canister. The effective multiplication factor is only in one instance slightly higher than the value obtained for the intact case "atr_int_1a-s-comb" from Table 15, which is reflected by the dry intact waste package internals. Positioning the DOE SNF canister in clay has a minor influence on k_{eff}, highest value corresponding to bottom positioning, which is the most probable. Adding water to clay reduces k_{eff} by increasing neutron absorption.

The following table (Table 20) present similar configurations to those presented in the above table but the content of each compartment of the DOE SNF canister is degraded and is similar to the case “atr_all_gd01-g60” in Table 18.

Table 20~~20~~. Results for Configurations with Intact DOE SNF Canister and Degraded Fuel Surrounded by Pre-breach Clay

Case (MCNP Input File)	Description	k_{eff}	σ	k_{eff}+2σ	AENCF (MeV)	H/X
Effect of DOE SNF canister position in the waste package						
atr_all_gd01-g60-pbc-0wb	DOE SNF canister similar to that from case “atr_all_gd01-g60” in Table 18. The canister is located at the bottom of the waste package and is surrounded by dry pre-breach clay. No water above clay.	0.5597	0.0005	0.5607	0.0141	365 - 378
atr_all_gd01-g60-pbc-0wm	Similar to case “atr_int_comb-pbc-0wb,” but canister placed in the middle of the clay	0.5565	0.0005	0.5575	0.0140	365 - 378
atr_all_gd01-g60-pbc-0wbs	Similar to above case, but DOE SNF canister is placed under the surface of the clay	0.5513	0.0005	0.5523	0.0146	365 - 378
Effect of water content in clay						
atr_all_gd01-g60-pbc-20%wb-w	Similar to case “atr_int_comb-pbc-0wb” above, but pre-breach clay has 20 vol% void filled with water	0.5490	0.0005	0.5500	0.0145	365 - 378
atr_all_gd01-g60-pbc-40%wb-w	Similar with above case, but pre-breach clay has 40 vol% void filled with water	0.5435	0.0005	0.5445	0.0146	365 - 378
atr_all_gd01-g60-pbc-50%wb-w	Similar with above case, but pre-breach clay has 50 vol% void filled with water	0.5424	0.0005	0.5434	0.0147	365 - 378

The results included in Table 20 suggest that the presence of the pre-breach clay around the DOE SNF canister does not significantly affect the k_{eff} of the system. By comparing with the results obtained for case “atr_all_gd01-g60” from Table 18, only the case with the canister at the bottom has a slightly higher k_{eff}. All other cases have lower k_{eff} values than the case presented in Table 18.

Regarding of the position of the canister in clay and the presence of water mixed with clay, the influence is very small and is similar to that observed in the cases from Table 19. The highest k_{eff} is obtained for the DOE SNF canister placed at the bottom of the waste package and for a dry clay composition, which provide a better reflection for neutrons.

6.2.3 Results for Configurations Containing Completely Degraded Components

This section presents the results of the cases described in Section 5.5.3. The fuel and the internals of the waste package are considered completely degraded and settled in layers of various compositions. The following table (Table 21) presents the results of the cases that describe a configuration class in which the degraded fuel (schoepite) and degraded Al fill material with Gd are placed in a homogeneous layer at the bottom of the waste package (Figure 10). The layer is covered by pre-breach clay mixture. This case is also representative for the configurations that can result from the accumulation of the mixture containing fissile material at the bottom of the waste package during earlier stages of degradation of the internals. All non-degraded components of the DOE SNF canister (including Ni-Gd alloy basket structure) are conservatively neglected. Variations of the water content of the layers are investigated, covering a very large spectrum of $H/^{235}U$ ratios. The composition of the layers is detailed in the spreadsheet “clay-composition.xls” from Attachment I.

