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**Civilian Radioactive Waste Management System
Management & Operating Contractor**

Evaluation of Codisposal Viability for HEU Oxide (Shippingport PWR) DOE-Owned Fuel

TDR-EDC-NU-000003 REV 00

February 2000

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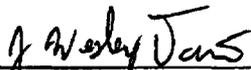


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EXECUTIVE SUMMARY

INTRODUCTION

There are more than 250 forms of U.S. Department of Energy (DOE)-owned spent nuclear fuel (SNF). Due to the variety of the SNF, the National Spent Nuclear Fuel Program (NSNFP) has designated nine representative fuel groups for disposal criticality analyses based on fuel matrix, primary fissile isotope, and enrichment. The Shippingport pressurized water reactor (PWR) fuel has been designated as the representative fuel for the highly enriched uranium oxide (HEU oxide) fuel group, which is a uranium oxide clad with Zircaloy-4. The Shippingport PWR fuel is "seed and blanket" type fuel. This technical document addresses the seed type fuel assemblies only. The blankets will be shipped and handled as bare assemblies and use the same packaging associated with either PWR or boiling water reactor (BWR) commercial fuels (DOE 1999a). Therefore, this report does not specifically address the disposal of blanket assemblies in the Monitored Geologic Repository (MGR). Demonstration that other fuels in this group are bounded by the Shippingport PWR analysis remains for the future before acceptance of these fuel forms. The results of the analyses performed will be used to develop waste acceptance criteria. The items that are important to safety are identified based on the analysis needs and result sensitivities. Prior to acceptance of fuel from the HEU oxide fuel group for disposal, the safety items for the fuel types that are being considered for disposal under the HEU oxide fuel group must be demonstrated to satisfy the conditions determined in this report.

The analyses have been performed by following the disposal criticality analysis methodology, which was documented in *Disposal Criticality Analysis Methodology Topical Report* (CRWMS M&O 1998a) submitted to the U.S. Nuclear Regulatory Commission. The methodology includes analyzing the geochemical and physical processes that can breach the waste package and degrade the waste forms and other internal components, as well as the structural, thermal, and shielding analyses, and intact and degraded component criticality analyses. One or more addenda to the topical report will be required to establish the critical limit for DOE SNF once sufficient critical benchmarks are identified and performed.

The waste package that holds the DOE SNF canister with Shippingport PWR HEU oxide fuel also contains five high-level waste (HLW) glass pour canisters and a carbon steel basket. The Shippingport PWR DOE SNF canister is placed in a carbon steel support tube that becomes the center of the waste package (see Figure ES-1). The waste package carbon steel basket height is 4,607 mm. The five HLW glass canisters are evenly spaced around the Shippingport PWR DOE SNF canister. The Shippingport PWR DOE SNF canister is designed for one intact Shippingport PWR fuel assembly placed in the center position of the 2,681-mm-long stainless steel basket. The canister basket consists of a rectangular grid that is 208-mm square. The canister basket plate is stainless steel (Type 316L) with a 9.5 mm thickness.

The 5-DHLW/DOE Spent Fuel-Long waste package is based on the Viability Assessment design of waste packages. The outer barrier is made of corrosion-allowance material, 100-mm thick carbon steel. The corrosion-resistant inner barrier is fabricated from a 20-mm thick high-nickel alloy. Both the top and bottom lids are also based on the two-barrier principle and use the same materials.

This report presents the results of analyzing the 5-DHLW/DOE Spent Fuel-Long waste package against various design criteria. Section 2.2 provides the criteria, and Section 2.3 provides the key assumptions for the various analyses. This report does not address codisposal waste packages with HLW glass canisters which contain immobilized plutonium.

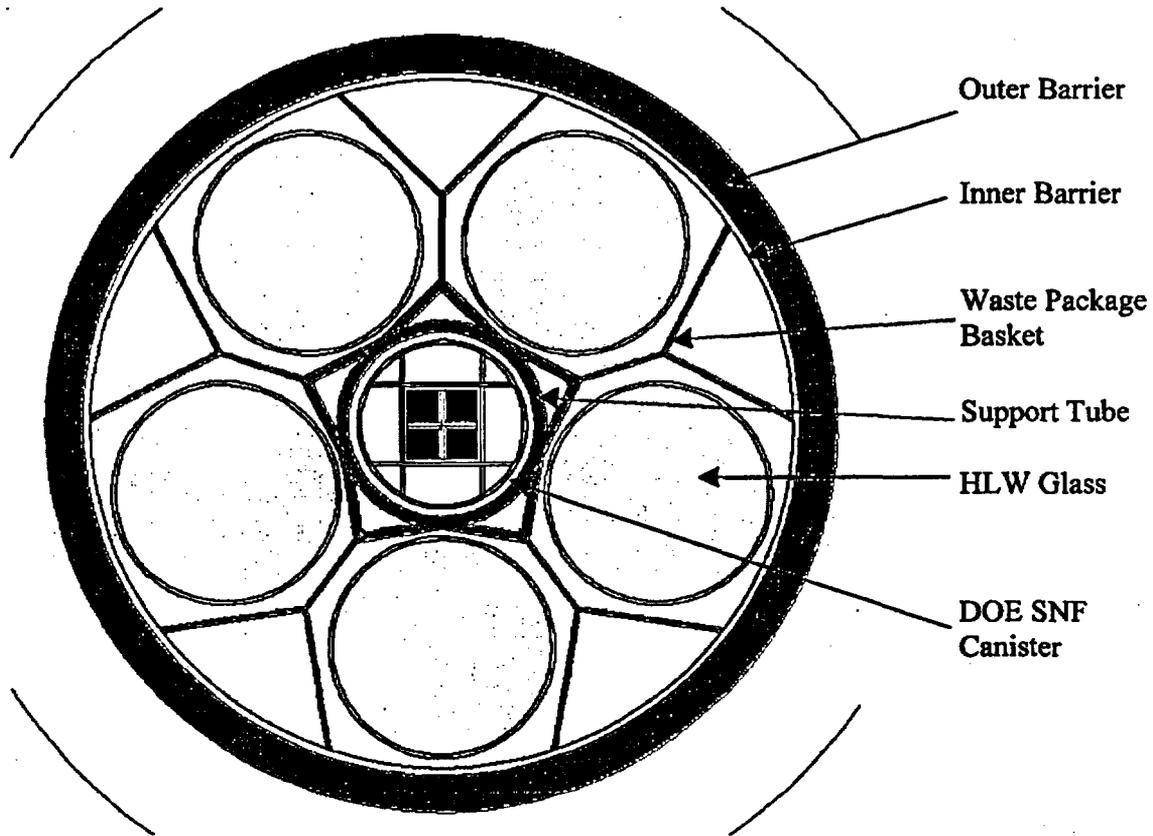


Figure ES-1. 5-DHLW/DOE Spent Fuel-Long Waste Package with Shippingport PWR SNF

STRUCTURAL ANALYSIS

ANSYS Version 5.4 – a finite-element analysis (FEA) computer code – is used for the structural analysis of the 5-DHLW/DOE Spent Fuel-Long waste package with the Shippingport PWR DOE SNF canister in the center. A two-dimensional (2-D) finite-element representation of this 5-DHLW/DOE Spent Fuel-Long waste package was developed to determine the effects of loads on the container's structural components due to a waste package tipover design-basis event (DBE). Calculations of maximum potential energy for each handling accident scenario (2.4-m horizontal drop, 2.0-m vertical drop, and tipover DBEs) show that the bounding dynamic load results from a tipover case in which the rotating top end of the waste package experiences the highest g-load. Therefore, tipover structural evaluations are bounding for all handling accident scenarios under the above constraints of 2.4-m horizontal drop, 2.0-m vertical drop, and tipover considered in the

DBEs document (CRWMS M&O 1997e). The analyses assume that the MGR surface design will prevent events which exceed these bounding assumptions.

The results show that the cavity between the Shippingport fuel assembly and the basket plates does not close, but on the contrary, becomes larger because of the dynamic load applied on the bottom plate by the Shippingport fuel assembly. Hence, there will be no interference between the fuel assembly and the basket plates because of tipover DBE. The maximum stress in the DOE SNF canister structural components including internals is determined to be 217 MPa. This magnitude of stress is less than the tensile strength of 316L stainless steel, 483 MPa.

The calculations also show that the maximum bending stress on the base plate due to the weight of the structural components and the fuel is 55 MPa, which is less than the yield strength of 316L stainless steel (172 MPa). Finally, the critical stress for buckling to take place on the spacer cylinder is 1.43 GPa whereas the compressive stress is only 2.5 MPa. Therefore, the Shippingport PWR fuel assembly will not be crushed within the basket structure.

THERMAL ANALYSIS

The FEA computer code used for the thermal analysis of the 5-DHLW/DOE Spent Fuel-Long waste package with the Shippingport PWR DOE SNF canister in the center is ANSYS Version 5.4. The maximum heat generation from a Hanford 15-foot HLW glass canister is projected to be 2,540 watts (Taylor 1997). Although this maximum heat generation may be reduced, which will result in even lower temperatures than the temperatures calculated in this report, the analysis was based on heat output of 2,540 watts. The thermal conductivity of the HLW glass is approximated as that of pure borosilicate glass, while the properties of density and specific heat are approximated as those of Pyrex glass. Only the axial cross section of the waste package at the center of the DOE SNF canister is represented in this 2-D calculation. The Shippingport PWR DOE SNF canister is analyzed with helium (He), nitrogen (N), and argon (Ar) as fill gases, while the waste package is filled with He.

Using conservative input values, the analyses show that the Shippingport PWR waste package satisfies all relevant governing criteria. The highest fuel temperature occurs with argon fill gas in the DOE SNF canister, and is 248.9 °C. The highest cladding temperature occurs with argon fill gas in the DOE SNF canister, and is 249.2 °C, which is below the design criterion of 350 °C.

SHIELDING ANALYSIS

The Monte Carlo particle transport code, MCNP, Version 4B2, is used to calculate average dose rates on the surfaces of the waste package. Dose rate calculations were performed for a waste package containing Hanford HLW and Shippingport PWR fuel.

The highest dose rate of 10.3 rem/h is calculated on a radial outer surface segment of the waste package that contains the Shippingport PWR DOE SNF canister. The maximum dose rate on the outer surfaces of the waste package is below the criterion limit of 355 rem/h for the cases investigated by over a factor of 34. The dose rate from primary gamma rays dominates the neutron dose rate by approximately three orders of magnitude.

DEGRADATION AND GEOCHEMISTRY ANALYSES

The degradation analyses follow the general methodology developed for application to all waste forms containing fissile material. This methodology evaluates potential critical configurations from the intact (geometrically intact components but otherwise breached waste package to include water as moderator) waste package through the completely degraded waste package. The waste package design developed for the intact configuration is used as the starting point. Sequences of events and/or processes of component degradation are developed. Standard scenarios from the master scenario list in the topical report (CRWMS M&O 1998a) are refined using unique fuel characteristics. Potentially critical configurations are identified for further analysis.

The EQ3/6 geochemistry code was used to determine the chemical composition of the solid degradation products with particular emphasis on the chemical conditions that could lead to a loss of neutron absorbers from the waste package and that would allow the fissile materials to remain. The DOE SNF canister with Shippingport PWR fuel does not contain any strong neutron absorbers such as gadolinium. Boron, which is a burnable poison that is an integral part of the fuel, is neglected for criticality calculations.

EQ3/6 cases are constructed to span the range of possible fuel corrosion. The effects of steel corrosion, glass degradation, and fluid influx rate on uranium oxide dissolution are also investigated. Uranium loss from the waste package varied from 0.06 to 100%, and was typically complete if greater than neutral pH's existed for any appreciable amount of time. At a given glass dissolution rate, uranium loss varies inversely with the influx of water.

INTACT AND DEGRADED COMPONENT CRITICALITY ANALYSES

The intact and degraded component criticality analyses consider a single Shippingport PWR assembly inside the DOE SNF canister, which contains a stainless steel Type 316L basket. Analyses consider optimum moderation, optimum distribution of fissile material and degradation products, and optimum reflection to determine the highest k_{eff} attainable by the system. Intact cases represent breached but otherwise intact waste package, DOE SNF canister, and fuel assembly. Degraded cases cover range of degradation of waste package internals, HLW glass canisters, DOE SNF canister, and the fuel assembly.

The results from the intact and degraded component criticality analyses show that $k_{eff} + 2\sigma$ (95% confidence) are less than or equal to 0.93 for one Shippingport PWR assembly in the DOE SNF canister. The configurations do not need any neutron absorber in the canister basket or elsewhere in the waste package, even without credit for burnable absorber (boron) that is present in the fuel assembly.

CONCLUSIONS

In summary, the structural, thermal, and shielding criteria are met for a DOE SNF canister containing Shippingport PWR SNF. The waste package can contain one fuel assembly and falls

below the interim critical limit of 0.93 without any neutron absorber in the DOE SNF canister basket or elsewhere in the waste package. With this design, there will be approximately 20 DOE SNF canisters loaded with Shippingport PWR SNF (Core 2 Seed 2). This corresponds to 20 waste packages.

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ACRONYMS AND ABBREVIATIONS

AP	administrative procedure
ASM	American Society for Metals
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
BOL	beginning of life
BPVC	Boiler and Pressure Vessel Code
BWR	boiling water reactor
CRWMS	Civilian Radioactive Waste Management System
CSCI	Computer Software Configuration Item
DBE	design basis event
DHLW	defense high-level waste
DOE	U.S. Department of Energy
FEA	finite-element analysis
HEU	highly enriched uranium
HLW	high-level waste
ID	inner diameter
IP	internal to the package
k_{eff}	effective multiplication factor
LCE	laboratory critical experiment
LLNL	Lawrence Livermore National Laboratory
M&O	Management and Operating Contractor
MGR	Monitored Geologic Repository
MTHM	metric tons of heavy metal
NSNFP	National Spent Nuclear Fuel Program
OD	outer diameter
PC	personal computer
PWR	pressurized water reactor
QARD	Quality Assurance Requirements and Description
SCM	Software Configuration Management
SCR	software change request
SDD	system description document
SNF	spent nuclear fuel
SQR	software qualification report
SRS	Savannah River Site
SS	stainless steel
TBV	to be verified
2-D	two-dimensional
3-D	three-dimensional

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1. INTRODUCTION AND BACKGROUND

There are more than 250 forms of U.S. Department of Energy (DOE)-owned spent nuclear fuel (SNF). Due to the variety of the spent nuclear fuel, the National Spent Nuclear Fuel Program (NSNFP) has designated nine representative fuel groups for disposal criticality analyses based on fuel matrix, primary fissile isotope, and enrichment. The Shippingport Pressurized Water Reactor (PWR) fuel has been designated as the representative fuel (DOE 1999a) for the Highly Enriched Uranium Oxide Fuels (HEU oxide) fuel group. Demonstration that other fuels in this group are bounded by the Shippingport PWR analysis remains for the future before acceptance of these fuel forms. As part of the criticality licensing strategy, NSNFP has provided a reviewed data report (DOE 1999a) with traceable data for the representative fuel type. The results of the analyses performed by using the information from this reviewed data report will be used to develop waste acceptance criteria which must be met by all fuel forms within the HEU oxide fuel group including Shippingport PWR SNF. The items that are important to safety are identified based on analysis needs and result sensitivities. Prior to acceptance of the fuel from HEU oxide fuel group for disposal, the safety items of the fuel types that are being considered for disposal under the HEU oxide fuel group must be demonstrated to satisfy the conditions set in Section 8.6, Items Important to Safety.

The commercial development of PWR technology was based on the Nuclear Navy program. The first reactor in this program was Shippingport. The Shippingport plant was a PWR design, based on Argonne National Laboratory's submarine reactor technology, the capacity being 60 MWe. In December of 1957, the first large-scale nuclear power plant in the world began operating in Shippingport, PA. This was the first commercial light water reactor plant, operating from 1958 to 1982.

The analyses have been performed by following the disposal criticality analysis methodology, which was documented in the topical report, submitted to U.S. Nuclear Regulatory Commission (CRWMS M&O 1998a). The methodology includes analyzing the geochemical and physical processes that can breach the waste package and degrade the waste forms as well as the structural, thermal, shielding analyses, and intact and degraded component criticality analyses. Addenda to the topical report will be required to establish the critical limit for the DOE SNF once sufficient critical benchmarks are identified and run. In this report, a conservative and simplified bounding approach is employed to designate an interim critical limit.

In this technical report, there are numerous references to "codisposal container" and "waste package." Since the use of these two terms may be confusing, a definition of the terms is included here:

"(Co)disposal container" means the container barriers or shells, spacing structures and baskets, shielding integral to the container, packing contained within the container, and other absorbent materials designed to be placed internal to the container or immediately surrounding the disposal container (i.e., attached to the outer surface of the disposal container). The disposal container is designed to contain SNF and high-level waste (HLW), but exists only until the outer weld is complete and accepted. The disposal container does not include the waste form or the encasing

containers or canisters (e.g., HLW pour canisters, DOE SNF codisposal canisters, multi-purpose canisters of SNF, etc.).

“Waste package” means the waste form and any containers (i.e., disposal container barriers and other canisters), spacing structures or baskets, shielding integral to the container, packing contained within the container, and other absorbent materials immediately surrounding an individual waste container placed internally to the container or attached to the outer surface of the disposal container. The waste package begins its existence when the outer lid weld of the disposal container is complete and accepted.

“5-DHLW/DOE Spent Fuel-Long waste package” is the waste package that can accommodate a 15-ft long (18-in. diameter) DOE SNF canister and five 15-ft HLW glass canisters.

1.1 OBJECTIVE

The objective of this report is to provide sufficient detail to establish the technical viability for disposing of HEU oxide (Shippingport PWR) SNF in the potential Monitored Geologic Repository (MGR). This report sets limits and establishes values that if and when these limits are met by a specific fuel type under the HEU oxide fuel group, the results for that fuel will be bounded by the results reported in this technical report.

Section 2, Design Inputs, describes the design basis, and identifies requirements and assumptions. Analytical results to demonstrate the adequacy of the design and evaluate the feasibility of codisposing the HEU oxide (Shippingport PWR) SNF in the MGR are presented in Section 3 for Structural Analysis, Section 4 for Thermal Analysis, Section 5 for Shielding Analysis, Section 6 for Degradation and Geochemistry Analyses, and Section 7 for Intact and Degraded Component Criticality Analyses. For purposes of this report, these five items may be collectively designated as waste package performance. Section 8, Conclusions, provides the connections between the design criteria and analytical results to establish technical viability. In addition, Section 8 gives recommendations regarding any additional needs for analysis or documentation. References are given in Section 9.

This technical document summarizes and analyzes the results of the detailed calculations that were performed in support of determining the evaluation of codisposal viability of HEU oxide (Shippingport PWR) fuel. These calculation documents and the section of this document in which they are summarized and analyzed are shown in Table 1-1.

1.2 SCOPE

This technical report *Evaluation of Codisposal Viability for HEU Oxide (Shippingport PWR) DOE-Owned Fuel* evaluates and reports the performance of HEU oxide (Shippingport PWR) SNF in a waste package. This technical report summarizes the evaluation of viability of the 5-DHLW/DOE Spent Fuel-Long waste package design with HEU oxide (Shippingport PWR) SNF, which is the representative fuel for HEU oxide fuel group. The remaining fuels in the same group must be demonstrated to be bounded by the values obtained from the reviewed data report, which is based on the Shippingport PWR SNF.

Table 1-1. List of Supporting Documents

Discipline	Document Title	Summarized/ Analyzed in	Reference
Structural	<i>Structural Calculations for the Codisposal of Shippingport Spent Nuclear Fuel in a Waste Package</i>	Section 3	CRWMS M&O (1999b)
Thermal	<i>Thermal Evaluation of the Shippingport PWR Codisposal Waste Package</i>	Section 4	CRWMS M&O (1999f)
Shielding	<i>Dose Calculation for the Co-Disposal WP of HLW Canisters and the Shippingport PWR Fuel</i>	Section 5	CRWMS M&O (1999h)
Degradation and Geochemistry	<i>EQ6 Calculations for Chemical Degradation of Shippingport PWR (HEU Oxide) Spent Nuclear Fuel Waste Packages</i>	Section 6	CRWMS M&O (1999e)
Intact and Degraded Component Criticality	<i>Intact and Degraded Criticality Calculations for the Codisposal of Shippingport PWR Fuel in a Waste Package</i>	Section 7	CRWMS M&O (2000)

1.3 QUALITY ASSURANCE

This technical document was prepared in accordance with AP-3.11Q, *Technical Reports*. The responsible manager for DOE Fuel Analysis has evaluated this report development activity in accordance with QAP-2-0, *Conduct of Activities*. The evaluation (CRWMS M&O 1999a, CRWMS M&O 1999i) concluded that the development of this report is subject to the DOE Office of Civilian Radioactive Waste Management Quality Assurance Requirements and Description (QARD) controls (DOE 2000). The information provided in this report is to be indirectly used in the evaluation of the codisposal viability of HEU oxide fuel.

There is no determination of importance evaluation developed in accordance with Nevada Line Procedure, NLP-2-0, *Determination of Importance Evaluations*, since the report does not involve any field activity.

This technical report is based in part on unqualified data. However, the unqualified data is only used to determine the bounding values and items that are important to safety for the fuel group by establishing the limits based on the representative fuel type (Shippingport PWR) for this group (HEU oxide fuel). Hence, the input values used for evaluation of codisposal viability of HEU oxide (Shippingport PWR) SNF do not constitute data that have to be qualified in this application. They merely establish the bounds for acceptance. Since the input values are not relied upon directly to address safety and waste isolation issues, nor do the design inputs affect a system characteristic that is critical for satisfactory performance, according to the governing procedure (AP-3.15Q), data do not need to be controlled as TBV (to be verified). However, prior to acceptance of the fuel for disposal, the items that are identified as important to safety in Section 8.6 must be qualified by any means identified in the QARD (e.g., experiment, non-destructive test, chemical assay, qualification under a program subject to the QARD requirements).

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2. DESIGN INPUTS

The data that were obtained from ASTM B 575-94, ASTM A 516/A 516M - 90, ASTM G 1-90, ASTM A 240/A 240M-97a, ASM (1990), ASTM A 276-91a, and ASME (1995) are considered accepted data. These references are standard handbooks, and due to the nature of these sources, the data in it are established fact and are therefore considered accepted. The data from other references used as direct input are considered unqualified.

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.

2.1 DESIGN PARAMETERS

Each of the following sections either describes the design of the waste package or identifies the basis of major parameters.

2.1.1 Codisposal Waste Package

The codisposal waste package contains five HLW glass canisters surrounding a DOE standardized 18-inch diameter SNF canister. The 5-DHLW/DOE Spent Fuel-Long waste package is based on the Viability Assessment (DOE 1998a) design of waste packages. The barrier materials of the waste package are typical of those used for commercial SNF waste packages. The inner barrier is composed of 20 mm of high-nickel alloy ASTM B 575 (Alloy 22) and serves as a corrosion-resistant material. The outer barrier comprises 100 mm of carbon steel (ASTM A 516 Grade 70) and serves as a corrosion-allowance material (CRWMS M&O 1997a, pp. 56 and 72). The outside diameter of the waste package is 2,120 mm and the length of the inside cavity is 4,617 mm (CRWMS M&O 1998b), which is designed to accommodate Hanford 15-foot HLW glass canisters. The lids of the inner barrier are 25 mm thick; those of the outer barrier, 110 mm thick. There is a 30-mm gap between the inner and outer barrier upper lids. Each end of the waste package has a 225-mm long skirt. Table 2-1 summarizes the dimensions and materials of the waste package.

The DOE SNF canister is placed in a 31.75-mm thick carbon steel (ASTM A 516 Grade 70) support tube with a nominal outer diameter of 565 mm. The support tube is connected to the inside wall of the waste package by a web-like structure of carbon steel (ASTM A 516 Grade 70) basket plates to support five long HLW glass canisters, as shown in Figure 2-1. The support tube and the plates are 4,607 mm long.