Table 2121. Results for Configurations with Completely Degraded Components Placed in Layers

Case (MCNP Input File)	Description	k_{eff}	σ	$k_{eff}+2σ$	AENCF (MeV)	H/X
Effect of water content in both layers						
atr_degf+clay0w	Homogeneous layer formed from degraded fuel (schoepite) and degraded fill material (gibbsite + gadolinium phosphate) placed at the bottom of the waste package. No voids and dry mixtures. Initial Gd content was 0.1 wt% in Al fill material. See Figure 10.	0.6394	0.0005	0.6404	0.0076	605
atr_degf+clay10%w	Similar to above case but both layers form with 10 vol% void that is filled with water	0.6310	0.0005	0.6320	0.0071	685
atr_degf+clay20%w	Similar to above case, but both layers form with 20 vol% void that is filled with water	0.6225	0.0005	0.6235	0.0063	785
atr_degf+clay30%w	Similar to above case, but both layers form with 30 vol% void that is filled with water	0.6141	0.0004	0.6149	0.0057	913
atr_degf+clay40%w	Similar to above case, but both layers form with 40 vol% void that is filled with water	0.6024	0.0005	0.6034	0.0053	1084
Effect of water content in upper layer						
atr_degf+clay0-10%w	Similar to case "atr_degf+clay0w" above, but upper layer has 10 vol% void that is filled with water	0.6355	0.0005	0.6365	0.0075	605
atr_degf+clay0-20%w	Similar to case "atr_degf+clay0w" above, but upper layer has 20 vol% void that is filled with water	0.6320	0.0005	0.6330	0.0075	605
Effect of 50% less gibbsite in fuel layer						
atr_degf+clay0w-50gb	Similar to case "atr_degf+clay0w" above, but lower layer has 50% less gibbsite (considered lost); thickness of layers was adjusted accordingly	0.6542	0.0006	0.6554	0.0133	305
atr_degf+clay10%w-50gb	Similar to case "atr_degf+clay10%w" above, but lower layer has 50% less gibbsite (considered lost); thickness of layers was adjusted accordingly	0.6454	0.0006	0.6466	0.0126	345
atr_degf+clay20%w-50gb	Similar to case "atr_degf+clay20%w" above, but lower layer has 50% less gibbsite (considered lost); thickness of layers was adjusted accordingly	0.6389	0.0005	0.6399	0.0110	396
atr_degf+clay30%w-50gb	Similar to case "atr_degf+clay30%w" above, but lower layer has 50% less gibbsite (considered lost); thickness of layers was adjusted accordingly	0.6344	0.0005	0.6354	0.0100	461
atr_degf+clay40%w-50gb	Similar to case "atr_degf+clay40%w" above, but lower layer has 50% less gibbsite (considered lost); thickness of layers was adjusted accordingly	0.6316	0.0005	0.6326	0.0086	547
Effect of 50% less gibbsite and $GdPO_4$ in fuel layer						
atr_degf+clay0w-50gb-Gd	Similar to case "atr_degf+clay0w" above, but lower layer has 50% less gibbsite and $GdPO_4$ (considered lost); thickness of layers was adjusted accordingly	0.8291	0.0007	0.8305	0.0102	305
atr_degf+clay0w-50gb-Gd-tf	Similar to above case, but the waste package is surrounded by dry tuff with composition given in Table 13	0.8281	0.0007	0.8295	0.0104	305
atr_degf+clay10%w-50gb-Gd	Similar to case "atr_degf+clay10%w" above, but lower layer has 50% less gibbsite and $GdPO_4$ (considered lost); thickness of layers was adjusted accordingly	0.8228	0.0007	0.8242	0.0096	345
atr_degf+clay20%w-50gb-Gd	Similar to case "atr_degf+clay20%w" above, but lower layer has 50% less gibbsite and $GdPO_4$ (considered lost); thickness of layers was adjusted accordingly	0.8195	0.0007	0.8209	0.0086	396
atr_degf+clay30%w-50gb-Gd	Similar to case "atr_degf+clay30%w" above, but lower layer has 50% less gibbsite and $GdPO_4$ (considered lost); thickness of layers was adjusted accordingly	0.8161	0.0006	0.8173	0.0078	461
atr_degf+clay40%w-50gb-Gd	Similar to case "atr_degf+clay40%w" above, but lower layer has 50% less gibbsite and $GdPO_4$ (considered lost); thickness of layers was adjusted accordingly	0.8146	0.0006	0.8158	0.0067	547

The results show that as long as the neutron absorber is present interspersed within the fissile material, the effective multiplication factor of the system has very low values. Increasing the H/X ratio by adding various fractions of water to the mixtures results in a small decrease of the k_{eff}. The presence of more hydrated layers on top of the most reactive bottom layer containing fissile material reduces the k_{eff} of the system.

A special attention was given to the amount of gibbsite mixed with the degraded fuel. Assuming that almost 50 % of gibbsite is not mixed with the fuel in the bottom layer, results in a slightly increase in the k_{eff}. Even in the hypothetical situation in which 50% of the additional Gd from the Al fill material is lost or separated from the fissile material, the k_{eff} of the system is well below the interim criticality limit of 0.93. The geochemistry calculation (BSC 2004f) shows that the Gd loss is almost insignificant in all scenarios analyzed. Using Al fill material with $GdPO_4$ assures that degradation of Al based fuel and fill material will always occur in the same time, keeping the neutron absorber in close proximity with the degraded fuel.

A final set of MCNP runs has investigated the configurations comprising post-breach clay composition (Table 14) that was obtained considering degradation of all waste package components in the same time (IP-2 scenario). The clay composition (at 20,400 years) was obtained from the geochemistry calculation (BSC 2004f) that investigated the initial design of the DOE SNF canister containing ATR SNF (without additional neutron absorber). All Uranium present in the clay was assumed to be fissile ^{235}U. The amount is slightly below the total amount of ^{235}U available in the intact waste package cases (spreadsheet "clay-composition.xls"). All non-degraded components of the waste package and DOE SNF canister were conservatively neglected. The results are summarized in Table 22.

Table 2222. Results for Configurations with Post-breach Clay Mixed with Water

Case (MCNP Input File)	Description	k_{eff}	σ	$k_{eff}+2\sigma$	AENCF (MeV)	H/X
Effect of water content in post-breach clay						
atr_post-b-clay0w	Homogeneous post-breach clay settled at the bottom of the waste package. No water mixed with the clay and above the clay.	0.1230	0.0001	0.1232	0.0344	160.6
atr_post-b-clay0w-f	Similar to above case, but water filling the space above clay in the waste package	0.1237	0.0001	0.1239	0.0341	160.6
atr_post-b-clay20%w	Similar to above case, but clay is mixed with 20 vol% water	0.0813	0.0001	0.0815	0.0331	658.0
atr_post-b-clay40%w	Similar to above case, but clay is mixed with 40 vol% water	0.0576	0.00003	0.0577	0.0304	1487.0

As expected, the k_{eff} of the system has very low values, given by the presence of various absorbing isotopes in the post breach clay composition. Clearly, there are no criticality concerns for the cases analyzed from this class of configurations.

6.2.4 Summary of Results

The results throughout Sections 6.2.1 to 6.2.3 present a large number of parametric evaluations for the internal configurations ranging from intact to completely degraded internals of the ATR SNF waste package. All outputs are reasonable compared to the inputs and the results of this calculation are suitable for their intended use.

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7.4 SOFTWARE CODES

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8. ATTACHMENTS

Attachment I: One Compact Disk (CD) containing the MCNP input and output files for the cases denoted in Section 6.

Attachment II: Description of files contained in Attachment I (1 page).

ATTACHMENT II

This attachment contains a listing and description of the zip file contained on the attachment CD – Disk 1 of 1 (Attachment I) of this calculation. The zip archive was created using Winzip 8.1. The zip file attributes are:

Archive File Name	File Size (bytes)	File Date	File Time
ATRCrit.zip	12,751,003	10/04/2004	1:36 PM

There are 195 total files contained in the unique directory structure. Upon file extraction, 190 MCNP files along with 5 Excel spreadsheet files will be found.