Table 2-1. Codisposal Waste Package Dimensions and Material Specifications

Component	Material	Parameter	Dimension (mm)
Outer barrier shell	ASTM A 516 Grade 70	Thickness	100
		Outer diameter	2,120
Inner barrier shell	ASTM B 575	Thickness	20
		Inner length	4,617
Top and bottom outer barrier lids	ASTM A 516 Grade 70	Thickness	110
Top and bottom inner barrier lids	ASTM B 575	Thickness	25
Gap between the upper inner and outer closure lids	Air	Thickness	30
Support tube	ASTM A 516 Grade 70	Outer diameter	565
		Inner diameter	501.5
		Length	4,607

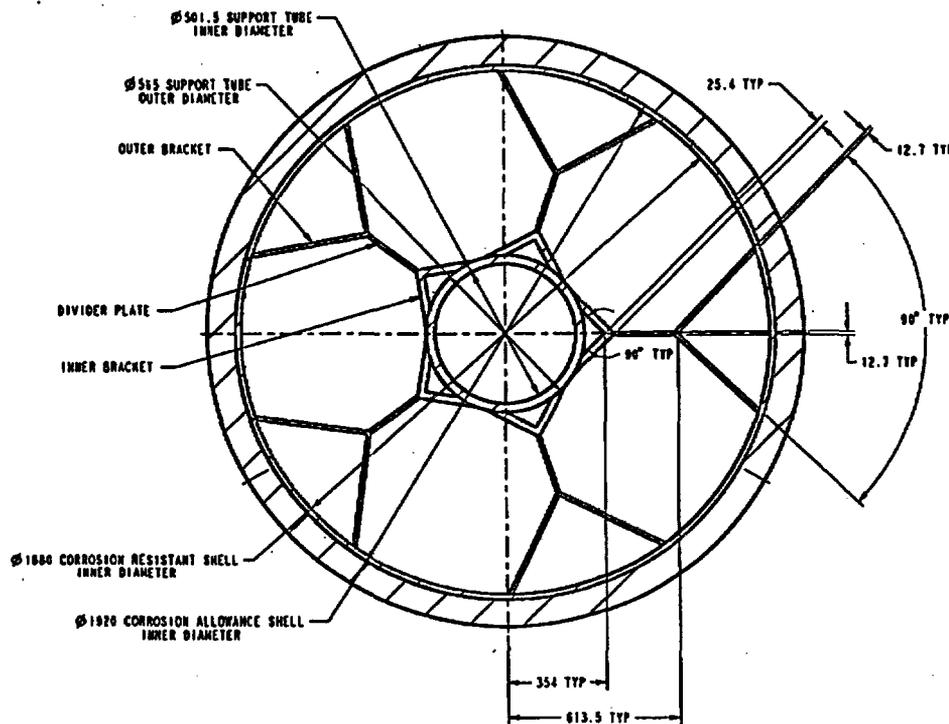


Figure 2-1. Cross Section of 5-DHLW/DOE Spent Fuel-Long Waste Package

2.1.2 HLW Glass Pour Canisters

There is no long Savannah River Site (SRS) HLW glass canister. Therefore, the Hanford 15-foot HLW glass canister (Figure 2-2) is used in the Shippingport PWR waste package. Since the specific composition of the Hanford HLW glass is not known at this time, the SRS glass composition is used in all analyses (Table 2-13). The Hanford 15-foot HLW glass canister is 4,572-mm long stainless steel Type 304L canister with an outer diameter of 610 mm (24.00 in.)

(Taylor 1997). The wall thickness is 10.5 mm. The maximum loaded canister weight is 4,200 kg and the fill volume is 87%. The heat generation from a single canister is 2,540 W. The geometry and material specifications for HLW glass canisters are given in Table 2-2.

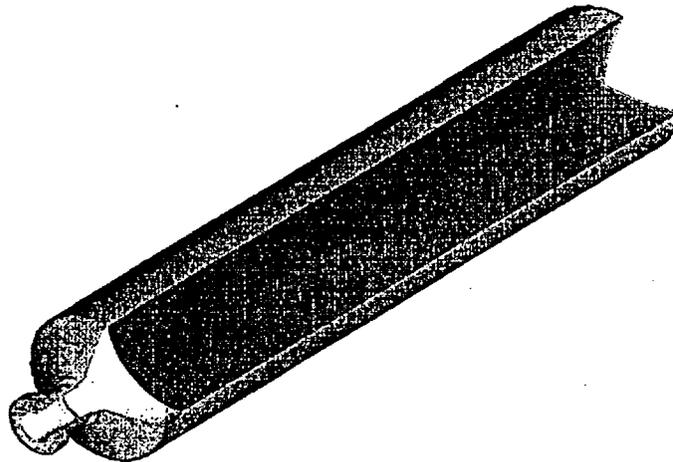


Figure 2-2. HLW Glass Pour Canister

Table 2-2. Geometry and Material Specifications for HLW Glass Canisters

Component	Material	Parameter	Value
Hanford 15-ft canister	Stainless Steel 304L	Outer diameter	610 mm
		Wall thickness	10.5 mm
		Length	4,572 mm
		Total weight of canister and glass	4,200 kg
		Fill volume of glass in canister	87%

Source: Taylor (1997).

2.1.3 DOE SNF Canister

The information on the 18-inch DOE SNF canister conceptual design is taken from DOE (1998b). It is recognized that DOE (1998b) has been revised (DOE 1999b); however, only Revision 1 was available at the time the calculations reported in this technical document were performed. A review of the most recent revision indicated that there is no impact on current results since neither the dimensions nor the materials of the canister changed. The canister is a right circular cylinder of stainless steel (Type 316L) that contains a stainless steel (Type 316L) basket. The basket is not a standard part of the DOE SNF canister. The basket design is modified for each specific fuel type. The basket provides structural support, and acts as a guide for the fuel assembly during loading. The dimensions for the DOE SNF canister are a 457.2-mm (18.00-inch) outer diameter with a 9.525-mm (0.375-inch) wall thickness (Table 2-3). The

minimum internal length of the canister is 4,117 mm (162.09 in.); the nominal overall length, 4,569 mm (179.87 in.). A curved bottom carbon steel impact disk that varies in thickness from 15.24 mm to 50.8 mm is located at both the top and bottom of the canister (see Figure 2-3). In addition, there is a 12.7-mm thick curved plate in each end of the canister. Maximum loaded weight of the canister is 2,721 kg.

The standard 18-inch DOE SNF canister (15-ft) is used for disposal of Shippingport PWR fuels, and holds a single Shippingport PWR C2 S2 SNF assembly in a specially designed basket. A cross-sectional and an isometric view of the DOE SNF canister containing one Shippingport PWR assembly are shown in Figures 2-4 and 2-5, respectively. The basket consists of a rectangular grid that is 208-mm square. The basket plate is stainless steel (Type 316L) with a 9.5 mm thickness. The basket height is 2,681 mm.

Table 2-3. Geometry and Material Specifications for the DOE SNF Canister

Component	Material	Parameter	Dimension (mm)
Circular cylinder	SS 316L	Outer diameter	457.2
		Wall thickness	9.525
		Internal length	4,117
Impact plate	ASTM A 516 Grade 70	Thickness	From 15.24 to 50.8 at the top and bottom
Top and bottom curved plates	SS 316L	Thickness	12.7

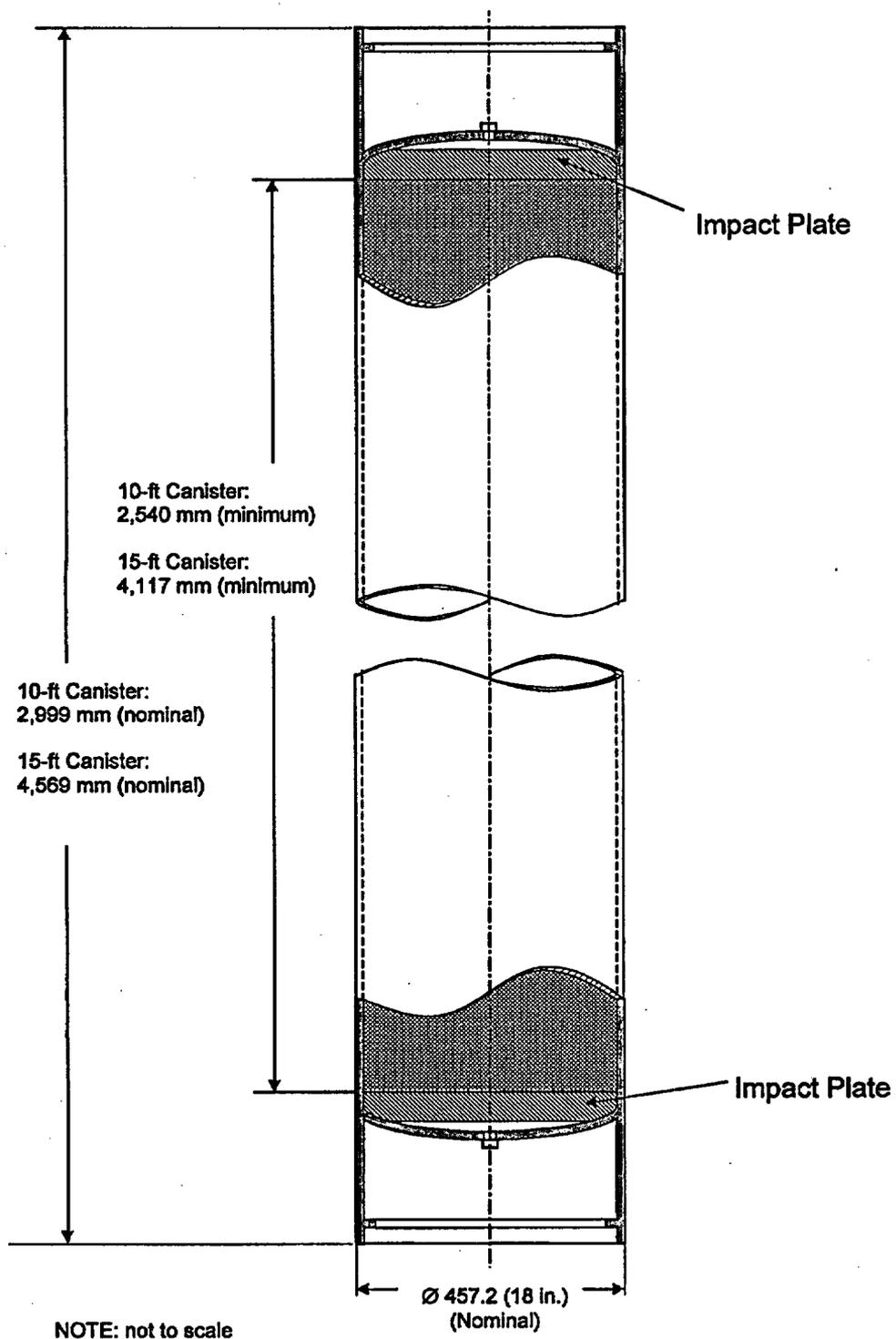


Figure 2-3. Plan View of the 18-in. DOE SNF Canister

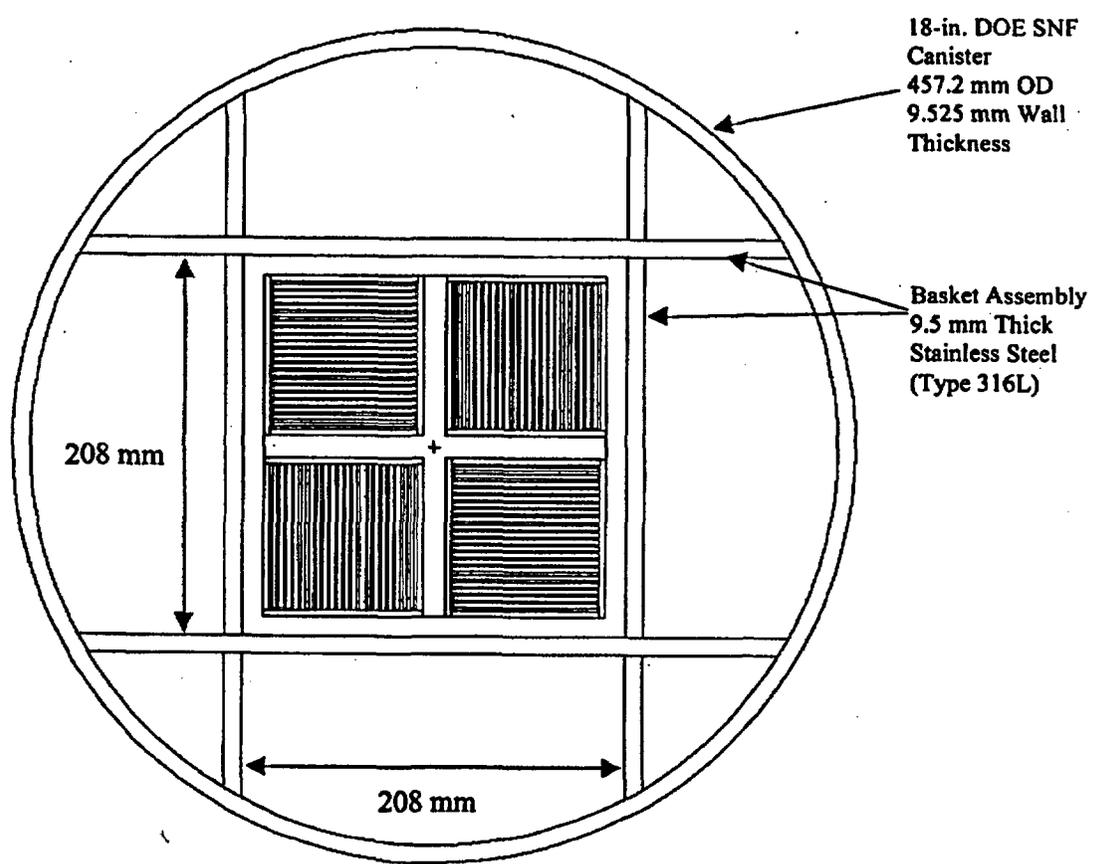


Figure 2-4. Cross Section of the Shippingport PWR DOE SNF Canister

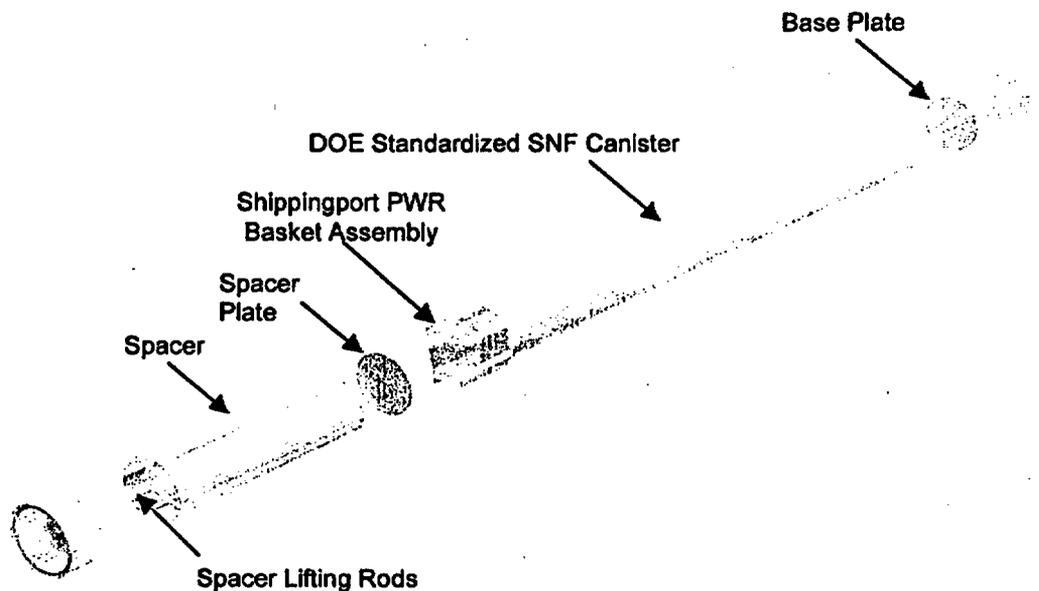


Figure 2-5. Isometric View of the Shippingport PWR DOE SNF Canister

2.1.4 Shippingport PWR DOE SNF

The Shippingport PWR was a “seed and blanket” reactor, which underwent multiple modifications to provide higher thermal outputs. The blankets will be shipped and handled as bare assemblies. The low enrichments (< 1%) allows use of the same packaging associated with either PWR or BWR commercial fuels (DOE 1999a, p. 1). Therefore, this report does not specifically address the disposal of blanket assemblies in the MGR.

Two seeds, Seed 1 (S1) and Seed 2 (S2), which had identical geometrical dimensions but different U-235 enrichment and chemical composition, were designed for Shippingport PWR Core 2 (C2) operation. The Shippingport PWR C2 S2 fuel assembly is shown in Figure 2-6 (DOE 1999a, p. 11). The assembly is composed of Zircaloy-4 and consists of four sub-assemblies and a cruciform-shaped channel in the center to accommodate a control rod. Figure 2-7 shows the cross section of a single sub-assembly. Each sub-assembly is composed of 19 fuel plates and 20 channels. Each plate is formed by sandwiching an enriched U-Zr alloy strip between two Zircaloy-4 cover plates and four side strips. Note that there are five types of fuel plates located in the assembly: end (Y), transition (T), secondary (W), standard (R), and intermediate (L). As shown in Table 2-4, the three assembly regions, i.e., Zones 1, 2, and 3, have different fissile loadings. Figure 2-8 gives a cross-sectional representation of a typical fuel plate (DOE 1999a, p. 10).

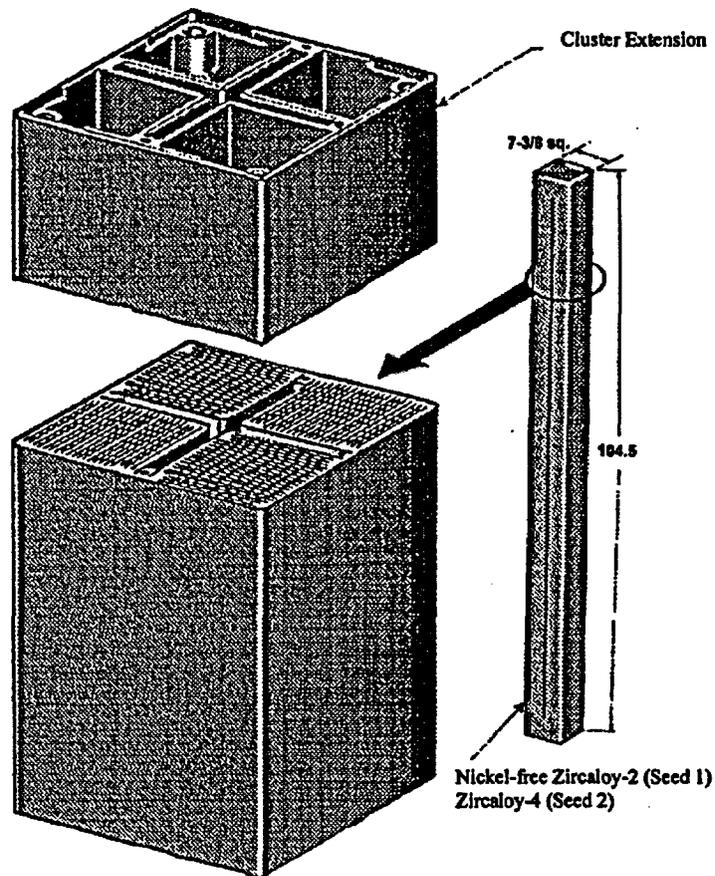


Figure 2-6. Shippingport C2 S2 SNF Assembly

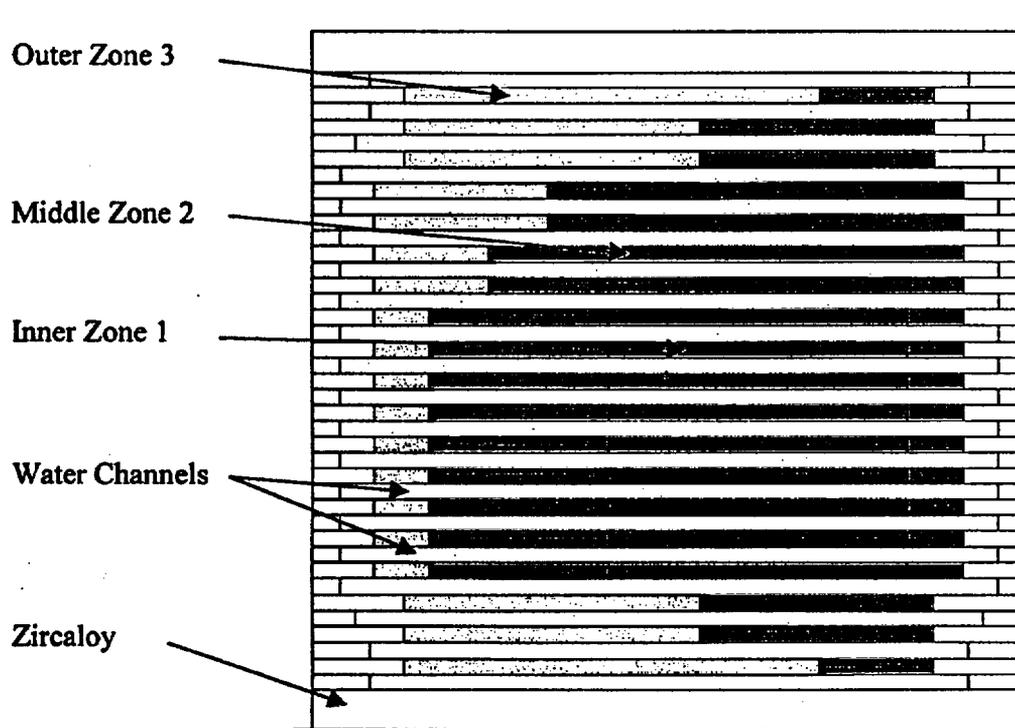


Figure 2-7. Shippingport C2 S2 SNF Sub-assembly Cross Section

Table 2-4. Geometry and Material Specifications for the Shippingport C2 S2 Assembly

Component	Material	Characteristic	Value
Assembly		Total mass (kg)	357
		Length (cm)	265.43
		Transverse dimensions (cm)	18.7325
Fuel plate		Active fuel length (cm)	246.38
Fuel wafer	UO ₂ -ZrO ₂ -CaO 93.2% U-235 beginning of life (BOL) enrichment	Length (cm)	2.07264
		Width (cm)	0.64008
		Thickness (cm)	0.09144
Fuel Zone 1	UO ₂ -ZrO ₂ -CaO	weight (wt)% UO ₂	54.9
		wt% CaO	5.2
		wt% ZrO ₂	39.9
		Fissile loading (kg)	7.076
Fuel Zone 2	UO ₂ -ZrO ₂ -CaO	wt% UO ₂	40.2
		wt% CaO	5.8
		wt% ZrO ₂	54
		Fissile loading (kg)	8.987
Fuel Zone 3	UO ₂ -ZrO ₂ -CaO	wt% UO ₂	26.5
		wt% CaO	6.4
		wt% ZrO ₂	67.1
		Fissile loading (kg)	3.437
Borated stainless steel	SS 304	Mass (g)	6,001
	B-10	Mass (g)	26
	B-11	Mass (g)	114
Spacer rings	Inconel X	Mass (g)	546
Chrome plating	Cr	Mass (g)	325
Cladding	Zircaloy-4	--	--

Source: DOE (1999a), pages 6, 7, 8, C-16, C-17, and C-18.

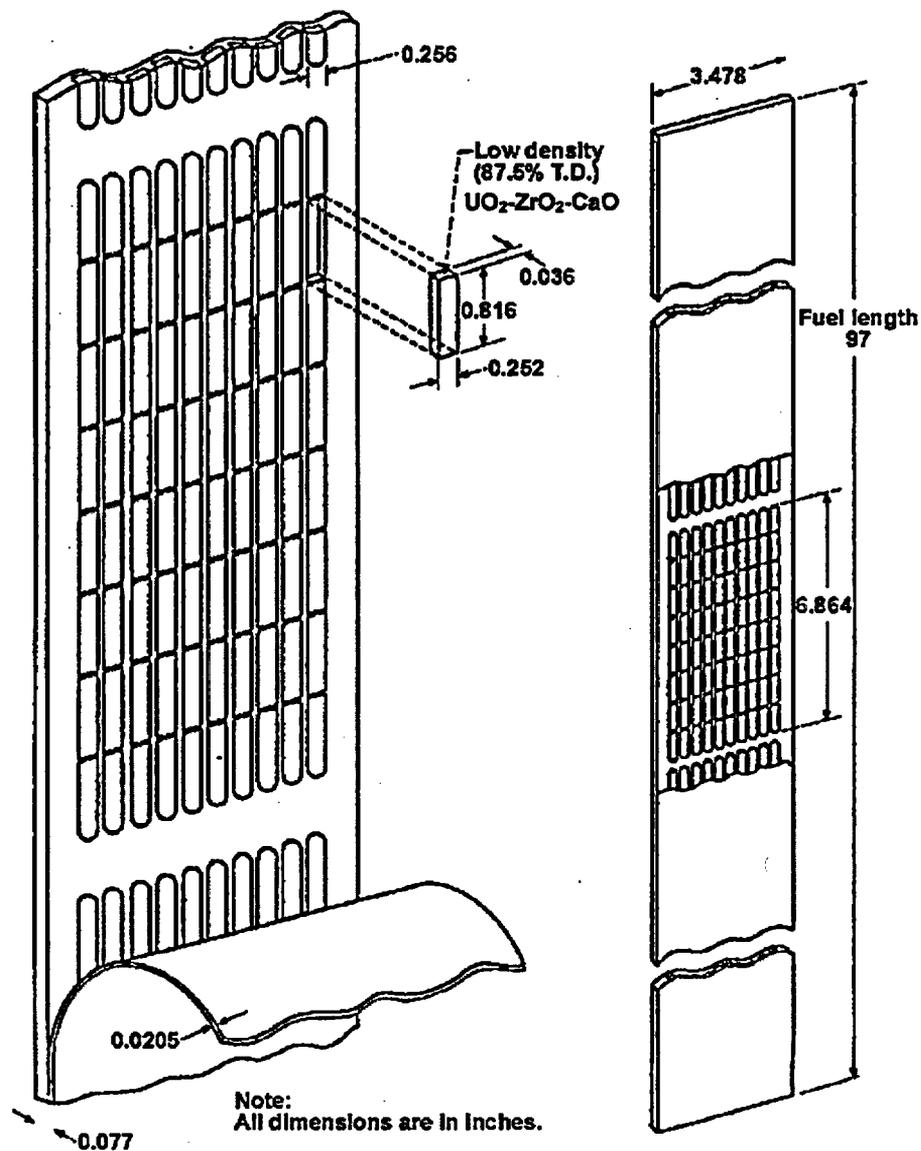


Figure 2-8. Fuel Plate

2.1.5 Thermal

The maximum heat generation rate from a Hanford 15-foot HLW glass canister is 2,540 W (Taylor 1997), which results in 12,700 W heat generation by five HLW glass canisters. Table 2-5 lists the heat output of each waste package component. The thermal properties of the Shippingport PWR fuel are determined as described in CRWMS M&O (1999f).

Table 2-5. Heat Output of Each Waste Package Component

Time Emplaced (years)	5 Hanford Long HLW Canisters (W)	Shippingport Fuel Zone 1 (W)	Shippingport Fuel Zone 2 (W)	Shippingport Fuel Zone 3 (W)	Waste Package Total (W)
0	2540.0	46.749	59.375	22.707	12828.8
0.1	2461.6	46.749	59.375	22.707	12436.8
0.2	2389.9	46.749	59.375	22.707	12078.3
0.3	2324.0	46.749	59.375	22.707	11748.8
0.4	2263.6	46.749	59.375	22.707	11446.8
0.5	2208.2	46.749	59.375	22.707	11169.8
0.6	2157.2	46.749	59.375	22.707	10914.8
0.7	2110.0	46.749	59.375	22.707	10678.8
0.8	2066.8	46.749	59.375	22.707	10462.8
0.9	2026.9	46.749	59.375	22.707	10263.3
1	1989.8	46.749	59.375	22.707	10077.8
2	1739.7	46.749	59.375	22.707	8827.3
3	1609.7	46.749	59.375	22.707	8177.3
4	1530.4	46.749	59.375	22.707	7780.8
5	1473.8	46.749	59.375	22.707	7497.8
6	1428.3	46.749	59.375	22.707	7270.3
7	1389.0	46.749	59.375	22.707	7073.8
8	1353.7	46.749	59.375	22.707	6897.3
9	1320.4	46.749	59.375	22.707	6730.8
10	1289.0	46.749	59.375	22.707	6573.8
20	1024.8	31.252	39.692	15.180	5210.1
30	819.0	31.252	39.692	15.180	4181.1
40	657.2	31.252	39.692	15.180	3372.1
50	529.5	31.252	39.692	15.180	2733.6
60	429.2	31.252	39.692	15.180	2232.1
70	349.9	31.252	39.692	15.180	1835.6
80	287.5	31.252	39.692	15.180	1523.6
90	237.9	31.252	39.692	15.180	1275.6
100	199.1	31.252	39.692	15.180	1081.6
200	61.8	31.252	39.692	15.180	395.1
300	41.7	31.252	39.692	15.180	294.6
400	33.2	31.252	39.692	15.180	252.1
500	27.4	31.252	39.692	15.180	223.1
600	22.4	31.252	39.692	15.180	198.1
700	18.4	31.252	39.692	15.180	178.1
800	15.2	31.252	39.692	15.180	162.1
900	12.5	31.252	39.692	15.180	148.6
1000	10.2	31.252	39.692	15.180	137.1

The thermal conductivity of the HLW glass is approximated as that of pure borosilicate glass, while the properties of density and specific heat are approximated as those of Pyrex glass. Only the axial cross section of the waste package at the center of the DOE SNF canister is represented in the calculations. The values of thermal conductivity, specific heat, and density for borosilicate glass are 1.1 W/m/K, 835.0 J/kg/K, and 2,225.0 kg/m³ respectively. The thermal conductivity is the mid-range value for a temperature range of 100 °C to 500 °C (CRWMS M&O 1995a, p. 13).

The density and specific heat are taken to be the same as that of Pyrex glass at 27 °C (300 K) (CRWMS M&O 1995a, p. 13).

2.1.6 Shielding Source Term

Although the material and geometry specifications of the Shippingport PWR C2 S2 fuel assembly are used in the calculations in Section 5, the gamma and neutron source terms are from the C2 S1 assembly. These sources are the bounding values for the Shippingport PWR fuel (DOE 1999a, pp. B-2 and B-3). Table 2-6 gives the details of the gamma sources and the total strength of each component.

Table 2-6. Gamma and Neutron Sources of the Shippingport C2 S1 Fuel Assembly at Year 2005

Upper Energy Boundary (MeV)	Gamma Intensity (photons/s)			Neutron Intensity (neutrons/s)
	Activation Products	Actinides and Daughters	Fission Products	
0.02	2.8410E+10	4.5890E+12	6.3430E+14	
0.03	9.1100E+09	5.9580E+10	1.1110E+14	
0.05	3.4820E+09	1.6890E+10	9.7230E+13	
0.07	2.3590E+09	8.6340E+11	1.0380E+14	
0.10	9.3670E+08	1.1830E+10	6.2850E+13	
0.15	3.9480E+08	6.3100E+09	4.2030E+13	
0.30	5.9420E+08	4.4630E+09	5.4170E+13	
0.45	2.8350E+09	2.3510E+09	2.3530E+13	
0.70	3.5670E+09	6.3060E+07	3.9300E+14	
1.00	4.4320E+09	4.9280E+07	5.5290E+12	
1.50	7.6130E+11	8.5050E+06	3.1620E+12	
2.00	2.9270E+05	4.4900E+06	1.5510E+11	
2.50	4.0350E+06	3.5760E+05	1.0790E+07	
3.00	1.2490E+04	3.9030E+07	2.2920E+00	
4.00	4.1600E-08	1.8430E+05	2.9960E-01	
6.00	8.8690E-09	7.8270E+04	1.5730E-05	
8.00	5.7540E-10	8.9510E+03	1.0210E-06	
14.00	3.6390E-11	1.0240E+03	6.4560E-08	
Total	8.1743E+11	5.5540E+12	1.4370E+15	2.680E+06

The SRS HLW glass canister gamma and neutron source spectra per canister (CRWMS M&O 1998c, Attachment III, p. 1; CRWMS M&O 1997b, Attachment IV, pp. 17 and 18) are given in Tables 2-7 and 2-8, respectively. Since the SRS HLW glass canisters are 3-m long, the sources for the 3-m long HLW glass canister are scaled up to correspond to a 15-ft HLW canister that will be placed in the 5-DHLW/DOE Spent Fuel-Long waste package.

Table 2-7. Gamma Sources for HLW Glass Canisters at One Day Decay Time

Upper Energy Boundary (MeV)	Average Energy (MeV)	SRS Total (photons/sec)
0.05	0.0300	2.0480E+15
0.10	0.0750	6.1351E+14
0.20	0.1500	4.7986E+14
0.30	0.2500	1.3546E+13
0.40	0.3500	9.9093E+13
0.60	0.5000	1.3681E+14
0.80	0.7000	2.0891E+15
1.00	0.9000	3.3083E+13
1.33	1.1650	4.5956E+13
1.66	1.4950	9.9450E+12
2.00	1.8300	7.9634E+11
2.50	2.2500	4.5524E+12
3.00	2.7500	3.1682E+10
4.00	3.5000	3.5394E+09
5.00	4.5000	8.1428E+09
6.50	5.7500	3.2640E+05
8.00	7.2500	6.3958E+04
10.00	9.0000	1.3589E+04
	Total	5.6962E+15

Table 2-8. Neutron Sources for HLW Glass Canisters at One Day Decay Time

Upper Energy Boundary (MeV)	Average Energy (MeV)	SRS Total (n/sec)
20.000	13.2150	4.7557E+05
6.430	4.7150	5.2948E+07
3.000	2.4250	4.0517E+07
1.850	1.6250	9.4907E+06
1.400	1.1500	1.0724E+07
0.900	0.6500	9.8224E+06
0.400	0.2500	2.9342E+06
0.100	0.0585	3.0535E+05
	Total	1.2722E+08

2.1.7 Material Compositions

The chemical compositions of the materials used in the analyses are given in Tables 2-9 through 2-12. The composition of the HLW glass shown in Table 2-13 is based on the assumption that both 3-m and 15-ft canisters have the same glass composition.

Table 2-9. Chemical Composition of ASTM B 575 (Alloy 22)

Element	Composition (wt%)	Value Used (wt%)
Carbon (C)	0.015 (max)	0.015
Manganese (Mn)	0.50 (max)	0.50
Silicon (Si)	0.08 (max)	0.08
Chromium (Cr)	20.0 - 22.5	21.25
Molybdenum (Mo)	12.5 - 14.5	13.5
Cobalt (Co)	2.50 (max)	2.50
Tungsten (W)	2.5 - 3.5	3.0
Vanadium (V)	0.35 (max)	0.35
Iron (Fe)	2.0 - 6.0	4.0
Phosphorus (P)	0.02 (max)	0.02
Sulfur (S)	0.02 (max)	0.02
Nickel (Ni)	Balance	54.765
Density = 8.69 g/cm ³		

Source: ASTM B 575-94, page 2.

Table 2-10. Chemical Composition of ASTM A 516 Grade 70 Carbon Steel

Element	Composition (wt%)	Value Used (wt%)
Carbon (C)	0.30 (max)	0.30
Manganese (Mn)	0.85-1.20	1.025
Phosphorus (P)	0.035 (max)	0.035
Sulfur (S)	0.035 (max)	0.035
Silicon (Si)	0.15-0.40	0.275
Iron (Fe)	Balance	98.33
Density ^a = 7.832 g/cm ³		

Source: ASTM A 516/A 516M - 90, page 2.

NOTE: ^a Density of this material is given as 7.850 g/cm³ in ASTM G 1-90, page 7.

Table 2-11. Chemical Composition of Stainless Steel Type 304L

Element	Composition (wt%)	Value Used (wt%)
Carbon (C)	0.03 (max)	0.03
Manganese (Mn)	2.00 (max)	2.00
Phosphorus (P)	0.045 (max)	0.045
Sulfur (S)	0.03 (max)	0.03
Silicon (Si)	0.75 (max)	0.75
Chromium (Cr)	18.00 - 20.00	19.00
Nickel (Ni)	8.00 - 12.00	10.00
Nitrogen (N)	0.10	0.10
Iron (Fe)	Balance	68.045
Density ^a = 7.94 g/cm ³		

Source: ASTM A 240/A 240M-97a, page 2.

NOTE: ^a Density of this material is given as 7.94 g/cm³ in ASTM G 1-90, page 7 and as 8.0 g/cm³ in ASM (1990, p. 871).

Table 2-12. Chemical Composition of Stainless Steel Type 316L

Element	Composition (wt%)	Value Used (wt%)
Carbon (C)	0.03 (max)	0.03
Manganese (Mn)	2.00 (max)	2.00
Phosphorus (P)	0.045 (max)	0.045
Sulfur (S)	0.03 (max)	0.03
Silicon (Si)	1.00 (max)	1.0
Chromium (Cr)	16.00 - 18.00	17.00
Nickel (Ni)	10.00 - 14.00	12.00
Molybdenum (Mo)	2.00 - 3.00	2.50
Nitrogen (N)	0.10 (max)	0.10
Iron (Fe)	Balance	65.295
Density ^a = 7.98 g/cm ³		

Source: ASTM A 276-91a, page 2.

NOTE: ^a Density of this material is given as 7.98 g/cm³ in ASTM G 1-90, page 7 and as 8.0 g/cm³ in ASM (1990, p. 871).

Table 2-13. Chemical Composition of SRS HLW Glass

Component	Water Free wt%	Radioisotope	g/Canister
Ag	0.06	Rh-103m	0.5028E-15
Al ₂ O ₃	3.96	Sm-149	0.742E+1
B ₂ O ₃	10.28	U-233	0.1636E-3
BaSO ₄	0.14	U-234	0.5485E+1
Ca ₃ (PO ₄) ₂	0.07	U-235	0.7278E+2
CaO	0.85	U-236	0.1742E+2
CaSO ₄	0.08	U-238	0.3122E+5
Cr ₂ O ₃	0.12	Np-237	0.1263E+2
Cs ₂ O	0.08	Pu-238	0.8667E+2
CuO	0.19	Pu-239	0.2076E+3
Fe ₂ O ₃	7.04	Pu-240	0.3809E+2
FeO	3.12	Pu-241	0.1620E+2
K ₂ O	3.58	Pu-242	0.3206E+1
Li ₂ O	3.16	Am-241	0.3210E+1
MgO	1.36	Am-242m	0.1488E-2
MnO	2.00	Am-243	0.2902E-1
Na ₂ O	11.00	Cm-245	0.3910E-4
Na ₂ SO ₄	0.36		
NaCl	0.19		
NaF	0.07		
NiO	0.93		
PbS	0.07		
SiO ₂	45.57		
ThO ₂	0.21		
TiO ₂	0.99		
U ₃ O ₈	2.20		
Zeolite	1.67		
ZnO	0.08		
Others	0.58		
Total	100.00		
Density at 25°C = 2.85 g/cm ³			

Sources: Stout, R.B. and Leider, H.R. (1991), pages 2.2.1.4-3 through 2.2.1.4-5, and page 2.2.1.4-11; (CRWMS M&O 1998c, Attachment V).

NOTE: HLW glass canisters with immobilized plutonium are not considered in the analyses.

2.1.8 Degradation and Geochemistry

This section identifies the degradation rate of the principal alloys, the chemical composition of J-13 well water, and the drip rate of J-13 well water into a waste package. These rates are used in Section 6, Degradation and Geochemistry Analyses.

2.1.8.1 Physical and Chemical Form of Shippingport Waste Package

Table 2-14 summarizes the degradation rates of the principal alloys used in the calculations. The lower rate for A 516 is 60 °C, 100-year rate, and the upper rate for A 516 is the 0-year rate (CRWMS M&O 1995b, Figure 5.4-3). The 304L and 316L rates are estimated from CRWMS M&O (1997c, pp. 11 through 13). For a comparable specific surface area, the carbon steel is expected to degrade much more rapidly than the stainless steels (Type 316L and Type 304L). In addition, the stainless steels contain significant amounts of chromium (Cr) and molybdenum (Mo), and under the assumption of complete oxidation, would produce more acid, per unit volume, than the carbon steel.

Table 2-14. Steel Degradation Rates

	A 516 Carbon Steel	SS 304L	SS 316L
Average rate ($\mu\text{m}/\text{yr}$)	35	0.1	0.1
Average rate ($\text{moles}/\text{cm}^2/\text{sec}$)	1.58E-11	4.58E-14	4.55E-14
High rate ($\mu\text{m}/\text{yr}$)	100.0	1.0	1.0
High rate ($\text{moles}/\text{cm}^2/\text{sec}$)	4.51E-11	4.58E-13	4.55E-13

The actual glass composition used in the HLW glass pour canisters may vary significantly from the values used in the calculations, since the sources of the glass and melting processes are not currently fixed. Compositions proposed for SRS glass vary by a factor of ~6 in U_3O_8 content, from 0.53 to 3.16 wt% (DOE 1992, p. 3.3-15). The silica and alkali (Na, Li and K) contents of the glass have perhaps the most significant bearing on EQ3/6 calculations. The amount of silica in the glass strongly controls the amount of clay that forms in the waste package, and the silica activity controls the presence of insoluble uranium phases such as soddyite ($(\text{UO}_2)_2\text{SiO}_4 \cdot 2\text{H}_2\text{O}$). The alkali content can induce the pH to rise in the early stages of the EQ3/6 run, as glass degrades; the alkaline earth elements (Ca, Ba, Mg), by forming sparingly soluble solid carbonates, can buffer the pH for longer times. The Si and alkali contents of the glass used are typical for proposed DOE glasses, but alkaline earth content is low, and the uranium content (of the glass) in Table 2-13 is high compared to compositions recently produced at Savannah River (Bibler et al. 1998, p. 10). However, this high uranium content is conservative, since it enhances the precipitation of uranium solids, and ultimately the retention of fissile materials within the package. Table 2-15 rates for glass degradation are taken from CRWMS M&O (1995b), Figure 6.2-5. The high rate corresponds approximately to a pH 9 at 70 °C; the low rate, to a pH 8 at 25 °C.

Table 2-15. Glass Degradation Rates

Low rate (g/m ² /day)	1E-04
Low rate ^a (moles/cm ² /sec)	1.1574E-15
High rate (g/m ² /day)	3E-02
High rate (moles/cm ² /sec)	3.4722E-13

NOTE: ^aFor 1 mole in 100 grams.

Table 2-16 summarizes the characteristics and degradation rates of the Shippingport PWR fuel. The calculations used the composition of fresh fuel. Using values for fresh fuel is conservative, since most fission products have significant neutron-absorption cross sections, and the unirradiated fuel has a higher fissile content than that of partially spent fuel. Also, since it is expected that very few waste packages will be breached before thousands of years post-emplacment, and that most of the calculation will involve post-emplacment periods greater than 10,000 years, the HLW glass composition used in EQ6 geochemistry calculations is altered to pre-decay some of the shorter-lived isotopes (Pu-238 and Pu-241). Since EQ3/6 does not have the capability to decay isotopes, this was done manually.

Table 2-16. Shippingport PWR Characteristics and Degradation Rates

Average molecular weight (UO ₂ , CaO, ZrO ₂)	50.79
Average density of fuel wafers (g/cm ³)	5.80
Low fuel degradation rate (mg/m ² /day)	0.05
Low fuel degradation rate (moles/cm ² /sec)	1.1394E-15
Moderate fuel degradation rate (mg/m ² /day)	1
Moderate fuel degradation rate (moles/cm ² /sec)	2.2788E-14
Fast fuel degradation rate (mg/m ² /day)	30
Fast fuel degradation rate (moles/cm ² /sec)	6.83643E-13

Sources: DOE (1999a), page C-14; and CRWMS M&O (1999e), page 21.

2.1.8.2 Chemical Composition of J-13 Well Water

The geochemistry calculations reported in this document have used the standard J-13 well water composition, which is reproduced in Table 2-17 (DTN: LL980711104242.054), for water dripping into the waste package. Since this water composition was determined from a well drilled into the saturated zone beneath the planned repository location, there is some question about the compositional deviations to be expected for water dripping into the repository drift, which is in the unsaturated zone. Several alternative versions of the J-13 well water composition have been proposed and used in other geochemistry calculations. The following two paragraphs summarize current thinking on the sensitivity of geochemistry results to potential variations in the composition of the water entering the waste package.

Table 2-17. Composition of J-13 Well Water

Component	mg/l
Na ⁺	45.8
K ⁺	5.04
Ca ²⁺	13.0
Mg ²⁺	2.01
NO ₃ ⁻	8.78
Cl ⁻	7.14
F ⁻	2.18
SO ₄ ²⁻	18.4
Si ²⁺	28.5
PO ₄ ³⁻	0.12
Alkalinity (assumed to be HCO ₃ ⁻)	128.9
pH = 7.41	

Source: LL980711104242.054.

Two major factors control how the J-13 well water chemistry might affect EQ6 calculations. The first factor is the presumed CO₂ pressure of equilibration, which is closely coupled to the pH of the J-13 well water. The second factor is the content of dissolved species, which may react with package materials and fuel, and thus affect solubilities. The pH is an important factor in the solubility of the fissile elements and neutron absorber. An example of the second factor is the amount of available dissolved silica, which can precipitate uranium as insoluble minerals like soddyite and uranophane.

In codisposal packages, the chemistry of the package water is influenced, overwhelmingly, by the degradation of glass and other package materials. The alkali and alkaline earth content of the glass completely swamped the native J-13 well water composition in the bulk of the EQ6 scenarios run for the EQ6 geochemical calculations (CRWMS M&O 1998e). The combination of steel and glass degradation drove the pH from ~3 to ~10, far greater than the range that exists in native J-13 well water (CRWMS M&O 1998e, Figures 5-2 through 5-20). The silica content built into the glass is enormously greater than the amount of silica that can be contributed from J-13 well water, even with long periods of flushing at high rates. The calculations in CRWMS M&O (1998e) showed that in cases of significant uranium and plutonium solubility, the dominant aqueous species were carbonate and phosphate complexes. The phosphate was supplied overwhelmingly from the glass, and the high aqueous carbonate was controlled by the pH (which resulted from glass dissolution and the assumption of fixed CO₂ pressure).

2.1.8.3 Drip Rate of J-13 Well Water into a Waste Package

The rates at which water drips onto a waste package and flows through it are represented as being equal. The drip rate is taken from a correlation between the percolation rate and the drip rate (CRWMS M&O 1998g, pp. 2.3-105 through 2.3-107, and Figure 2.3-110). Specifically,

percolation rates of 40 mm/yr and 8 mm/yr correlate with drip rates onto the waste package of 0.15 m³/yr and 0.015 m³/yr, respectively.

For the present study, the range of allowed drip rates is extended to include an upper value of 0.5 m³/yr and a lower value of 0.0015 m³/yr. The upper value corresponds to the 95 percentile upper limit for a percolation rate of 40 mm/yr (as determined in CRWMS M&O 1998g, pp. 2.3-105 through 2.3-107), and the lower value is simply 0.1 times the mean value for the present 8 mm/yr percolation rate. These extreme values are used, because prior studies (CRWMS M&O 1998f, pp. 18 and 19) suggested that when ceramic waste forms are codisposed with glass, the greatest chance of Gd removal occurs when: (1) initial high drip rates cause glass leaching and removal of alkali and (2) subsequent low drip rates allow acid to build up from the degradation of the steel. Although the waste package with Shippingport PWR fuel does not need any neutron absorber, these extreme values were conservatively used.

2.2 FUNCTIONS AND DESIGN CRITERIA

The design criteria are based on *DOE Spent Nuclear Fuel Disposal Container System Description Document* (CRWMS M&O 1998h), which is referred to as the SDD. The SDD numbers, which follow, are paragraph numbers from that document. In this section, the key waste package design criteria from the SDD are identified for the following areas: structural, thermal, shielding, intact criticality, degradation and geochemistry, and degraded component criticality.

2.2.1 Structural

2.2.1.1 "The disposal container shall retain the capability to be unloaded after the occurrence of the events listed in Section 1.2.2.1."

[SDD 1.2.1.17]

2.2.1.2 "The disposal container shall be designed to withstand transfer, emplacement, and retrieval operations without breaching."

[SDD 1.2.1.22]

2.2.1.3 "During the preclosure period, the disposal container, while in a vertical orientation, shall be designed to withstand a drop from a height of 2 m (6.6 ft) (TBV-245) without breaching. (TBV-245)"

[SDD 1.2.2.1.3] [TBV-245]

2.2.1.4 "During the preclosure period, the disposal container, while in a horizontal orientation, shall be designed to withstand a drop from a height of 2.4 m (7.9 ft) (TBV-245) without breaching. (TBV-245)"

[SDD 1.2.2.1.4] [TBV-245]

2.2.1.5 "During the preclosure period, the disposal container shall be designed to withstand a tip over from a vertical position with slap down onto a flat, unyielding surface without breaching. (TBV-245)"

[SDD 1.2.2.1.6] [TBV-245]

Calculations of maximum potential energy for each handling accident scenario (horizontal drop, vertical drop, and tipover design-basis events [DBEs]) showed that the bounding dynamic load is obtained from a tipover case in which the rotating top end of the waste package experiences the highest g-load with maximum velocity of 9.5 m/sec (CRWMS M&O 1999b, p. 16). The maximum velocities of the waste package for 2.4 m horizontal and 2.0 m vertical drops are approximately 6.86 m/sec ($v = \sqrt{2gh}$, where g is the gravitational acceleration, and h is height) and 6.26 m/sec, respectively. Therefore, tipover structural evaluations are bounding for all handling accident scenarios considered in the SDD. Section 3.3 addresses these requirements. All other accident scenarios (from CRWMS M&O 1997e) are considered non-credible. This analysis assumes that MGR surface design will prevent events that exceed the bounding assumptions made in deriving the conclusions in this report.

The tipover DBE may only take place during a waste package transfer operation from vertical to horizontal (just after waste package closure) or horizontal to vertical (upon retrieval). Section 3, Structural Analysis, demonstrates that the waste package will not breach under such a handling-accident scenario.

2.2.2 Thermal

2.2.2.1 "The disposal container shall limit the zircaloy and stainless steel cladding temperature to less than 350 °C (TBV-241). Temperature of other types of DOE fuel cladding shall be limited to (TBD-179) °C. Exceptions to these temperature limits are given in Section 1.2.2.1."

[SDD 1.2.1.8] [TBV-241][TBD-179]

2.2.2.3 "The disposal container shall be designed to have a maximum thermal output of 18 kW (1025 BTU/min.) (TBV-251) or less. This criteria identifies the primary disposal container interface with the Ex-Container System."

[SDD 1.2.4.9] [TBV-251]

The criteria are met as described in Sections 4 and 8.2.

2.2.3 Shielding

"Disposal container design shall reduce the dose rate at all external surfaces of a loaded and sealed disposal container to 355 rem/hr (TBV-248) or less. This criteria identifies the primary disposal container interface with the Waste Emplacement System and the Disposal Container Handling System."

[SDD 1.2.4.7] [TBV-248]

The criterion is met as described in Sections 5 and 8.3.

2.2.4 Degradation and Geochemistry

There are no degradation and geochemistry criteria in the SDD to address.

2.2.5 Intact and Degraded Component Criticality

2.2.5.1 "The disposal container provides sufficient criticality control during loading and after it is loaded with waste."

[SDD 1.1.3]

The function is met as described in Sections 7.3, 7.4, 7.5 and 8.5.

2.2.5.2 "During the preclosure period, the disposal container shall be designed 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 system must be designed for criticality safety assuming occurrence of design basis events, including those with the potential for flooding the disposal container prior to disposal container sealing (TBD-235) or misloading canisters (TBD-235). 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 method of calculation."

[SDD 1.2.1.5] [TBD-235]

As stated in Section 8.5, the results from the intact criticality analysis show that the requirement of k_{eff} plus bias and uncertainty less than or equal to 0.95 is satisfied.

2.3 ASSUMPTIONS

In the course of developing this document, assumptions are made regarding the waste package structural, thermal, shielding, intact criticality, degradation and geochemistry, and degraded component criticality analyses. The list of the major assumptions that are essential to this technical document is provided below.

2.3.1 Structural

The assumptions in this section are used throughout Section 3.

2.3.1.1 The waste package containment barriers are assumed to have solid connections at the adjacent surfaces. The basis for this assumption is that the inner and outer barriers will be either shrunk fit or the inner barrier will be weld clad onto the outer barrier inner surface (CRWMS M&O 1997a).

2.3.1.2 The target surface is conservatively assumed to be essentially unyielding by using a large elastic modulus for the target surface compared to the waste package. The basis for this assumption is that a bounding set of results is required in terms of stresses and displacements and it is known that the use of an essentially unyielding surface results in slightly higher stresses in the waste package.

2.3.2 Thermal

The assumptions in this section are used throughout Section 4.

2.3.2.1 The volumetric heat generation of the HLW and the Shippingport PWR C2 S2 SNF assembly is assumed constant over the axial and radial cross section of each heat-generating element. The basis of this assumption is the following: heat generation for the HLW, which is geometrically uniform, does not exhibit any peaking behavior. Heat generating elements are dispersed (from vitrification) throughout the glass matrix. In addition, the Shippingport PWR C2 S2 SNF assembly has small heat generating fuel wafers distributed in axial and radial arrays. This even distribution of heat generating elements would negate any thermal peaking effect.

2.3.2.2 Representing only conduction and radiant heat transfer inside the waste package is assumed to provide conservative results (higher temperature) for the calculations. The basis for this assumption is the following: fill gas within the waste package will allow natural convective heat transfer to exist. However, since only a few small enclosed basket cavities exist and the temperature gradient in the enclosure is not significant, circulation of the fill gas is insignificant. Thus, the problem may be represented with only the dominant heat transfer modes, with a negligible or conservative impact upon the results.

2.3.2.3 It is assumed that a 2-D finite-element representation of a cross section at the midsection of the waste package will be the hottest portion of the waste package. Inherent to this assumption is that axial heat transfer does not significantly affect the solution. The basis for this assumption is that the metal thermal conductivity and heat generation distributions are such that axial heat transfer is very small or negligible at the midsection.

2.3.2.4 The surface temperature history of the 5-DHLW/DOE Spent Fuel-Long waste package is assumed to be equivalent to the 12 PWR average waste package given in CRWMS M&O (1998d) (Scenario 3, WP1). The basis for this assumption is the similarity in the thermal decay heat curves for each waste package type. In addition, CRWMS M&O (1999m) performed a calculation of the Hanford long HLW waste package loaded with Fast Flux Test Facility mixed oxide fuel. This calculation was performed with a simulated waste package surface temperature history (calculated from a curve fit) and the surface temperature history of the 12 PWR average waste package. It was found that using the boundary conditions from the 12 PWR average waste package was slightly more conservative (resulted in slightly higher temperatures).

2.3.3 Shielding

The assumptions in this section are used throughout Section 5.

2.3.3.1 The Shippingport PWR C2 S1 fuel assembly is homogenized inside its transverse dimensions. The basis for this assumption is that the calculated surface dose rates will be conservative, because the homogenization process essentially moves the radiation

source closer to the outer surfaces of the fuel assembly, allowing more particles to reach the outer surface, and decreases the self-shielding of the fuel (CRWMS M&O 1998k, p. 23).

- 2.3.3.2 A power peaking factor of 1.25 is used for the Shippingport PWR fuel source for bounding the axial source distribution. This value is based on the predicted heat profile shown in Creer et al. (1987, p. 3-29, Fig. 3-18). The basis for this is that the source term, provided by a depletion calculation, was uniformly created within the fuel volume and the axial source profile must be considered in shielding calculations.
- 2.3.3.3 The Watt fission neutron spectrum (Briesmeister 1997, p. 3-50) is used for the Shippingport PWR neutron fuel-source distribution. This option assumes that the most likely neutron energy is about 1 MeV. The basis for this is that the resulting biological neutron dose is bounding, since the quality factor has the highest value for this energy (Briesmeister 1997, App. H, p. 5).
- 2.3.3.4 The neutron source intensity is nine and eight orders of magnitude smaller than the gamma source intensity for the Shippingport PWR fuel and HLW, respectively. No coupled neutron-photon calculation is performed. The basis for this is that the dose rate due to secondary gamma rays is negligible.

2.3.4 Degradation and Geochemistry

The assumptions in this section are used throughout Section 6.

- 2.3.4.1 It is assumed that water may circulate sufficiently freely in the partially degraded waste package that all degraded solid products may react with each other through the aqueous solution medium. The basis for this assumption is that this provides one bound for the extent of chemical interactions within the waste package.
- 2.3.4.2 It is assumed that the corrosion resistant material (inner barrier) of the waste package will react so slowly with the infiltrating water (and water already in the waste package) that it will have a negligible effect on the chemistry. The basis of this assumption is the fact that the corrosion resistant material is fabricated from Alloy 22, which corrodes very slowly compared (1) to other reactants in the waste package, and (2) to the rate at which soluble corrosion products will likely be flushed from the waste package.
- 2.3.4.3 It is assumed that precipitated solids that are deposited remain in place and are not mechanically eroded or entrained as colloids in the advected water. The basis of this assumption is that since dissolved fissile material may be adsorbed on colloids (clays, iron oxides) or precipitated as colloids during waste package degradation, it is conservative, for internal criticality, to assume that all precipitated solids, including mobile colloids, will be deposited inside the waste package rather than transported out of the waste package.
- 2.3.4.4 It is assumed that over times of interest sufficient decay heat is retained within the waste package to cause convective circulation and mixing of the water inside the waste

package. The analysis that serves as the basis of this assumption is discussed in CRWMS M&O (1996, Attachment VI).

2.3.5 Intact and Degraded Component Criticality

The assumptions in this section are used throughout Section 7.

2.3.5.1 Beginning of life (BOL), pre-irradiation fuel compositions of Shippingport PWR SNF were used for all calculations. The basis of this assumption is that for Shippingport PWR SNF, it is conservative to assume fresh fuel as it is more neutronically reactive than spent fuel.

2.3.5.2 Burnable neutron absorber material (boron) in two end plates (referred to as "poison wafers") of the fuel subassembly were represented as water. The basis of this assumption is that it is conservative to neglect burnable neutron absorber material since it provides some additional amount of neutron absorption.

2.4 BIAS AND UNCERTAINTY IN CRITICALITY CALCULATIONS

The purpose of this section is to document the MCNP (CRWMS M&O 1998i), which is identified as Computer Software Configuration Item (CSCI) 30033 V4B2LV, evaluations of Laboratory Critical Experiments (LCEs) performed as part of the Disposal Criticality Analysis Methodology program. Only LCEs relevant to Shippingport PWR fuel are studied. LCE's results listed in this section are given in CRWMS M&O (1999c) for the thermal compound HEU systems and in CRWMS M&O (1999d) for the thermal solution uranium systems. The objective of this analysis is to quantify the MCNP Version 4B2 code system's ability to accurately calculate the effective neutron multiplication factor (k_{eff}) for various configurations. MCNP is set to use continuous-energy cross sections processed from the evaluated nuclear data files ENDF/B-V (Briesmeister 1997, App. G). These cross section libraries are part of the MCNP code system that has been obtained from the Software Configuration Management (SCM) in accordance with appropriate procedures. Each of the critical core configurations is simulated, and the results reported from the MCNP calculations are the combined average values of k_{eff} from the three estimates (collision, absorption, and track length) and the standard deviation of these results (σ) listed in the final generation summary in the MCNP output. When MCNP underpredicts the experimental k_{eff} , the experimental uncertainty is added to the uncertainty at 95% confidence from the MCNP calculation to obtain the bias. This bias along with the 5% margin (see Section 2.2.5.2) is used to determine the interim critical limit for all MCNP calculations of the waste package with Shippingport PWR DOE SNF canister.

2.4.1 Benchmarks Related to Intact Waste Package Configurations

Several critical experiments with highly enriched fuel rods are relevant for the Shippingport PWR fuel with respect to intact criticality analyses: HEU-COMP-THERM-003, HEU-COMP-THERM-005, HEU-COMP-THERM-006, and HEU-COMP-THERM-007 (NEA 1998).

A series of critical experiments with water-moderated hexagonally-pitched lattices of highly enriched fuel rods of cross-shaped cross section was performed over several years in the Russian

Research Center "Kurchatov Institute." The 22 experiments analyzed under this category in this report consist of the following:

1. Fifteen critical two-zone lattice experiments corresponding to different combinations of inner and peripheral zones of cross-shaped fuel rods at two pitches. For detailed descriptions of these experimental configurations see pages 2, and 7 through 14 of NEA (1998), HEU-COMP-THERM-003 (HCT-003).
2. One critical configuration of hexagonal pitched clusters of lattices of fuel rods with copper (Cu) rods. Detailed experimental configuration descriptions are available on pages 2 through 8 of NEA (1998), HEU-COMP-THERM-005 (HCT-005).
3. Three critical configurations with uniform hexagonal lattices with pitch values of 5.6, 10.0, and 21.13 mm. Detailed experimental configuration descriptions are available on pages 2, 5, and 6 of NEA (1998), HEU-COMP-THERM-006 (HCT-006).
4. Three critical configurations with double hexagonal lattices of fuel rods and zirconium (Zr) hydride rods. Detailed experimental configuration descriptions are available on pages 2 through 8 of NEA (1998), HEU-COMP-THERM-007 (HCT-007).

The pitch, number of rods, and number of fuel rods were the parameters that were varied. The maximum bias for this set of calculations is 0.019 (CRWMS M&O 1999c, pp. 16 through 19, and 76).

2.4.2 Benchmarks Related to Degraded Waste Package Configurations

Critical experiments with HEU (approximately 90 wt%) nitrate solution are described in detail in NEA (1998) (HEU-SOL-THERM-001, HEU-SOL-THERM-002, HEU-SOL-THERM-003). The concentration of fissile element in the solution, enrichment, reflector type and thickness, tank diameter, and solution height were among the parameters that were varied. The maximum bias for this set of experiments is 0.016 (CRWMS M&O 1997d, pp. 26 through 32; CRWMS M&O 1999d, pp. 14 through 18).

2.4.3 Critical Limit

The worst-case bias, calculated from the MCNP simulations of the experiments described in Sections 2.4.1 and 2.4.2, is 0.02. This bias includes the bias in the method of calculation and the uncertainty in the experiments. Based on this bias, the interim critical limit is determined to be 0.93 after a 5 percent margin; allowance for the bias in the method of calculation, and the uncertainty in the experiments used to validate the method of calculation. This interim critical limit will be used until the addenda to the topical report is prepared to establish the final critical limit.

3. STRUCTURAL ANALYSIS

3.1 USE OF COMPUTER SOFTWARE

The finite-element analysis (FEA) computer code used to analyze the 5-DHLW/DOE Spent Fuel-Long waste package with the Shippingport PWR DOE SNF canister in the center is ANSYS version V5.4. ANSYS V5.4 is identified with the CSCI 30040 V5.4 and is obtained from SCM in accordance with appropriate procedures. ANSYS V5.4 is a commercially available FEA code. ANSYS V5.4 software is qualified as documented in the Software Qualification Report (SQR) for ANSYS V5.4 (CRWMS M&O 1998j).

3.2 DESIGN ANALYSIS

Finite-element solutions resulted from structural analyses for the components of the 5-DHLW/DOE Spent Fuel-Long waste package. A detailed description of the finite-element representations, the method of solution, and the results are provided in CRWMS M&O (1998b) and CRWMS M&O (1999b). The results of these analyses are compared to the design criteria obtained from the 1995 American Society of Mechanical Engineers (ASME) Boiler and Pressure Vessel Code (BPVC), Section III, Subsection NB (ASME 1995), so that conclusions can be drawn regarding the structural performance of the 5-DHLW/DOE Spent Fuel-Long waste package design.

The design approach for determining the adequacy of a structural component is based on the stress limits given in the 1995 ASME BPVC. S_u is defined as the ultimate tensile strength of the materials, and S_m is defined as the design stress intensity of the materials. Table 3-1 summarizes design criteria as obtained from appropriate sections of the 1995 ASME BPVC.

Table 3-1. Containment Structure Allowable Stress-limit Criteria

Category	Containment Structure Allowable Stresses	
	Normal Conditions (ASME 1995, Division 1, Subsection NB, Articles NB-3221.1 and NB-3221.3)	Accident Conditions (ASME 1995, Division 1, Appendix F, Article F-1341.2)
Primary membrane stress intensity	S_m	$0.7S_u$
Primary membrane and bending stress intensity	$1.5S_m$	$0.9S_u$

The stresses calculated in this analysis are within the bounds of the structural criteria from the SDD (CRWMS M&O 1998h). This analysis does not consider other DBEs (e.g., crane two-block events), which are considered non-credible.

3.3 CALCULATIONS AND RESULTS

3.3.1 Description of the Finite-element Representation

A two-dimensional (2-D) finite-element representation of the 5-DHLW/DOE Spent Fuel-Long waste package is developed to determine the effects of loads from the tipover DBE on the

structural components (CRWMS M&O 1999b). The representation of the waste package includes the outer and inner barriers, the basket, the support tube, the DOE SNF canister and its basket and support tube, and the HLW pour canisters. This representation corresponds to a 2-D (x-y) slice from the middle of the waste package. After a tipover DBE onto an unyielding surface, the waste package lies horizontally as shown in Figure 3-1. A half-symmetry finite-element representation of the waste package was used. The barriers are assumed to have solid connections at the adjacent surfaces (Assumption 2.3.1.1) and are constrained in a direction perpendicular to the symmetry plane. It was shown in CRWMS M&O (1998b) that there is no closure of gap between the support tube and the DOE SNF canister, and there is no structural load transferred from the support tube to the DOE SNF canister. Since all calculations are 2-D, masses per unit length are calculated based on the maximum allowable weight limits. The maximum weight limits, which are higher than the weight limits in DOE (1998b, p. 6), from the SDD (CRWMS M&O 1998h, Table 1-2) is used to calculate the stresses on the support tube and waste package basket plates.

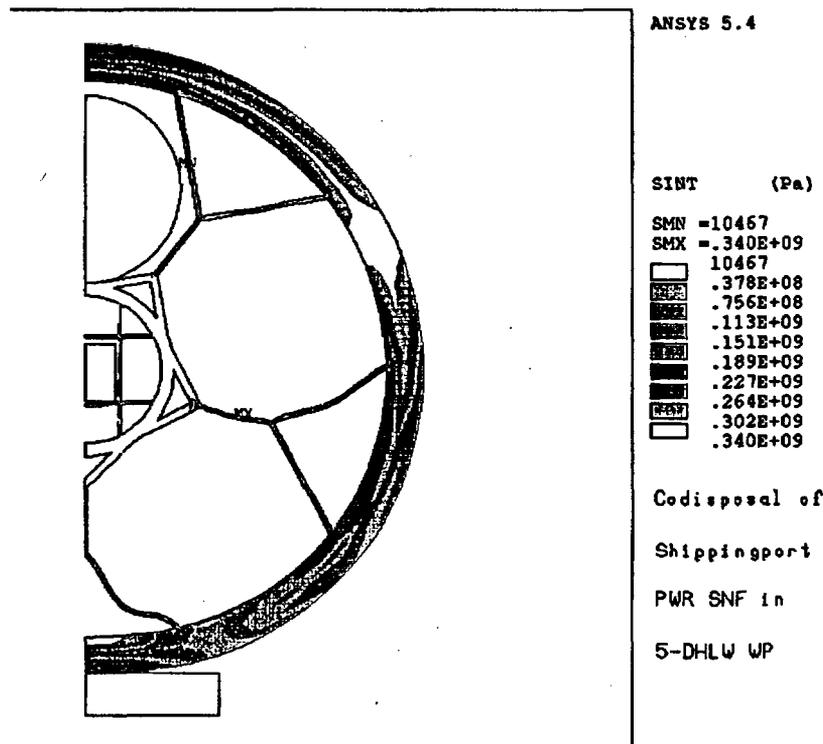


Figure 3-1. Stresses in 5-DHLW/DOE Spent Fuel-Long Waste Package

The finite-element representation is used to determine the maximum closure of the clearance gaps inside the DOE SNF canister-basket plates so that they can be compared to the Shippingport fuel assembly dimensions to determine whether there is contact between the basket plates and the fuel assembly. A 2-D finite-element representation of the 5-DHLW/DOE Spent Fuel-Long waste package is developed to determine the effects of tipover DBE loads on the structural components of the DOE SNF canister. The design concept is developed to contain one Shippingport fuel assembly in the DOE SNF canister (see CRWMS M&O 1999b, p. I-3 and p.

II-2). Since the Shippingport PWR assembly mass is far below the DOE SNF canister mass limit, a second design is developed to contain two Shippingport PWR fuel assemblies in the DOE SNF (CRWMS M&O 1999b, p. I-2 and p. II-1) to show that the 5-DHLW/DOE Spent Fuel-Long waste package for Shippingport PWR can handle loads greater than the ones with a single assembly in a DOE SNF canister. The difference between the two designs is limited to the internal components of the DOE SNF canister only.

First, the impact velocity of the outer surface of the inner lid is calculated for a waste package tipover DBE. Then, this velocity is conservatively used in the 2-D finite-element analysis. Since the 2-D representation does not model a lid, the calculations will indicate that the waste package components undergo more deflection and stress than would actually occur. The target surface is conservatively assumed to be essentially unyielding by using a large elastic modulus for the target surface compared to the waste package (Assumption 2.3.1.2). The target surface is constrained at the bottom to prevent horizontal and vertical motion. Contact elements are defined between the top HLW pour canister and the inner brackets, and between the outer barrier and the target surface. The initial configuration of the finite-element representation includes a negligibly small gap for each contact element defined in the representation. This configuration allows enough time and displacement for the waste package and its internals to ramp up to the specified initial velocity before the impact. With this initial velocity, the simulation is then continued through the impact until the waste package begins to rebound. At that time, the stress peaks and the maximum displacements have been obtained.

The vitrified HLW glass material properties are represented by ambient material properties of general borosilicate glass. This document does not specifically report any results for the individual HLW glass canisters.

3.3.2 Results of Structural Calculations

The structural response of the waste package to tipover accident loads is reported using maximum stress values and displacements obtained from the finite-element solution to the problem. The results show that the cavity between the Shippingport basket and the basket plates does not close, but on the contrary, becomes larger because of the dynamic load applied on the bottom plate by the Shippingport fuel assembly as shown in Figure 3-2. Hence, there will be no interference between the fuel assembly and the basket plates because of tipover DBE. The maximum stress in the DOE SNF canister-structural components including internals is determined to be 217 MPa (CRWMS M&O 1999b, p. 20). This magnitude of stress is also less than the tensile strength of 316L stainless steel, 483 MPa.

The results obtained with two Shippingport PWR assemblies are similar to the results with one Shippingport PWR assembly. The results show that the cavity between the Shippingport fuel assembly and the basket plates does not close, but on the contrary, becomes larger because of the dynamic load applied on the bottom plate by the Shippingport fuel assembly (see CRWMS M&O 1999b, Figure II-3). Hence, there will be no interference between the fuel assembly and the basket plates because of tipover DBE. The maximum stress in the DOE SNF canister-structural components including internals is determined to be 228 MPa (CRWMS M&O 1999b, p. 20). This magnitude of stress is less than the tensile strength of 316L stainless steel, 483 MPa (CRWMS M&O 1999b, p. 20).

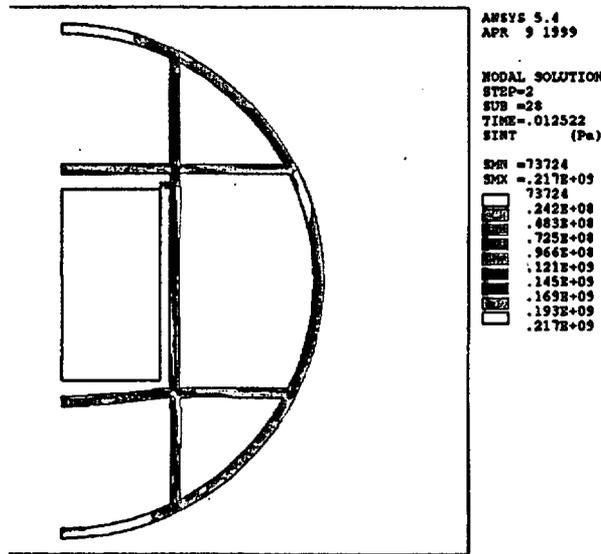


Figure 3-2. Stresses in the DOE SNF Canister

The calculations in CRWMS M&O (1999b) also show that the maximum bending stress on the base plate due to the weight of the structural components and the fuel is 55 MPa which is less than the yield strength of 316L stainless steel (172 MPa, CRWMS M&O 1999b, p. 20).

The calculations given in CRWMS M&O (1999b), Sections 5.7 and 5.8 utilize the maximum DOE SNF canister mass; therefore, the results of the bending and buckling calculations given in Section 3.3.2 are bounding for all design concepts.

3.4 SUMMARY

The results given in Section 3.3 show that there is sufficient clearance between the inner diameter of the support tube and the outer diameter of the DOE SNF canister in the case of a tipover DBE. Hence, there will be no interference between the two components, and the DOE SNF canister can be removed from the support tube if needed to be set inside another waste package.

4. THERMAL ANALYSIS

4.1 USE OF COMPUTER SOFTWARE

The FEA computer code used to analyze the 5-DHLW/DOE Spent Fuel-Long waste package containing a Shippingport PWR DOE SNF canister is ANSYS Version V5.4. ANSYS V5.4 is identified as CSCI 30040 V5.4 and is obtained from SCM in accordance with appropriate procedures. ANSYS is a commercially available finite-element thermal- and mechanical-analysis code. ANSYS V5.4 software is qualified as documented in the SQR for ANSYS V5.4 (CRWMS M&O 1998j).

4.2 THERMAL DESIGN ANALYSIS

A detailed description of the finite-element representations, the method of solution, and the results are provided in CRWMS M&O (1999f). This waste package is loaded with five Hanford 15-foot HLW glass canisters (Figure 2-2) and one DOE SNF canister (Figures 2-3 and 2-4). The DOE SNF canister holds one Shippingport PWR C2 S2 SNF assembly (Figures 2-5 through 2-7). Three different fill gases are considered for the Shippingport PWR DOE SNF canister: helium, argon, and nitrogen. The waste package is filled with helium.

The finite-element representation used in this calculation is shown in Figures 4-1 and 4-2. Figure 4-1 presents a finite-element representation of the 5-DHLW/DOE Spent Fuel-Long waste package with the DOE SNF canister containing Shippingport PWR SNF. Figure 4-2 presents a finite-element representation of the Shippingport PWR C2 S2 SNF assembly.

As shown in these figures, symmetry is across the center of the waste package. Therefore, this representation includes half of the 5-DHLW/DOE Spent Fuel-Long waste package, half of the DOE SNF canister, two-and-a-half Hanford long HLW glass canisters, and two sub-assemblies of the Shippingport PWR assembly. In addition, the HLW glass canisters and the Shippingport PWR assembly are positioned in the center of their compartments to maximize radiation heat transfer to waste package surfaces.

4.3 CALCULATIONS AND RESULTS

Table 4-1 lists the locations of components of interest. Table 4-2 summarizes the peak temperatures and time of occurrence for each DOE SNF canister fill gas. The results indicate that argon fill gas in the Shippingport PWR DOE SNF canister causes the peak Shippingport PWR fuel temperature, which occurs after ten years, to be approximately 1% higher than for helium fill gas. The peak HLW glass and waste package surface temperatures are not affected by the choice of the fill gas in the Shippingport PWR DOE SNF canister. Figure 4-3 plots peak temperatures versus radial location from the center of the waste package with the Shippingport PWR DOE SNF canister filled with argon, nitrogen or helium gas.

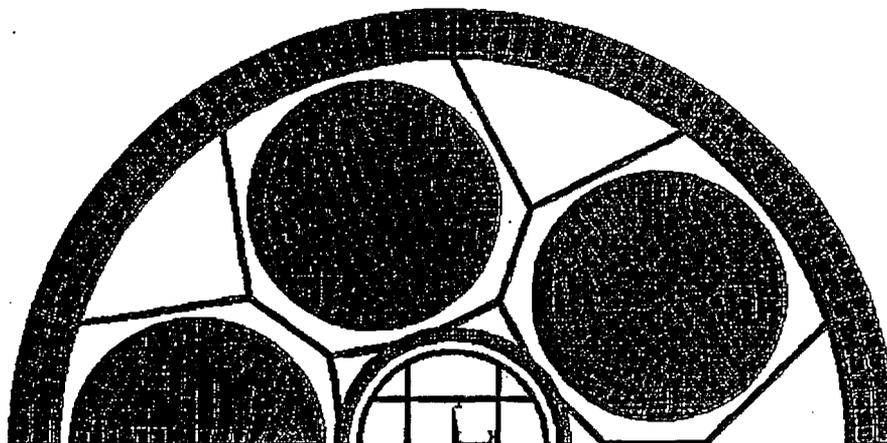


Figure 4-1. Finite-element Representation of the 5-DHLW/DOE Spent Fuel-Long Waste Package

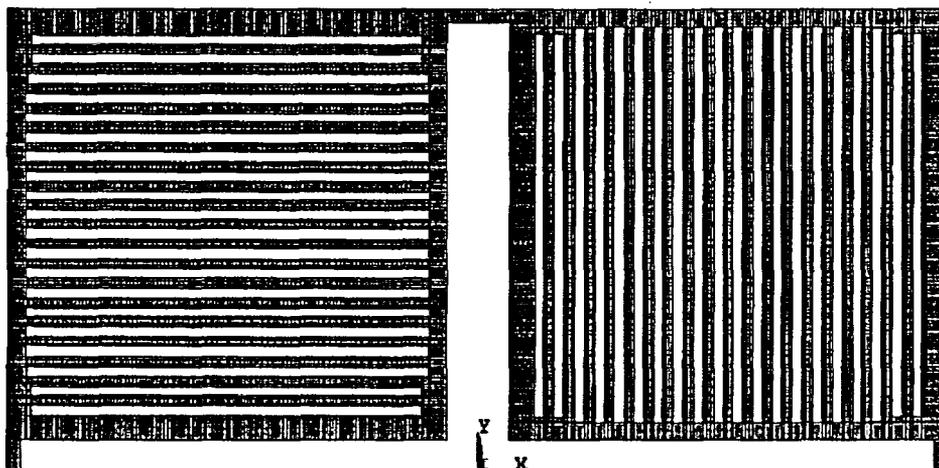


Figure 4-2. Finite-element Representation of the Shippingport PWR C2 S2 SNF Assembly

Table 4-1. Physical Locations of Nodes of Interest

Component and location	Location from Center of Waste Package (m)
Center of Shippingport assembly	0.00
Center of Shippingport canister A-guide	0.11
Center of Shippingport canister wall	0.22
Center of 5-DHLW/DOE waste package support tube	0.27
Center of 5-DHLW/DOE waste package divider plate	0.48
Inside of waste package inner barrier	0.94
Waste package inner and outer barrier interface	0.96
Outside of waste package outer barrier	1.06

Table 4-2. Peak Temperatures and Time of Occurrence for Each DOE SNF Canister Fill Gas

	DOE SNF Canister Fill Gas		
	Helium	Nitrogen	Argon
Peak Fuel Temperature (°C)	246.7	248.7	248.9
Time of Peak Fuel Temperature (yr)	10	10	10
Peak Waste Package Outer Barrier Surface Temperature (°C)	211.7	211.7	211.7
Time of Peak Waste Package Outer Barrier Surface Temperature (yr)	20	20	20
Peak HLW Glass Temperature (°C)	252.3	252.3	252.3
Time of Peak HLW Glass Temperature (yr)	10	10	10
Peak Fuel Cladding Temperature (°C)	246.8	248.9	249.2
Time of Peak Fuel Cladding Temperature (yr)	10	10	10

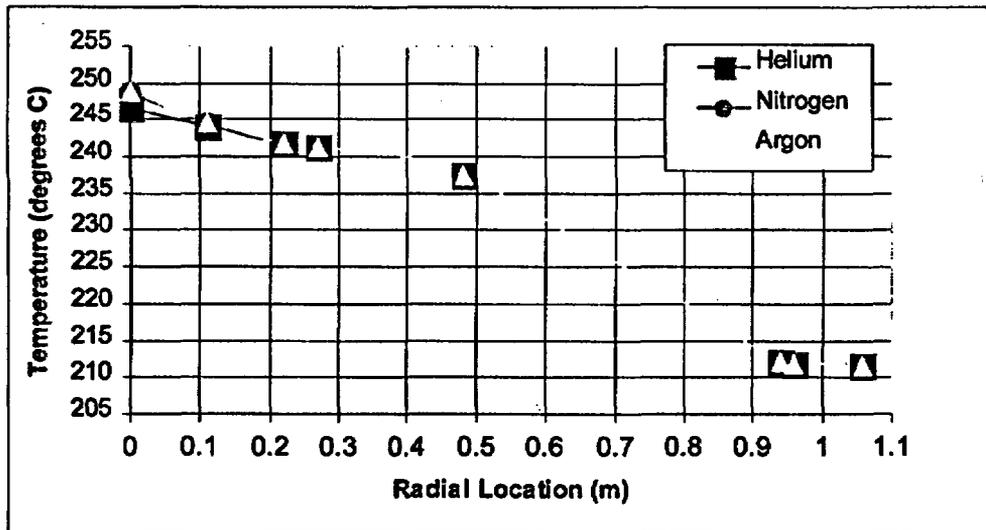


Figure 4-3. Axial Temperature Profile of the 5-DHLW/DOE Spent Fuel-Long Waste Package

4.4 SUMMARY

The results indicate that the maximum fuel and fuel cladding temperatures are 248.9 °C and 249.2 °C, respectively, with argon fill gas in the DOE SNF canister. Also the maximum HLW glass temperature occurs, after 10 years, with argon fill gas in the DOE SNF canister and is 252.3 °C.

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5. SHIELDING ANALYSIS

5.1 USE OF COMPUTER SOFTWARE

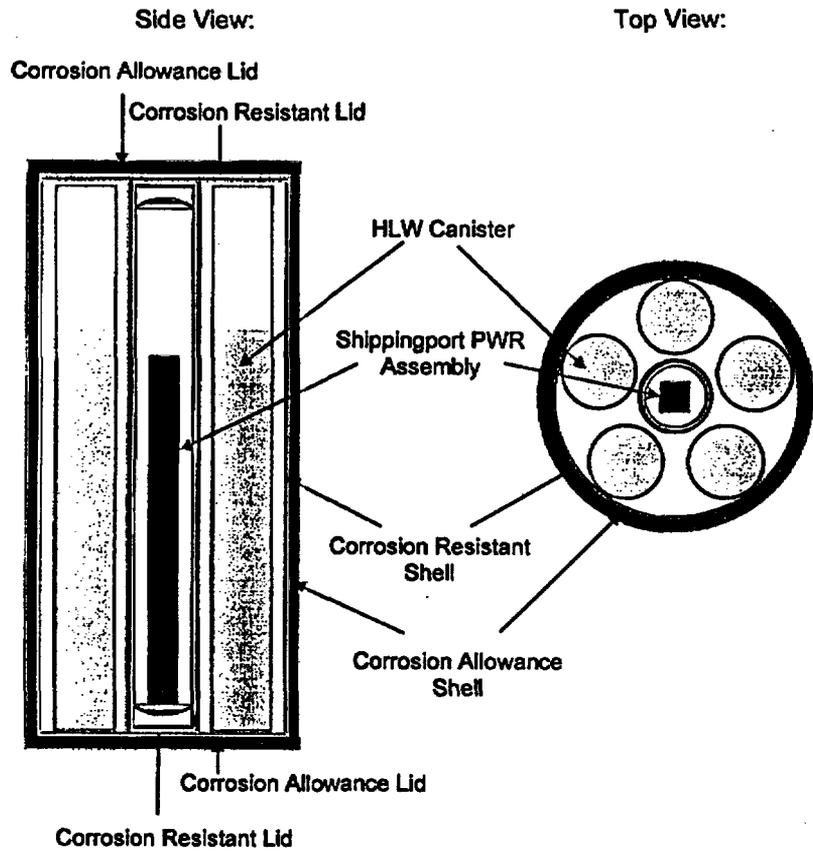
The Monte Carlo radiation transport code, MCNP, Version 4B2, is used to calculate average dose rates on the surfaces of the waste package. This code, identified as CSCI 30033 V4B2LV, was previously obtained from the SCM in accordance with appropriate procedures. MCNP software is qualified as documented in the SQR for the MCNP, Version 4B2 (CRWMS M&O 1998i).

5.2 DESIGN ANALYSIS

The Monte Carlo method for solving the integral transport equation, which is implemented in the MCNP computer program, is used to calculate radiation dose rates for the waste packages. MCNP is set to use continuous energy cross sections processed from the evaluated nuclear data files ENDF/B-V (Briesmeister 1997, App. G). These cross-section libraries are part of the qualified MCNP code system (CSCI 30033 V4B2LV). The flux averaged over a surface is tallied and the neutron and gamma flux-to-dose rate conversion factors (Briesmeister 1997, App. H) are applied to obtain surface dose rates.

5.3 CALCULATIONS AND RESULTS

The details of the calculations and the results are provided in CRWMS M&O (1999h). The geometric model used in MCNP calculations is shown in Figure 5-1. Previous dose-rate calculations for the waste package containing SRS HLW glass canisters show that the angular dose over the waste package radial surfaces is uniform (CRWMS M&O 1998c, pp. 30 and 33). Therefore, only axial variation of the dose rate on the waste package radial surfaces and the radial variation of the dose rate on the waste package axial surfaces are studied. The surfaces and segments that are used in the dose-rate calculations are shown in Figure 5-2. The radial surfaces, cut by the bottom and top planes of HLW glass, are equally divided into five segments, each of which is 67.108-cm high. The sixth radial segment, 125.11-cm high, is the portion between the top of waste package cavity and the top of HLW glass. Previous analyses used Hanford HLW glass neutron and gamma sources, which resulted in approximately 20% higher dose rates, for long waste packages (5-DHLW/DOE Spent Fuel-Long.) Although the results were more than a factor of 20 below the criteria, this approach yielded overly conservative results. Therefore, SRS HLW glass neutron and gamma sources were used in the analyses of the Shippingport PWR SNF. Although the sources are from 3-m SRS HLW glass canisters, they were scaled up to account for longer (15-foot) HLW glass canisters.



NOTE: not to scale

Figure 5-1. Vertical and Horizontal Cross Sections of MCNP Geometry Representation

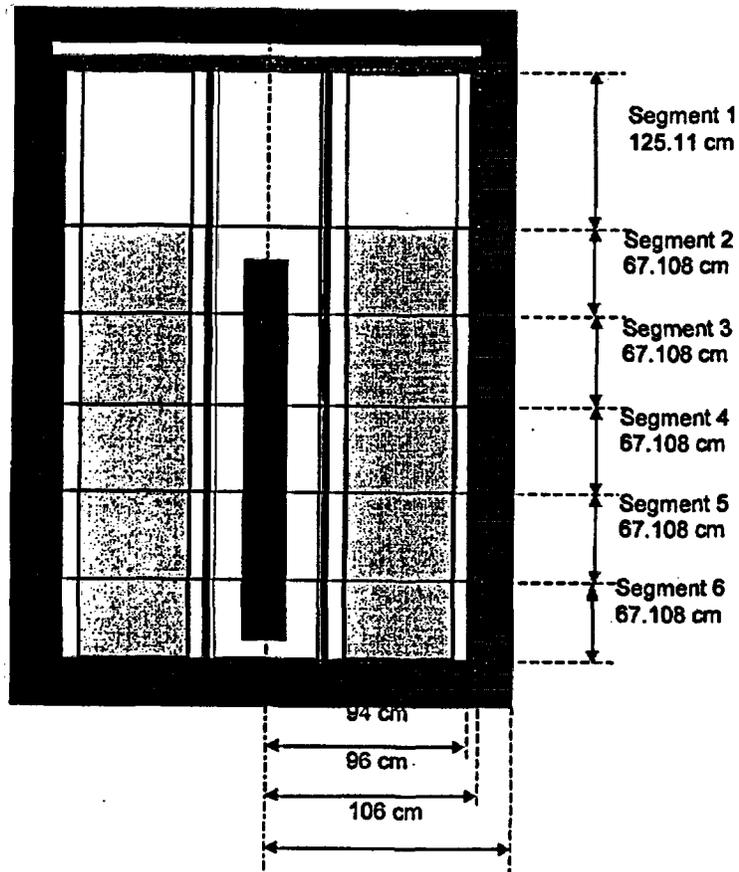


Figure 5-2. Radial Surfaces and Segments of the Waste Package Used in Dose Rate Calculations

Tables 5-1 and 5-2 show the dose rates in rem/h on the surfaces of interest of the waste package containing the SRS HLW glass and Shippingport PWR DOE SNF canister. The dose rates in rem/h and rad/h are practically the same due to the insignificant contribution of the neutron dose rate to the total dose rate (CRWMS M&O 1999h, pp. 21 through 25).

Table 5-1. Dose Rates on Waste Package Outer Radial Surface

Axial Location	Gamma		Neutron		Total	
	Dose Rate (rem/h)	Relative Error (%)	Dose Rate (rem/h)	Relative Error (%)	Dose Rate (rem/h)	Relative Error (%)
Segment 1	1.0624	0.0431	2.3274E-02	0.0065	1.0856	0.0422
Segment 2	9.4949	0.0191	6.9035E-02	0.0047	9.5640	0.0190
Segment 3	9.9406	0.0180	8.4840E-02	0.0042	10.025	0.0178
Segment 4	10.231	0.0176	8.5894E-02	0.0042	10.317	0.0175
Segment 5	9.7283	0.0174	8.5034E-02	0.0042	9.8133	0.0172
Segment 6	9.2088	0.0184	7.3792E-02	0.0046	9.2826	0.0183

Table 5-2. Dose Rates on Waste Package Axial Surfaces

Axial Location	Gamma		Neutron		Total	
	Dose Rate (rem/h)	Relative Error (%)	Dose Rate (rem/h)	Relative Error (%)	Dose Rate (rem/h)	Relative Error (%)
Bottom surface of waste package	2.5216	0.0368	5.2263E-02	0.0063	2.5738	0.0361
Top surface of waste package	0.49322	0.0805	1.3585E-02	0.0118	0.5068	0.0783

5.4 SUMMARY

For the radial surfaces, the maximum surface dose rate occurs at the middle segments of the HLW glass canisters. The maximum surface dose rates, for the middle segment of the waste package outer radial surface is 10.32 ± 0.36 rem/h which is below the design criteria of 355 rem/h. The maximum dose rates on the axial surfaces for the bottom and top surfaces are about one to one-half orders of magnitude lower than the maximum dose rates on the corresponding radial surfaces.

6. DEGRADATION AND GEOCHEMISTRY ANALYSES

6.1 USE OF COMPUTER SOFTWARE

The EQ3/6 software package identified as CSCI UCRL-MA-110662 V 7.2b, SCR: LSCR198. It was obtained from the SCM in accordance with appropriate procedures. The major components of the EQ3/6 package include the following: EQ3NR, a speciation-solubility code; EQ3/6, a reaction path code that calculates water/rock interaction or fluid mixing in either a pure reaction progress mode or a time mode; EQPT, a data-file preprocessor; EQLIB, a supporting software library; and several supporting thermodynamic data files. The software implements algorithms describing thermodynamic equilibrium, thermodynamic disequilibrium and reaction kinetics. The supporting data files contain both standard-state and activity-coefficient-related data.

EQ3/6 calculates the irreversible reactions that occur between an aqueous solution and a set of solid, liquid, or gaseous reactants. The code can calculate fluid mixing and the consequences of changes in temperature. This code operates both in a pure reaction progress frame as well as in a time frame.

In this study, EQ3/6 is used to provide:

- A general overview of the nature of chemical reactions to be expected.
- The degradation products likely to result from corrosion of the TRIGA SNF and canisters.
- An indication of the minerals, and their amounts, likely to precipitate within the waste package.

The EQ3/6 calculations reported in this document used version 7.2b of the code, which is appropriate for the application, and were executed on Pentium series personal computer (PCs). The EQ3/6 package has been verified by its present custodian, Lawrence Livermore National Laboratory. The source codes were obtained from SCM in accordance with the OCRWM procedure AP-SI.1Q. The code was installed on Pentium PCs according to an M&O-approval Installation and Test procedure (CRWMS M&O 1998m). The EQ3/6 version 7.2b is qualified as documented in the SQR for EQ3/6 V7.2b (CRWMS M&O 1998m). EQ3/6 V7.2b is also referred to as EQ6.

6.2 DESIGN ANALYSIS

6.2.1 Systematic Investigation of Degradation Scenarios and Configurations

Degradation scenarios comprise a combination of features, events, and processes that result in degraded configurations to be evaluated for criticality. A configuration is defined by a set of parameters characterizing the amount and physical arrangement, at a specific location, of the materials that can significantly affect criticality (e.g., fissile materials, neutron-absorbing

materials, reflecting materials, and moderators). The variety of possible configurations is best understood by grouping them into classes. A configuration class is a set of similar configurations whose composition and geometry is defined by specific parameters that distinguish one class from another. Within a configuration class the values of configuration parameters may vary over a given range.

A master scenario list and set of configuration classes relating to internal criticality is given in the *Disposal Criticality Analysis Methodology Topical Report* (CRWMS M&O 1998a, pp. 3-2 through 3-12) and also shown in Figures 6-1 and 6-2. This list was developed by a process that involved workshops and peer review. The comprehensive evaluation of disposal criticality for any waste form must include variations of the standard scenarios and configurations to ensure that no credible degradation scenario is neglected. All of the scenarios that can lead to criticality begin with the breaching of the waste package, followed by entry of the water, which eventually leads to degradation of the SNF and/or other internal components of the waste package. This degradation may permit neutron absorber material to be mobilized (made soluble) and either be flushed out of the waste package or displaced from the fissile material, thereby increasing the probability of criticality.

The standard scenarios for internal criticality divide into two groups:

1. When the waste package is breached only on the top, water flowing into the waste package builds up a pond. This pond provides water for moderation to support a criticality. Further, after a few hundred years of steady dripping, the water can overflow through the hole on the top of the waste package and flush out any dissolved degradation products.
2. When the waste package breach occurs on the bottom as well as the top, the water flows through the waste package. This group of scenarios allows the soluble degradation products to be removed more quickly, but does not directly provide water for moderation. Criticality is possible, however, if the waste package fills with corrosion products that can add water of hydration and/or plug any holes in the bottom of the waste package. The waste package supports this latter behavior because the silica released by the degrading HLW glass may form clay with enough water of hydration to support criticality.

The standard scenarios for the first group are designated IP-1, -2, and -3 (IP stands for internal to the package) according to whether the waste form degrades before the other waste package internal components, at approximately the same time (but not necessarily at the same rate), or later than the waste package internal components. The standard scenarios for the second group are designated IP-4, -5, or -6 based on the same criteria. The internal criticality configurations resulting from these scenarios fall into six configuration classes described below (CRWMS M&O 1998a, pp. 3-10 through 3-12):

1. Basket is degraded but waste form is relatively intact and sits on the bottom of the waste package (or the DOE SNF canister), surrounded by, and/or beneath, the basket corrosion products (see Figure 6-3). This configuration class is reached from scenario IP-3.

2. Both basket and waste form are degraded (see Figure 6-4). The composition of the corrosion product is a mixture of fissile material and iron oxides, and may contain clay. It is more complex than for configuration class 1, and is determined by geochemical calculations as described in Section 6.3. This configuration class is most directly reached from standard scenario IP-2, in which all the waste package components degrade at the same time. However, after many tens of thousands of years the scenarios IP-1 and IP-3, in which the waste form degrades before or after the other components, also lead to this configuration.
3. Fissile material is moved some distance from the neutron absorber, but both remain in the waste package (see Figure 6-5). This configuration class can be reached from IP-1.
4. Fissile material accumulates at the bottom of the waste package, together with moderator provided by water trapped in clay (see Figure 6-6). The clay composition is determined by geochemical calculation, as described in Section 6.3. This configuration class can be reached by any of the scenarios, although IP-2 and IP-5 lead to this configuration by the most direct path; the only requirement is that there be a large amount of glass in the waste package (as in the codisposal waste package) to form the clay.
5. Fissile material is incorporated into the clay, similar to configuration class 4, but with the fissile material not at the bottom of the waste package (see Figure 6-7). Generally the mixture is spread throughout most of the waste package volume, but could vary in composition so that the fissile material is confined to one or more layers within the clay. Generally, the variations of this configuration are less reactive than for configuration class 4, therefore, they are grouped together, rather than separated according to where the fissile layer occurs or whether the mixture is entirely homogeneous. This configuration class can be reached by either standard scenario IP-1 or -4.
6. Fissile material is degraded and spread into a more reactive configuration but not necessarily moved away from the neutron absorber, as in configuration class 3 (see Figure 6-8). This configuration class can be reached by scenario IP-1.

The configuration classes 1, 2, 4, and 5 require that most of the neutron absorber be removed from the waste package. However, in configuration classes 3 and 6, the fissile material is simply moved away from the absorber or into a more reactive geometry.

Note that most of these configurations or configuration pairs (Figures 6-3 through 6-8) look quite different even though both pair members belong to the same configuration class. This apparent dissimilarity arises from the configuration class definition strategy, which classifies critical configurations according to the geometry and composition of the materials, irrespective of the container (either the DOE SNF canister, or the entire waste package).

In Sections 6.2.1.1 through 6.2.1.7, the scenarios and the resulting configuration classes that are applicable to the 5-DHLW/DOE Spent Fuel-Long waste package with Shippingport PWR fuel in the DOE SNF canister are discussed. The naming convention used for the standard scenarios in

Sections 6.2.1.1 through 6.2.1.7 is slightly different from the convention used in the topical report (CRWMS M&O 1998a), which can be seen in Figures 6-1 and 6-2. The naming convention used in these sections is based on CRWMS M&O (1999k), which contains refinements to the configurations described in the topical report.

Note: W.P. = waste package
 W.F. = waste form
 F.M. = fissile material

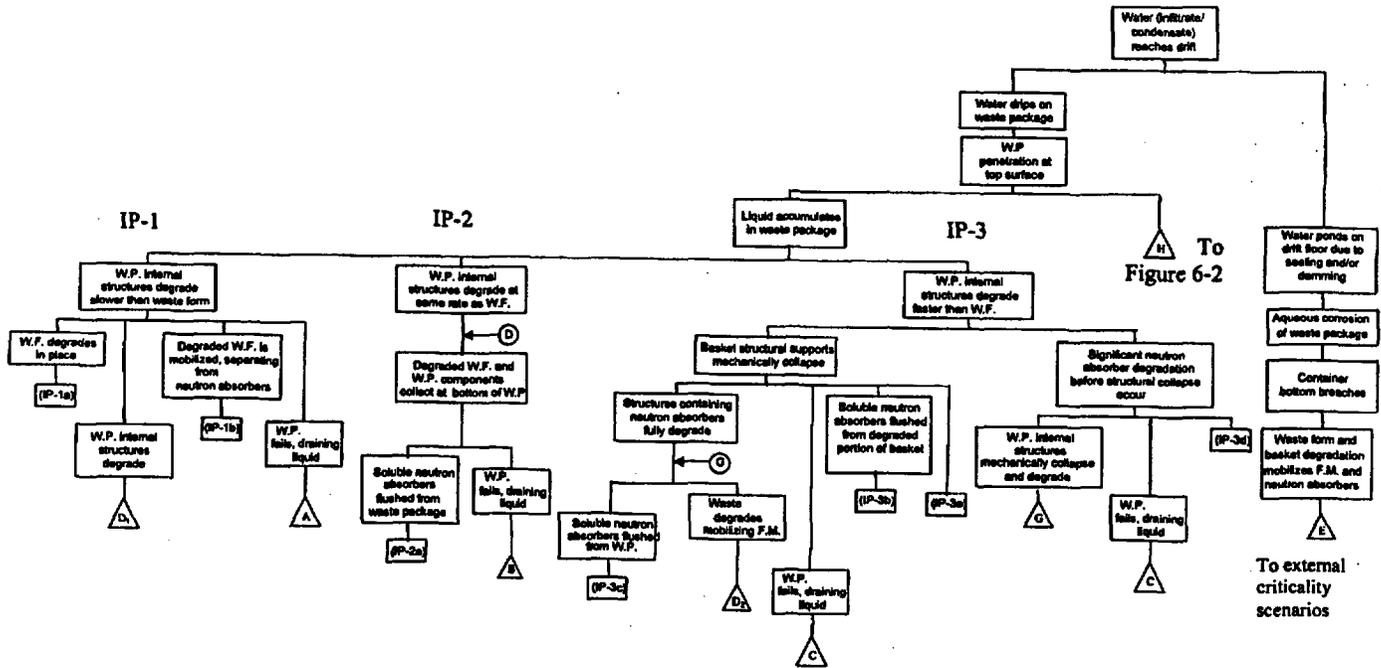


Figure 6-1. Internal Criticality Master Scenarios, Part 1

From Figure 6-1

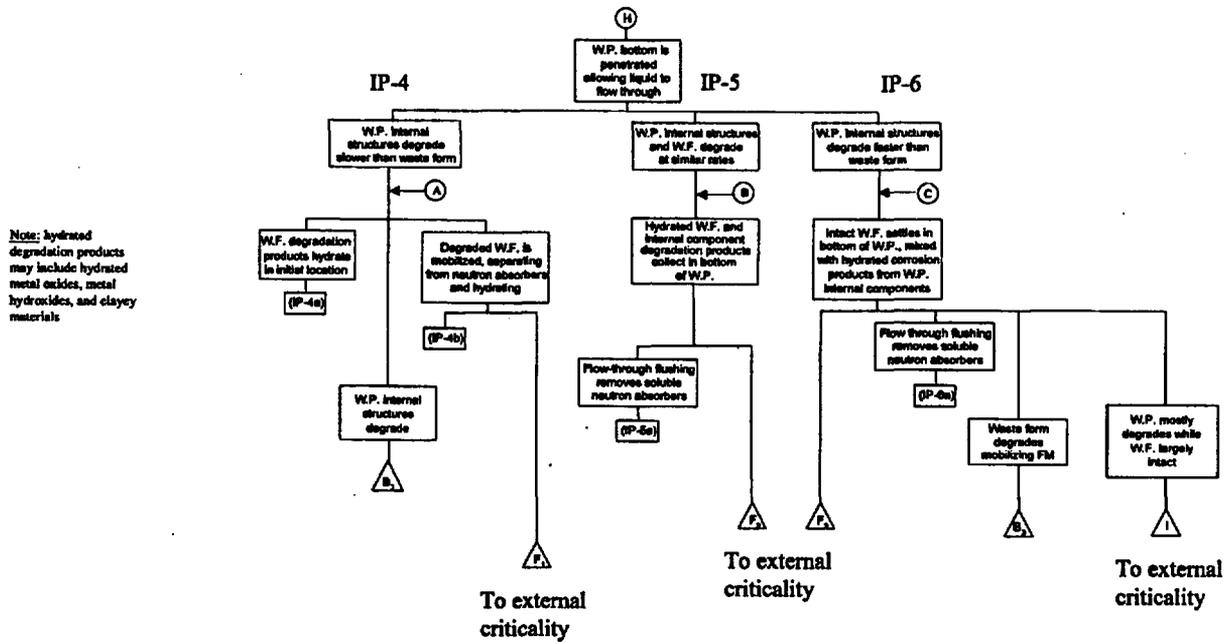


Figure 6-2. Internal Criticality Master Scenarios, Part 2

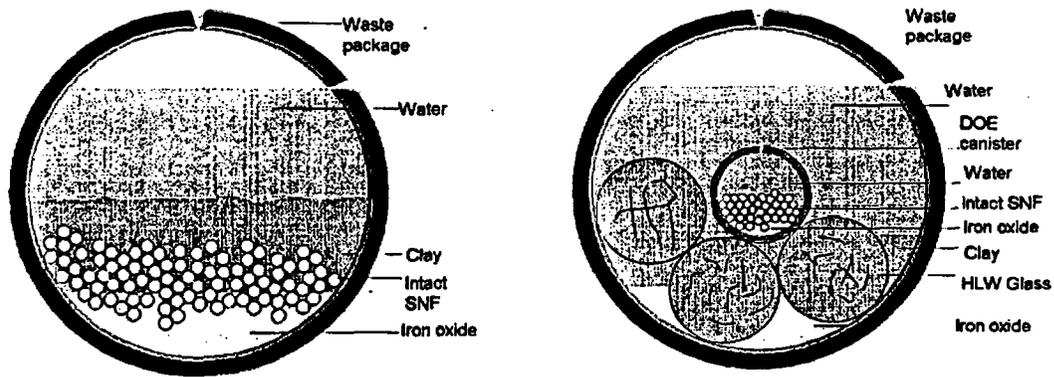


Figure 6-3. Examples of Degraded Configurations from Class 1

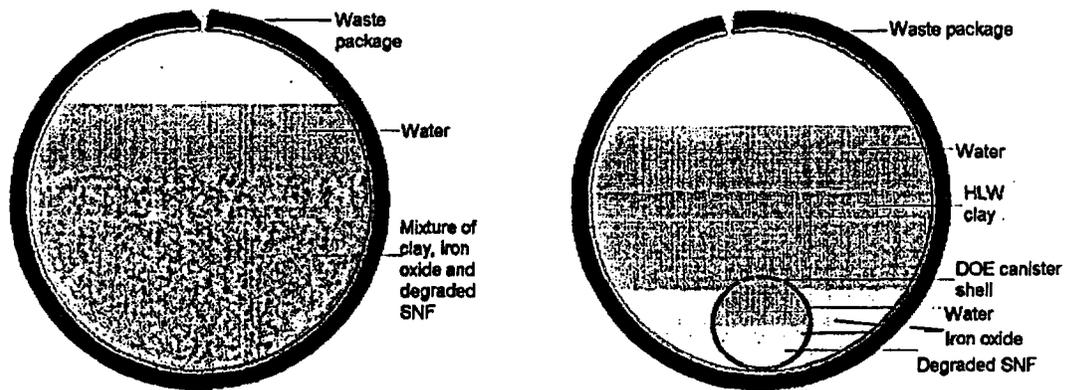


Figure 6-4. Examples of Degraded Configurations from Class 2

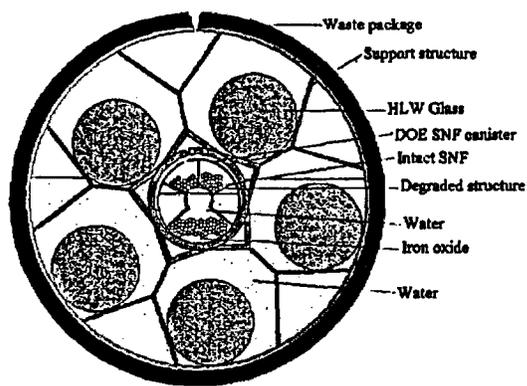


Figure 6-5. Example of Degraded Configuration from Class 3

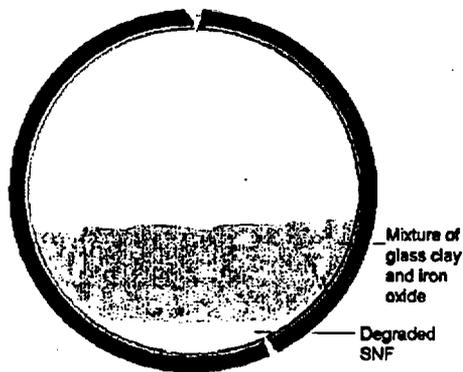


Figure 6-6. Example of Degraded Configuration from Class 4

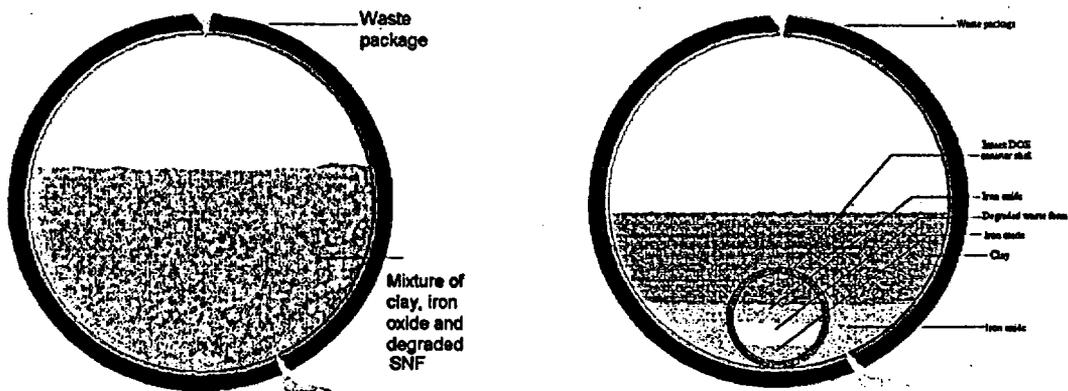


Figure 6-7. Examples of Degraded Configurations from Class 5

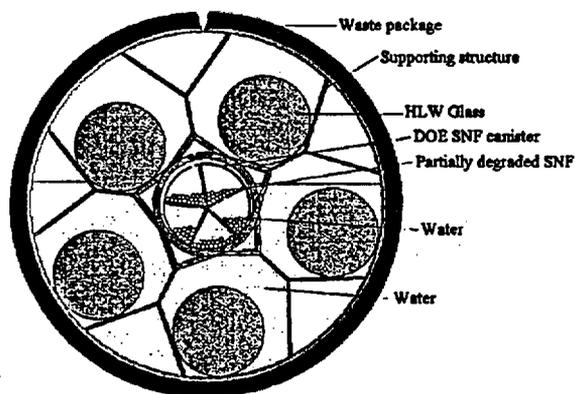


Figure 6-8. Example of Degraded Configuration from Class 6

6.2.1.1 Most Probable Scenario for Shippingport PWR SNF

The parameters that need to be considered to develop the most likely or probable degradation scenario/configuration for the Shippingport PWR SNF are: the materials of the components associated with the waste package; the DOE SNF canister and the SNF; thickness of the materials and the associated corrosion rates. The sequence of degradation can be developed, and the most probable degradation scenario/configuration can be identified by using these parameters, which are discussed below.

Corrosion rates- Stainless steels Type 304L and Type 316L degrade at approximately the same rate, and A516 carbon steel degrades faster than either of the stainless steels Type 304L and Type 316L (Table 2-14). The corrosion rate of Zircaloy-4 is conservatively selected as 0.0079 $\mu\text{m}/\text{yr}$ (3.1 mils in 10,000 years) (Hillner, et al. 1998, Table 1). When compared to the corrosion rates of stainless steel Zircaloy-4 can be considered inert. The corrosion rate of the SNF (uranium ceramic) is represented by the corrosion rate of plutonium ceramic (LLNL 1998). This is reasonable because the compositions of the plutonium ceramic are similar to the uranium ceramic. The wafer pyrolytic carbon coating also provides additional protection for the Shippingport PWR SNF.

Most Probable Degradation Path- Based on the corrosion rates and the material thicknesses that are given in Table 6-1, the most probable degradation path for the waste package, the DOE SNF canister, and the Shippingport PWR SNF follows the following sequence:

1. Waste package is penetrated and flooded internally. The waste package basket (inner brackets and support tube) is likely to degrade first because of the A516 carbon steel material.
2. HLW glass stainless steel shell and glass begin to degrade. After this, there are two degradation paths.
- 3a. DOE SNF canister stays intact. Intact DOE SNF canister and intact SNF assembly fall on top of degraded products near the bottom of the waste package.
- 3b. DOE SNF canister starts to degrade.
4. DOE SNF canister is penetrated and flooded inside.
5. DOE SNF canister basket and SNF assembly gets in contact with water.
6. SNF plates get in contact with water.
7. DOE SNF canister basket degrades. After this, there are two paths:
 - 7a. SNF assembly and plates stay intact and fall on top of degraded DOE SNF canister basket and settle on the bottom of the DOE SNF canister (Section 6.2.1.2).

- 7b. DOE SNF canister degrades. Intact SNF assembly and plates fall and scatter on top of all degradation products near the bottom of the waste package. There could be some separation between the stainless steel and fuel assembly (Section 6.2.1.4).
8. Given a very long period of time, it is postulated that everything will degrade including cladding and fuel. This corresponds to degradation scenario group IP-2. This is not likely because of very long lifetime of Zircaloy-4, which will most likely outlast the waste package. To bound the potential degraded cases, degradation of the SNF can be considered. The degraded SNF and other degradation products could mix and pile up near the bottom of waste package. However, there is no mechanism to cause complete and uniform mixing of all the degradation products inside the waste package.

Table 6-1. Materials and Thicknesses

Components	Material	Thickness (mm)
Waste package basket	A516 carbon steel	12.7
Waste package inner bracket	A516 carbon steel	25.4
Waste package support tube	A516 carbon steel	31.75
HLW glass shell	304L stainless steel	9.5
HLW glass	Glass	N/A
DOE SNF canister	316L stainless steel	9.5
DOE SNF canister basket	316L stainless steel	9.5
SNF cover plate	Zircaloy-4	0.52
Neutron absorber (in wafer form)	Borated stainless steel	0.91
SNF (wafer form)	UO ₂ -ZrO ₂ -CaO ₂	0.91
SNF wafer coating	Pyrolytic carbon	a few microns

Sources: CRWMS M&O (1999e) and DOE (1999a).

Most Probable Degradation Scenario/Configuration- Based on *Generic Degradation Scenario and Configuration Analysis for DOE Codisposal Waste Package* (CRWMS M&O 1999k), the above degradation sequences match with the degradation scenario/configurations of IP-3-A to IP-3-C (equivalent to IP-2). The details of these degradation scenario/configurations are discussed in Sections 7.4.1 and 7.4.2. The most probable degradation configuration is the one with the degradation of all components inside the waste package and the DOE SNF canister. The SNF assembly remains intact and positioned on the bottom of the waste package (Section 7.4.1.3). The degradation scenario of IP-1, i.e., SNF degrades faster than the other materials, is not probable, since the SNF is sealed inside the Zircaloy-4 plates, which practically do not degrade as compared to stainless steel.

The configurations described in Sections 6.2.1.2 through 6.2.1.4 are the most probable configurations. The configurations discussed in Sections 6.2.1.5 through 6.2.1.7 are not likely.

6.2.1.2 Degraded DOE SNF Canister Basket and Intact SNF

For these cases of intact fuel assembly within degraded basket, the scenarios and configuration classes are applied to the DOE SNF canister and its contents. This configuration is a variation of

configuration class 1 and can be reached from standard scenario IP-3-A. The results of the criticality calculations for this configuration are given in Section 7.4.1.1.

6.2.1.3 Intact DOE SNF Canister and Degraded Waste Package Internals

In this case, the concepts of scenario and configuration are applied to the entire waste package. The fuel assembly and the DOE SNF canister internals are intact. This configuration is a variation of configuration class 1 and can be reached from standard scenario IP-3-A. The results of the criticality calculations for this configuration are given in Section 7.4.1.2.

6.2.1.4 Degraded DOE SNF Canister and Waste Package Internals

In this case, the concepts of scenario and configuration are applied to the entire waste package. The DOE SNF canister, waste package internals, and HLW glass canisters are degraded. The fuel assembly is intact. This configuration is achievable because of very low degradation rate of Zircaloy-4, which envelops and protects the fuel. This configuration is a variation of configuration class 1 and can be reached from standard scenario IP-3-B. The results of the criticality calculations for this configuration are given in Section 7.4.1.3.

6.2.1.5 Intact DOE SNF Canister and Waste Package Internals and Degraded SNF

For these cases of degraded fuel assembly within intact basket, the scenarios and configuration classes are applied to the DOE SNF canister and its contents. This configuration is a variation of configuration class 6 and can be reached from standard scenario IP-1-A. The results of the criticality calculations for this configuration are given in Section 7.4.2.1.

6.2.1.6 Intact Waste Package Internals and Degraded DOE SNF Canister and SNF

For these cases of degraded fuel assembly within degraded basket, the scenarios and configuration classes are applied to the DOE SNF canister and its contents. This configuration is a variation of configuration class 3 and can be reached from standard scenario IP-1-B. The results of the criticality calculations for this configuration are given in Section 7.4.2.2.

6.2.1.7 Completely Degraded DOE SNF Canister and Waste Package Internals

In this case, the concepts of scenario and configuration are applied to the entire waste package. Degradation products from the DOE SNF canister and contents form a layer on the bottom of the waste package. The degradation products (clay) from waste package internals and HLW glass canisters form a layer above. This configuration is a variation of configuration class 2 and can be reached from standard scenario IP-1-C and IP-2. The results of the criticality calculations for this configuration are given in Sections 7.4.2.3 and 7.4.2.4.

6.2.2 Basic Design Approach for Geochemical Analysis

The method used for this analysis involves the steps described below.

1. Use the basic EQ3/6 capability to trace the progress of reactions as the chemistry evolves, including estimating the concentrations of material remaining in solution as well as the composition of precipitated solids. EQ3 is used to determine a starting fluid composition for a series of EQ6 calculations; it does not simulate reaction progress.
2. Evaluate available data on the range of dissolution rates for the materials involved, to be used as material/species input for each time step.
3. Use the "solid-centered flow-through" mode in EQ6. In this mode, an increment of aqueous "feed" solution is added continuously to the waste package system, and a like volume of the existing solution is removed. This mode simulates a continuously stirred tank reactor.
4. Determine the concentrations of fissile materials in solution as a function of time (from the output of EQ6-simulated reaction times up to $6 \cdot 10^5$ years).
5. Calculate the amount of fissile material released from the waste package as a function of time, which thereby reduces the chance of criticality within the waste package.
6. Calculate the composition and amounts of solids (precipitated minerals or corrosion products and unreacted package materials).

Two approaches were used in the geochemistry analysis for Shippingport PWR SNF: single-stage and double-stage. In single-stage, all waste package internals including SNF come in contact with water and degrade simultaneously thereby exposing the fissile and neutron absorber materials to the degraded solutions, which could result in losing the fissile and/or neutron absorber materials. The objective of the single-stage approach is to evaluate the effect of degraded products on the fissile and neutron absorber material, particularly the pH effect. In general, the single-stage cases are considered as the extreme or not probable cases due to the fact that all components are assumed to begin to degrade immediately after the waste package breach without considering the degradation sequences. In double-stage, the internals of waste package degrade first followed by the degradation of the DOE SNF canister and SNF. Therefore, the multiple-stage cases represent the most probable degradation scenarios. For most of the runs, only 1% of the fuel was exposed to the degraded environment due to the highly corrosion resistant Zircaloy-4 cladding. In some runs, 100% of the fuel was exposed.

6.3 CALCULATIONS AND RESULTS

The calculations begin by selecting representative values from known ranges for composition, amounts, and reaction rates of the various components of the 5-DHLW/DOE Spent Fuel-Long waste package with DOE SNF canister containing Shippingport PWR SNF. Surface areas are calculated based on the known package geometry. The input to EQ6 consists of the composition of J-13 well water, together with a rate of influx to the waste package (Section 2.1.8.3).

Sometimes the degradation of the waste package is divided into stages (e.g., degradation of HLW glass before breach, and exposure of the fuel assemblies and basket materials to the water). The EQ6 outputs include the compositions and amounts of solid products and the solution composition. Details of the results are presented below. The calculation process is described in more detail in CRWMS M&O (1999e).

Uranium and plutonium are quite soluble in alkaline, carbonate-rich solutions produced when the HLW glass degrades (solubility up to $\sim 10^{-1}$ molal [CRWMS M&O 1999e, p. 38]). A condition of low pH might be produced as stainless steel degrades separately from the HLW glass. To obtain sustained low-pH conditions, it is generally necessary to break the degradation process into two stages. The first stage involves an early breach of the 304L stainless steel canisters holding the HLW glass, followed by fast degradation of the HLW glass and removal of the alkaline components during a period of relatively high drip rate. In the second stage, the 316L stainless steel DOE SNF canister breaches, exposing some of the Shippingport PWR (HEU oxide) fuel. In this second stage, the pH of the ambient solutions remains low (~ 5 to ~ 6), due in part to the degradation of the stainless steel. To keep the pH low, the drip rate must be reduced for the second stage.

6.3.1 Results of EQ6 Runs

In total, thirty cases of single- and double-stage EQ6 simulations were run. In these cases, degradation rates of steel, glass, and Shippingport PWR (HEU oxide) SNF, and water fluxes were varied. Table 6-2 summarizes all the cases run, as well as total percentage of boron, uranium and plutonium loss at the end of the EQ6 runs. Note that although boron is included in the calculations, the criticality calculations did not take any credit for its presence. This is conservative, and also realistic, consistent with Table 6-2 showing all but six cases losing almost all their boron.

Cases 1-20 and 25-30 are single-stage, and involve simultaneous exposure of the fuel and the package materials to J-13 well water. Cases 25 to 27 were done to consider the effect of the degree of fuel exposure on reaction. Case 28 was done to determine if the alteration product density depended on the identity of the iron oxide that formed – hematite or goethite. This case was just a first stage, with hematite suppressed (with goethite), run to the same ending time and rates as the first-stage run of Case 21, wherein hematite was allowed to form. Cases 29 and 30 were specifically done to assess the relative contribution of uranium from dissolving fuel and glass.

Cases 21-24 are double-stage runs in which J-13 well water first interacts with everything inside the waste package except the SNF canister, followed in the second stage by interaction of the resulting fluids with the SNF. It is also assumed that Zr cladding would breach, exposing 1% of the fuel, just after the breach of the DOE SNF canister. In three of the double-stage runs (Cases 22-24) hematite formation is suppressed and goethite is the major iron oxide formed. Both hematite and goethite are products of steel corrosion with nearly equal thermodynamic stability. However, hematite is slightly more stable so it has been used for most of the cases considered in this report.

Table 6-2. Summary of Geochemistry Results

Case	% Fuel Exposure	%B Loss	%Pu Loss	%U Loss	Rates ^d				Fe Oxide
					Steel	Glass	Fuel	J-13	
1	1	100	12.3	100	1	1	1	1	Hematite
2	1	16.2	0.09	0.06	1	1	1	3	Hematite
3	1	100	12.3	100	1	1	3	1	Hematite
4	1	16.3	0.10	0.06	1	1	3	3	Hematite
5	1	100	1.28	100	1	1	2	2	Hematite
6	1	100	100	94.5	1	2	1	1	Hematite
7	1	100	41.2	100	1	2	1	3	Hematite
8	1	100	100	94.5	1	2	3	1	Hematite
9	1	100	41.2	100	1	2	3	3	Hematite
10	1	100	100	100	1	2	2	2	Hematite
11	1	100	7.68	100	2	1	1	1	Hematite
12	1	16.2	1.50	0.24	2	1	1	3	Hematite
13	1	100	7.68	100	2	1	3	1	Hematite
14	1	16.9	1.50	0.31	2	1	3	3	Hematite
15	1	100	1.84	100	2	1	2	2	Hematite
16	1	100	66.3	100	2	2	1	1	Hematite
17	1	100	55.3	100	2	2	1	3	Hematite
18	1	100	66.3	100	2	2	3	1	Hematite
19	1	100	55.3	100	2	2	3	3	Hematite
20	1	100	99.9	100	2	2	2	2	Hematite
21	1	99.5	31.7	100	2/2	2/0	0/2	4/2	Hematite
22 ^a	1	99.5	74.6	100	2/2	2/0	0/2	4/2	Goethite
23 ^a	1	99.5	0	24.2	2/2	2/0	0/2	3/1	Goethite
24 ^a	1	99.5	0	100	1/1	2/0	0/2	3/1	Goethite
25	100	16.2	0.09	0.07	1	1	1	3	Hematite
26	100	16.4	0.14	0.08	1	1	3	3	Hematite
27 ^a	100	99.5	0	4.60	2	0	2	1	Goethite
28 ^{a,b}	0	--	--	--	2	2	0	4	Goethite
29 ^c	1	100	12.7	100	1	1	1	1	Hematite
30 ^c	1	100	100	100	1	2	2	2	Hematite

NOTES: ^a These cases were run with hematite suppressed.

^b This case was run with the same ending time as Case 21.

^c These cases were run with uranium removed from the HLW glass composition.

^d Rates encoding:

Steels: 1=average rate; 2=high rate.

Glass: 0=no glass present; 1=low rate; 2=high rate.

Fuel: 0=no fuel present; 1=low rate; 2=average rate; 3=high rate.

J-13: 1=0.0015 m³/yr; 2=0.015 m³/yr; 3=0.15 m³/yr; 4=0.5 m³/yr.

Figures 6-9 through 6-12 illustrate the limits of system behavior. Specifically, single-stage runs show boron, uranium, and plutonium loss from the fuel and glass to alteration products and solution as a function of reaction time. It also shows how each output varies depending upon input steel corrosion rates, glass corrosion rates, fuel corrosion rates, and fluid flow rates. The double-stage runs provide information on how the system might behave under a number of extreme scenarios. Cases 1 through 10 involve average steel degradation rates. Cases 11 through 20 entail high steel degradation. Examination of the results in Table 6-2 indicates that uranium and plutonium loss are greatest when glass dissolution rates are high. At a given glass dissolution rate, uranium loss varies inversely with the flux of water, as does plutonium loss. Steel corrosion and fuel degradation are third order controls over uranium and plutonium release.

The general trend of iron oxide corrosion product accumulation seen in Figure 6-9 is that iron oxides accumulate until roughly 100 years have elapsed, followed by either a plateauing of accumulation after about 250 years (Cases 1, 4, 10, and 24), or a quantitative decrease in total iron oxide after about a hundred years (Cases 22 and 19). The first group accumulated iron oxides slowly, in part, because steel corrosion rates were low. The second group accumulated iron oxides rapidly because higher steel degradation rates were used as input. The plateauing of iron oxide accumulation in the first group, and the decrease in iron oxide accumulation in the second group, arose because of the rapid, parallel increase in Fe-containing smectite (see Figure 6-10) which formed at the expense of, respectively, potentially new, and existing corrosion products.

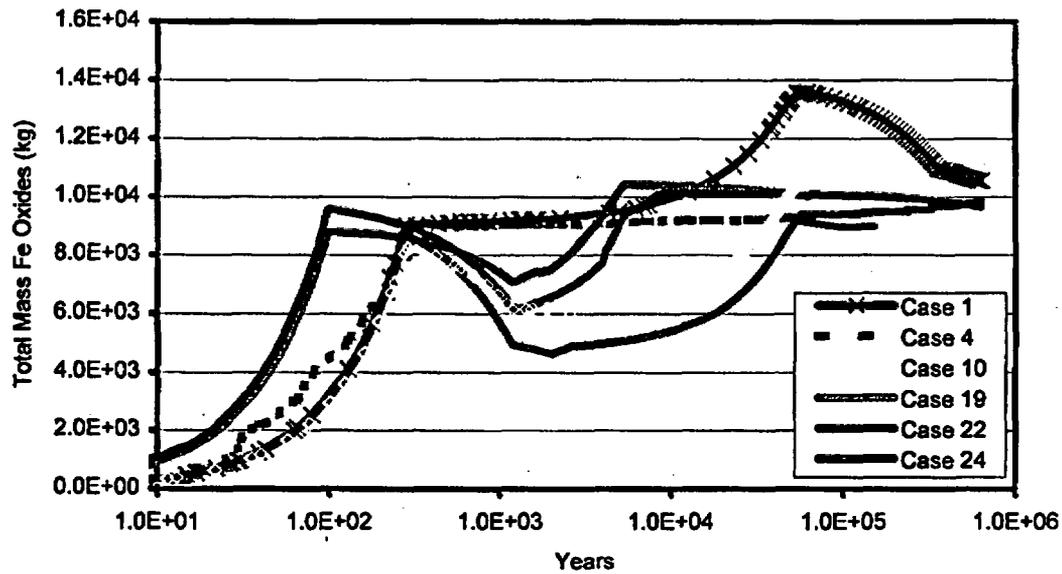


Figure 6-9. Predicted Accumulation of Iron Oxide Degradation Products over Time

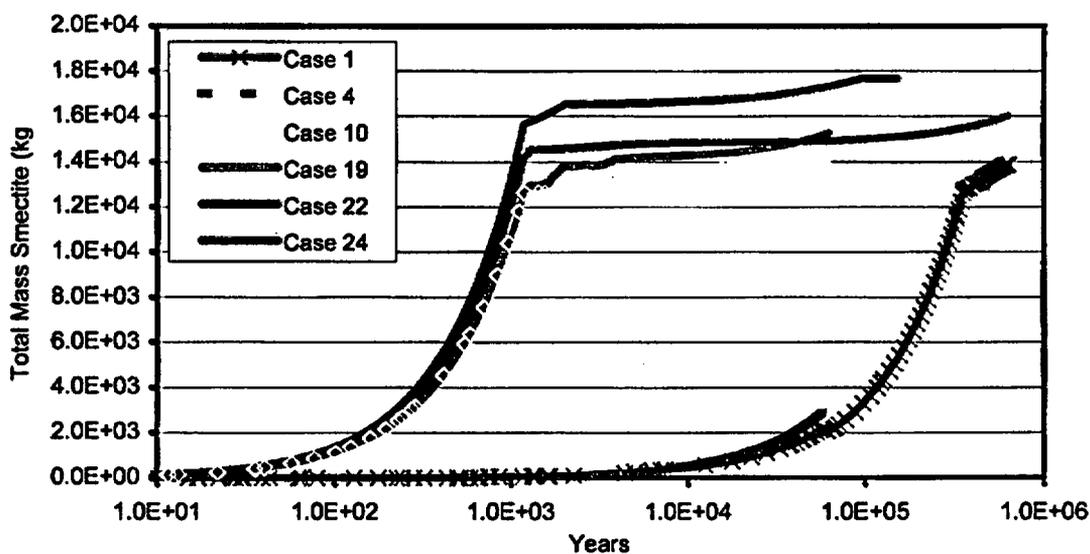


Figure 6-10. Predicted Accumulation of Smectite Degradation Products over Time

Smectite accumulation as a function of time (Figure 6-10) likewise shows two types of behavior. Only minor amounts of smectite accumulate in the first 10,000 years in some runs (Cases 1 and 4), while in others, smectite accumulation becomes significant within the first hundred years, ultimately plateauing at roughly 1,000 years. The runs in which smectite formed late are runs in which pH's were acidic for the first several thousand years of reaction. Smectites are more stable at neutral to high pH and are less likely to form under mildly acidic conditions. The runs where smectite formed early are those runs that were initially, or became, neutral to alkaline early. Recall that uranium is contained in both the Shippingport fuel and in the HLW glass, and that the isotopic ratios of the two sources differ.

It is important for subsequent neutronics calculations that the relative contribution of the two be estimated over time. This estimate was done in part through Cases 29 and 30 which had inputs identical to Cases 1 and 10, except that the original uranium component in the glass (~1.8%) was replaced with Ti in the input. This allows the uranium release from the fuel to be isolated. Comparison of the results of Cases 29 and 30 (uranium in fuel) against the results of Cases 1 and 10 (uranium in glass and fuel) allows the relative uranium contribution from the glass and fuel over time to be assessed. This comparison is made in Figures 6-11 and 6-12. In the first case (average steel corrosion, low glass corrosion, low fuel corrosion, and low fluid flux [Figure 6-11]), the total uranium in the waste package is primarily from the glass until $\sim 5 \cdot 10^5$ years have elapsed.

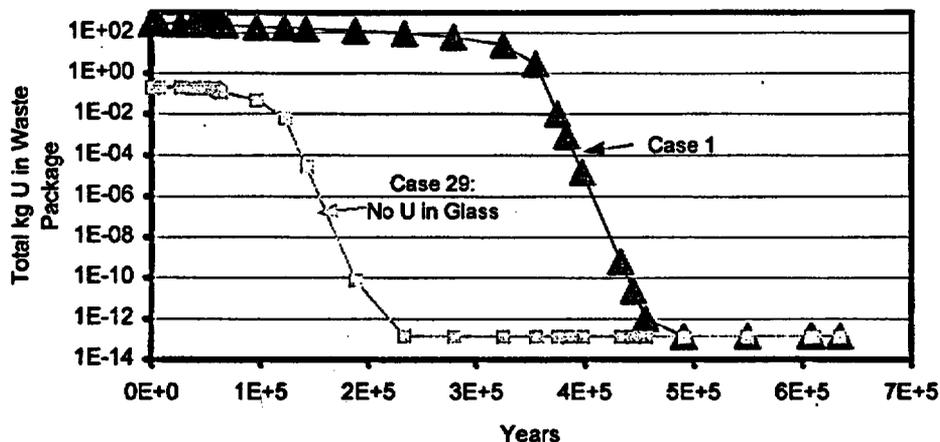


Figure 6-11. Predicted Total Uranium Mass in Waste Package for Cases 1 and 29

In the second case (average steel corrosion, high glass corrosion, average fuel corrosion, and average flow [Figure 6-12]), the total uranium in the waste package is primarily from the fuel, except over the first 500 years wherein the situation is reversed.

Part of the output from the EQ6 runs are files containing the elemental composition of the solids predicted to form during the degradation of Shippingport PWR SNF waste packages. The final ($\sim 6 \cdot 10^5$ years) predicted solids composition for the second stage of Case 22 (post-breach) was used for criticality calculations and is shown in Table 6-3 (CRWMS M&O 1999e, Table 5-20).

Since the degradation rate of the Zircaloy fuel cladding was assumed to be very slow, most of the cases were run assuming that only 1% of the moles and surface area of the fuel wafers was exposed to degradation during the simulations, i.e., the moles and surface area values entered for the fuel reactant were actually multiplied by 0.01 before entry in the input files. Cases 25-27 were done to test the effect of 100% fuel exposure on boron, plutonium, and uranium release from the waste package (compared to Cases 2, 4 and 23, respectively, with 1% fuel exposure). As shown in Table 6-2, the effect was found to be minimal with regard to losses based on total available boron, uranium, and Pu. An exception was Case 27, wherein the percentage of available uranium loss was decreased by about 20% compared to Case 23 with 1% fuel exposure.

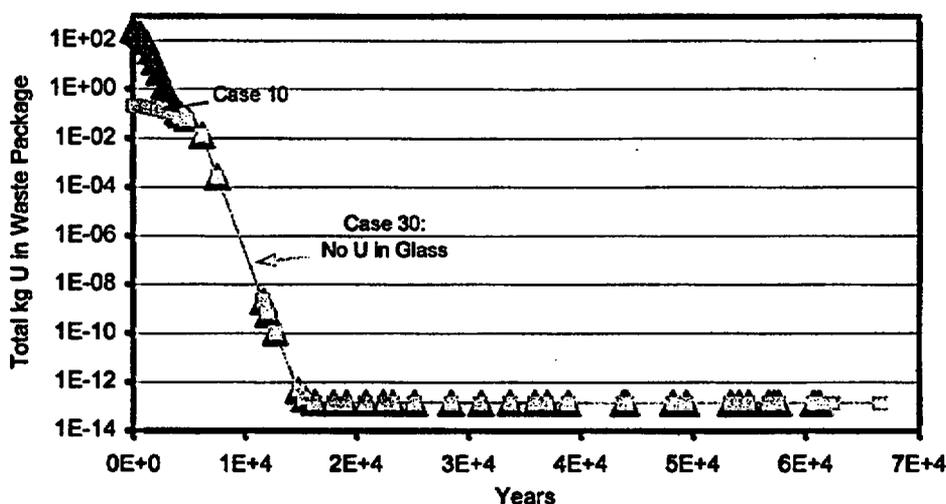


Figure 6-12. Predicted Total Uranium Mass in Waste Package for Cases 10 and 30

Table 6-3. Chemical Composition of Post-Breach Clay

Element	Mole Percent	Element	Mole Percent
O	56.3	P	0.0116
H	14.5	K	0.0321
Fe	15.5	Mg	0.199
Al	1.07	Mn	0.593
Ba	0.0102	Na	0.0448
Ca	0.268	Ni	0.53
Cl	2.7E-20	Pb	0.00365
Cu	0.0151	Si	10.8
F	0.00385	Ti	0.155
C	0.0139	Zr	0.000215

Cases 28 and 21a compared the total density of the corrosion products estimated under conditions when hematite was allowed to form and when hematite was suppressed and goethite was allowed to form. Very little difference was observed between the densities and elemental compositions of the corrosion products calculated for these two cases (see CRWMS M&O, 1999e, Table 5-24, p. 45).

6.4 SUMMARY

The objective of these calculations was to assess the chemical characteristics that might lead to the retention of uranium and plutonium in a waste package containing Shippingport PWR SNF. Thirty EQ6 reaction path calculations were carried out to span the range of possible system behavior and to assess the specific and coupled effects of fuel degradation, steel corrosion, glass degradation, and fluid influx rate on uranium and plutonium mobilization. Fluids having a composition of J-13 well water were modeled as steady-state reactants with waste package components over time spans of up to $6 \cdot 10^5$ years. Corrosion product accumulation (primarily of iron oxides and smectites) and uranium and plutonium mobilization were examined as well.

The controls on uranium and plutonium release from the waste package can be summarized as follows:

1. Uranium and plutonium loss are greatest when glass dissolution rates are high. High glass dissolution and low water fluxes favor alkalinity buildup and the formation of mobile actinide-carbonate complexes. Steel corrosion and fuel degradation are third order controls over uranium and plutonium release.
2. Uranium loss from the waste package varied from 0.06% to 100% and was typically complete if greater than neutral pH's (and attendant high alkalinity) existed for any appreciable amount of time. At a given glass dissolution rate, uranium loss varies inversely with the flux of water. Immobilized uranium was modeled as occurring due to the formation of the uranium-silicate, soddyite.
3. Plutonium loss was typically much less than uranium loss, though waste package accumulations were also quantitatively smaller than that observed for uranium. Plutonium accumulation was modeled as being due to formation of PuO_2 .
4. The relative contributions of uranium from glass and uranium from fuel are predicted to vary. Under conditions of average steel corrosion, low glass corrosion, low fuel corrosion, and low fluid flux, the total uranium in the waste package is primarily from the glass until $\sim 5 \cdot 10^5$ years have elapsed. When average steel corrosion, high glass corrosion, average fuel corrosion, and average flow are used as input, the total uranium in the waste package is predicted to come primarily from the fuel, except over the first 500 years wherein the glass contribution is greater.

As mentioned in the discussion of the calculation results above, the mobilities of uranium and plutonium are pH dependent. The degradation rates of waste package components, which affect acidity and alkalinity, as well as the flow rate of J-13 well water, will have a bearing on the possibility for internal criticality.

The scenario for the double-stage cases matches with the generic scenario group of IP-3 (CRWMS M&O 1999k), i.e., waste form degrade after the materials outside the DOE canister degrade. Thus, double-stage cases represent the most probable degradation scenario. Six cases were run with one percent of the fuel exposed to degradation. In one of the four cases, 24% of the uranium originating from 1% of the fuel was flushed from the waste package, leaving 99% of the original fuel intact. In one multiple stage case, which was run with 100% fuel exposure, only 5% of the total uranium was flushed from the waste package, leaving behind 95% of the original uranium as a corrosion product in the waste package. The case with 100% fuel exposure, however, is not very probable due to the highly corrosion resistant Zr-4 cladding. In all double-stage cases, various degradation rates of the steel, and J-13 water were used with fuel and steel degrading at a high rate.

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7. INTACT AND DEGRADED COMPONENT CRITICALITY ANALYSES

7.1 USE OF COMPUTER SOFTWARE

The Monte Carlo code, MCNP, Version 4B2, is used to calculate the k_{eff} of the waste package. This code, identified as CSCI 30033 V4B2LV, was obtained from SCM in accordance with appropriate procedures, and is qualified as documented in the SQR for the MCNP, Version 4B2 (CRWMS M&O 1998i).

7.2 DESIGN ANALYSIS

The calculation method used to perform the criticality calculations consisted of using the MCNP Version 4B2 code (Briesmeister 1997) to calculate the k_{eff} for various geometrical configurations of Shippingport PWR fuel in the 5-DHLW/DOE Spent Fuel-Long waste package. The k_{eff} results represent the average combined collision, absorption, and track-length estimator from the MCNP calculations. The standard deviation (σ) represents the standard deviation of k_{eff} about the average combined collision, absorption, and track-length estimate due to the Monte-Carlo-calculation statistics. The calculations are performed using continuous energy cross-section libraries that are part of the qualified MCNP code system (CSCI 30033 V4B2LV). All calculations are performed with fresh-fuel isotopics (Assumption 2.3.5.1). The DOE SNF canister with Shippingport PWR fuel does not contain any strong neutron absorbers such as gadolinium. Boron, which is a burnable poison that is an integral part of the fuel, is neglected in all criticality calculations.

The issue of minor actinides, which are fast-fissionable and non-fissile, is investigated. The critical mass of neptunium (Np-237) moderated and reflected by granite is 45,000 g, and that for americium (Am) at 10,000 years is 78,900 g (Allen 1978). The DOE SNF canister with one Shippingport PWR C2 S1 assembly has a total of approximately 38 g Pu-238 and 19 g Am-241, as a result of 426.4 MWd/kg exposure (DOE 1999a, Table B-3; Parrington et al. 1996, p. 9). No appreciable amount of Np-237 was generated as a result of exposure (DOE 1999a, Table B-3). Due to these very low quantities (less than 0.1% of required minimum critical mass), these minor actinides do not present a potential for criticality, and therefore, have not been included in the criticality calculations. The use of fresh fuel compositions and neglect of burnable neutron absorber conservatively bounds any changes associated with burnup.

7.3 CALCULATIONS AND RESULTS – PART I: INTACT CRITICALITY ANALYSIS

In this section, the criticality analyses for intact configurations are discussed. Although the components (fuel plates, assembly, and DOE SNF canister) are considered structurally intact, water intrusion into the components is allowed to determine the highest k_{eff} resulting from optimum moderation. It must be noted that no credit for burnable poison material (boron) is taken in any of the calculations that are analyzed in this section.

The intact canister with the intact fuel cluster is represented in the intact codisposal waste package as shown in Figure 7-1. The k_{eff} of the intact fuel cluster is calculated based on the fuel

cluster centered in the DOE SNF canister and the DOE SNF canister centered inside the waste package. The DOE SNF canister is assumed to be fully flooded internally, and reflected externally (outside of the waste package) with water. The empty space outside the canister and inside the waste package is represented as water. The densities of water inside the waste package and the DOE SNF canister are simultaneously varied between 0.0 and 1.0 g/cm³ to find the highest value of k_{eff} . The highest $k_{eff} + 2\sigma$ of 0.8437 is obtained with water with 1.0 g/cm³ density in both the DOE SNF canister and the waste package (CRWMS M&O 2000, Section 6.1.1). The density of water in the center cruciform area only is also varied to determine the effect of water density around the fuel assembly. The results indicated that decreasing the density of water in the cruciform area results in decrease in k_{eff} . Therefore, in all configurations in the following sections the DOE SNF canister and the waste package are modeled as being flooded.

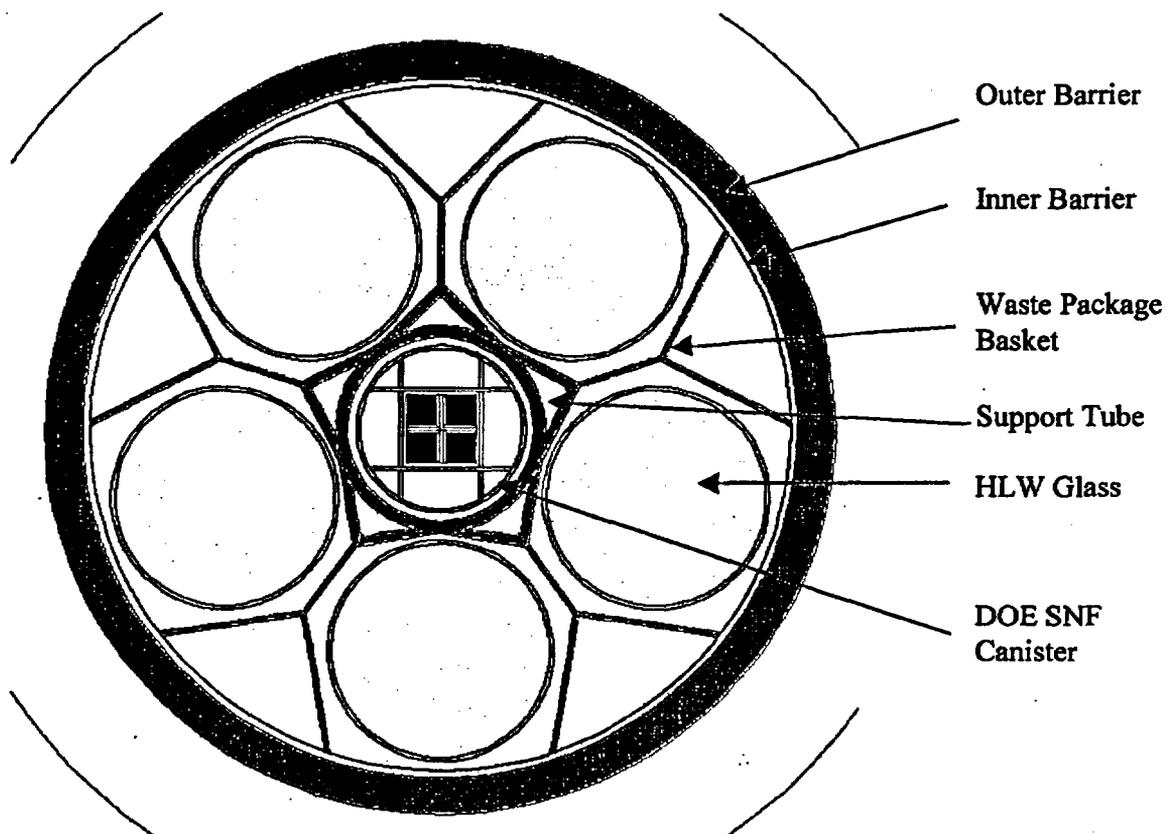


Figure 7-1. Cross-sectional View of the 5-DHLW/DOE Spent Fuel-Long Waste Package

In all cases the waste package is water reflected. A case was run to demonstrate that the environment outside the waste package, whether tuff, water, or a mixture, has no significant impact on the configuration k_{eff} . Instead of water reflection outside the waste package, reflective boundary conditions were used. The k_{eff} of the waste package with reflected boundary conditions (0.8408 ± 0.0011) was statistically identical to the k_{eff} of the water-reflected waste

package (0.8415 ± 0.0011). In addition, a case with fuel assembly placed against the waste package inner barrier wall was analyzed for neutron reflection by the outside material. The number of outgoing neutrons penetrating the waste package barriers is less than 1% of the total number of neutrons in the system; and typically less than 0.2 based on the evaluation of the neutron activity reported in the outputs. When the factor of four attenuation through the waste package barriers is factored in, having a different reflector (e.g., tuff, rock, clay, etc.) on the outside of the waste package would have negligible or no effect on the results.

Effect of water intrusion into the plate void space is also investigated. The plate void space is calculated by subtracting the total fuel wafer volume from the actual fuel volume of the fuel cluster. The fuel meat occupies 87.5% of the fuel wafer volume. The remaining portion (wafer porosity volume) is void space. The effect of water intrusion into the fuel wafer porosity volume is also calculated. Water densities in the fuel wafer porosity and/or the plate void space are varied between 0.0 and 1.0 g/cm³ to find the highest value of k_{eff} . Water intrusion into plate void space (with 1.0 g/cm³ density) increases k_{eff} by approximately 3% with a maximum $k_{eff} + 2\sigma$ of 0.8678 (CRWMS M&O 2000, Section 6.1.2). Water intrusion into fuel wafer porosity volume (with 1.0 g/cm³ density) increases k_{eff} by approximately 2% with a maximum $k_{eff} + 2\sigma$ of 0.8574 (CRWMS M&O 2000, Section 6.1.2). Water intrusion into both of these regions simultaneously increases k_{eff} by approximately 5% with a maximum $k_{eff} + 2\sigma$ of 0.8819 (CRWMS M&O 2000, Section 6.1.2).

Effect of mineral deposits from the J-13 well water accumulation around the fuel cluster, area between plates, and the cruciform area are calculated. Figure 7-1 gives a representation of this configuration. Water around the fuel cluster, the area between plates, and the cruciform area is mixed with mineral deposit. The J-13 well water mineral deposits are introduced in three different configurations: in the coolant channel and the cruciform areas, in the area around the fuel cluster inside the square central guide plate area where the water acts more as a reflector, and inside the canister outside the square guide plate area. The results indicated that mineral deposits from the J-13 well water have no significant effect on k_{eff} of the system (results are within statistical uncertainty) (CRWMS M&O 2000, Table 6-7).

7.4 CALCULATIONS AND RESULTS – PART II: DEGRADED COMPONENT CRITICALITY ANALYSIS

In analyzing the configurations described above, parametric studies have been performed to determine the optimum moderation and configuration. These parametrics include optimizing the moderation in the DOE SNF canister and the waste package by varying the amount of water in the degradation products, and by varying the density of water in the degradation products. As with the intact configurations no credit for the burnable poison (boron) is taken.

7.4.1 Intact SNF

7.4.1.1 Degraded Guide Plates

The guide plates, which comprise the DOE SNF canister basket (see Figure 2-4), are represented as being completely degraded and converted into goethite. This configuration is described in Section 6.2.1.2 and corresponds to the configuration class 1. Figure 7-2 shows the cross-

sectional view of the waste package in this configuration. The intact fuel cluster is positioned at the bottom of the canister. The water volume fraction in the goethite is varied. Water occupies the remaining portion of the canister. All other components in the canister and codisposal waste package are represented as being fully intact. Although this configuration is unlikely, the intact waste package basket maximizes the neutron reflection and, therefore, the value of calculated k_{eff} . This is confirmed by the results of the cases described in Section 7.4.1.2, where the waste package components are degraded. The effect of filling the coolant channel and cruciform areas with water instead of goethite/water mixture is investigated first. Filling the coolant channel and cruciform areas with water results in approximately 24% increase in k_{eff} (CRWMS M&O 2000, Table 6-6.) Therefore, the coolant and cruciform areas are filled with water for the remainder of the configurations in this section. The highest $k_{eff} + 2\sigma$ of 0.9042 is obtained when the DOE SNF canister is filled with only water at 1 g/cm³ density (goethite volume fraction of 0) (CRWMS M&O 2000, Table 6-6.)

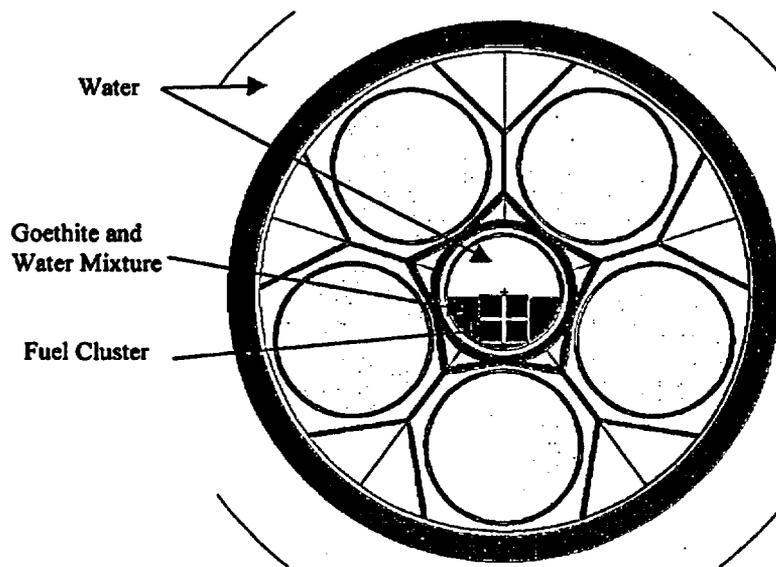


Figure 7-2. Cross-sectional View of the Configuration with Degraded Guide Plates and Intact SNF

7.4.1.2 Clay Accumulation Inside Canister

Effect of clay intrusion into the canister is calculated based on total degradation of the HLW glass pour canisters and retained integrity of the canister. The canister is positioned at the bottom of the inner barrier of the waste package. This configuration is described in Section 6.2.1.3 and corresponds to the configuration class 1. Figure 7-3 shows the cross-sectional view of the waste package in this configuration. Pre-breach clay is degraded material prior to breach of the canister. Post-breach clay is degraded material formed after breach of the canister. The pre-breach clay composition is represented outside the canister while the post-breach clay composition is used in representing clayey material inside the canister. Water inside the canister is replaced with clay. Water and clay volume fractions are varied. The results show that the k_{eff} is highest when there is no clay in the DOE SNF canister with maximum $k_{eff} + 2\sigma$ of 0.8429 (CRWMS M&O 2000, Table 6-8.)

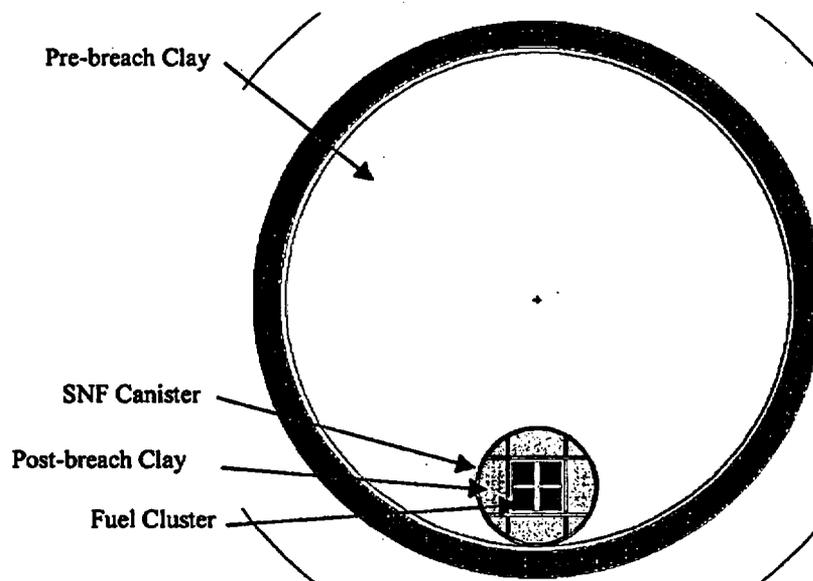


Figure 7-3. Cross-sectional View of Clay-accumulated Configuration

7.4.1.3 Degraded DOE SNF Canister and Waste Package

In these configurations, the materials surrounding the fuel cluster degrade faster than the fuel, which is likely given the extremely low degradation rate of Zircaloy-4. The DOE SNF canister shell, five HLW glass pour canisters, waste package basket, and the DOE SNF canister basket are fully degraded. The canister is positioned on the bottom of the waste package before being degraded. This configuration is described in Section 6.2.1.4 and corresponds to the configuration class 1. Figure 7-4 shows the cross-sectional view of the waste package in this configuration. The intact fuel cluster is surrounded by goethite (from degraded canister) and clay (degraded waste package, internals, HLW glass pour canisters, etc.). The goethite is mixed with clay and water with varying volume fractions. The coolant and cruciform areas are filled with water. The region above the clay, goethite, and water mixture is filled with post-breach clay. The fractions of goethite, water, and clay are varied to determine the effects of these parameters. The maximum difference in k_{eff} of the system is less than 4% with maximum $k_{eff} + 2\sigma$ of 0.922 with goethite, clay, and water fractions of 0.0, 1.0, and 0.0, respectively (CRWMS M&O 2000, Table 6-9.) This case corresponds to the fuel cluster reflected by clay only. When the fuel cluster is reflected by water or goethite only, the k_{eff} decreases by approximately 1%, therefore indicating that all three materials are similar from stand point of neutron reflection.

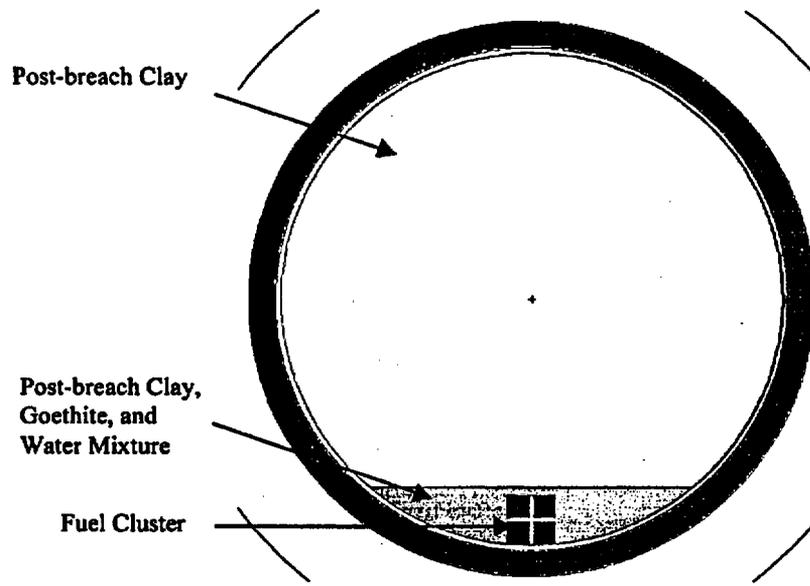


Figure 7-4. Cross-sectional View of the Intact Fuel Cluster in the Degraded Waste Package

7.4.2 Degraded Fuel Cluster

The Shippingport PWR SNF cluster is degraded for all cases in this section. Partially and fully degraded fuel cases are calculated. The partial degradation is represented as a fraction of fuel ($\text{UO}_2\text{-ZrO}_2\text{-CaO}$) redistributed outside the fuel plates and homogeneously mixed with water, goethite, and/or clay. The fuel cluster is assumed to be physically intact in the partial degradation calculations. The fully degraded fuel is represented as a homogeneous mixture of UO_2 , water, goethite, and clay. The degraded fuel is assumed to be chemically unchanged. The codisposal waste package is assumed to be fully reflected by water for all cases.

The degradation configurations presented in this section are for analyzing the effect of the generic degradation scenario group IP-1, i.e., SNF degrades faster than the other surrounding components. As discussed in Sections 6.2.1.5 through 6.2.1.7, the degradations associated with IP-1 are not probable since for Shippingport PWR the SNF is sealed inside the highly corrosion resistant material of Zircaloy-4, which is considered inert.

7.4.2.1 Partially Degraded Fuel Cluster in the Intact DOE SNF Canister

The fuel cluster is partially degraded and $\text{UO}_2\text{-ZrO}_2\text{-CaO}$ is redistributed into the coolant channels and the cruciform areas as well as into the central-basket area of the canister. The central-basket area is the central square area excluding the fuel cluster. The intact waste package representation of Figure 7-1 gives a representation of this partial fuel degradation case. The redistributed fuel (ranging from 10 to 99% of the total fuel mass) is mixed with water in the coolant channel, the cruciform, and/or central-basket areas. The remaining portion of the fuel mass stays inside the fuel plates. This configuration is described in Section 6.2.1.5 and corresponds to the configuration class 6.

The k_{eff} for the configuration with 10% of the fuel redistributed (due to aqueous transport) into the coolant channel, cruciform, and central-basket areas is first calculated. It is observed that the 10% fuel redistribution to the coolant channel, cruciform, and the central-basket areas results in the largest $k_{eff} + 2\sigma$ (0.8736) compared to the fuel redistribution to the coolant channel only (0.8460), or to the coolant channel and the cruciform areas (0.8625). Therefore, when the fuel redistribution fraction is varied from 10 to 99%, the redistributed fuel is placed in the coolant channel, cruciform, and central-basket areas. The results indicate that k_{eff} increases as the amount of redistributed fuel increases (CRWMS M&O 2000, Table 6-12.) The highest $k_{eff} + 2\sigma$ of 0.9300 is obtained with 80% fuel redistribution. This would require essentially all the cladding to fail and expose the fuel wafers, which is extremely unlikely as discussed in Section 6.2.1.6.

7.4.2.2 Partially Degraded Fuel Cluster in Degraded DOE SNF Canister

The partially redistributed fuel is mixed with goethite and water with varying volume fraction simulating degradation of the guide plates and the canister. This configuration is described in Section 6.2.1.6 and corresponds to the configuration class 3. Figure 7-5 gives a representation of this partial degradation case. The fuel cluster is physically intact in this representation. The coolant channel and cruciform areas of the fuel cluster are filled with water instead of goethite and water mixture.

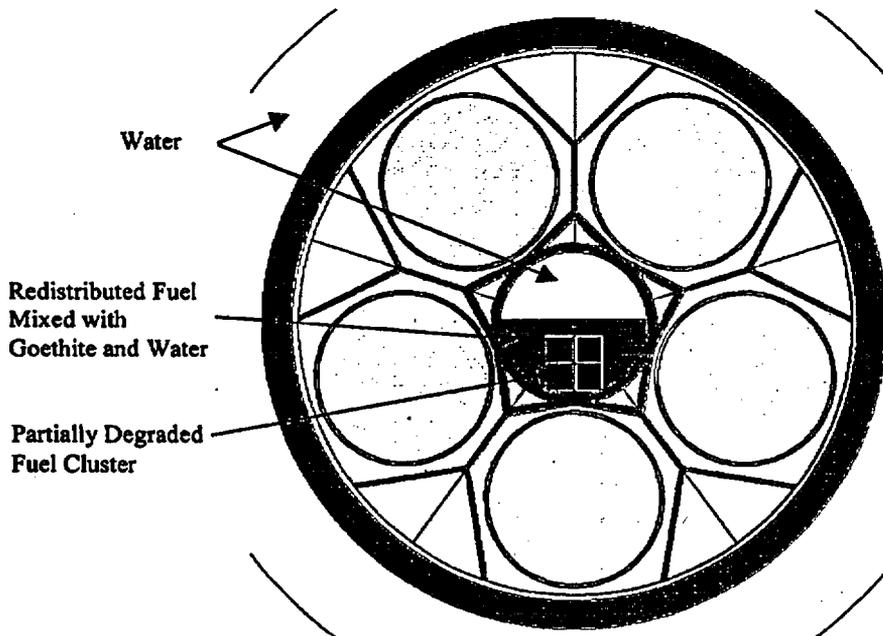


Figure 7-5. Partially Degraded Fuel Cluster in the Waste Package

The results indicate that varying the fraction of fuel that is redistributed through aqueous transport effects the k_{eff} by as much as 28% with a maximum $k_{eff} + 2\sigma$ of 0.9188 with 40% fuel

redistribution (CRWMS M&O 2000, Table 6-13.) This configuration does not contain any water mixed with the fuel/goethite mixture. Varying the amount of water mixed with the fuel/goethite mixture effects the k_{eff} by as much as 1% with a maximum $k_{eff} + 2\sigma$ of 0.9254 with 40% fuel redistribution and 40% water in the fuel/goethite/water mixture. The effect of having redistributed fuel, goethite, and water mixture in the coolant channel and cruciform control rod channel areas instead of water is also investigated. Replacing water with fuel/goethite/water mixture reduces k_{eff} by as much as 21%. As described in Section 6.2.1.6, this level of fuel redistribution is extremely unlikely.

7.4.2.3 Partially Degraded Fuel Cluster with Degraded Canister and Degraded Waste Package

In this scenario, the fuel materials and everything surrounding the fuel degrades at the same rate. The partially degraded fuel (UO_2) is mixed with degradation products from guide plates, DOE SNF canister, waste package basket, HLW glass pour canisters, and HLW glass. This configuration is described in Section 6.2.1.7 and corresponds to the configuration class 2. Figure 7-6 gives a representation of this configuration. Although the fuel cluster loses fuel due to aqueous transport, the cover plates are assumed to remain intact (fuel is carried out by aqueous transport through possible cracks in welds). The partially redistributed fuel is mixed with goethite, clay, and water with varying fractions and fuel mass. The fraction of clay and fraction of goethite are also varied. Decrease in the goethite fraction in the fuel/goethite/clay mixture (consequently increase in the clay fraction) decreases k_{eff} by as much as 9% with a maximum $k_{eff} + 2\sigma$ of 0.9167 for a 0.4 fuel redistribution fraction. This redistributed fuel is mixed with goethite and clay with volume fractions of 0.9 and 0.05, respectively (CRWMS M&O 2000, Table 6-14.). This indicates that goethite in this configuration is a better neutron reflector than clay for the partially intact fuel cluster, and a better moderator for the redistributed fuel mixture. Note that the goethite and clay occupy 60% of the fuel/goethite/clay mixture. The fraction of fuel redistribution is varied for the configuration with 90% goethite and 5% clay in the remaining part of the mixture. The maximum $k_{eff} + 2\sigma$ of 0.9194 is obtained when the fuel redistribution fraction is 0.3.

Effect of spacing variation inside the cruciform area due to fuel assembly welds failure is also investigated. The mixture outside the fuel cluster contains 90% goethite, 5% clay, and 5% water, which results in $k_{eff} + 2\sigma$ of 0.9054 with original spacing of 1.19 cm between fuel sub-clusters (CRWMS M&O 2000, Table 6-15.) Decreasing the spacing between the sub-clusters decreases the k_{eff} by up to 7% (sub-clusters are touching.) Increasing the spacing decreases k_{eff} with approximately 15% decrease for a spacing of 5.08 cm.

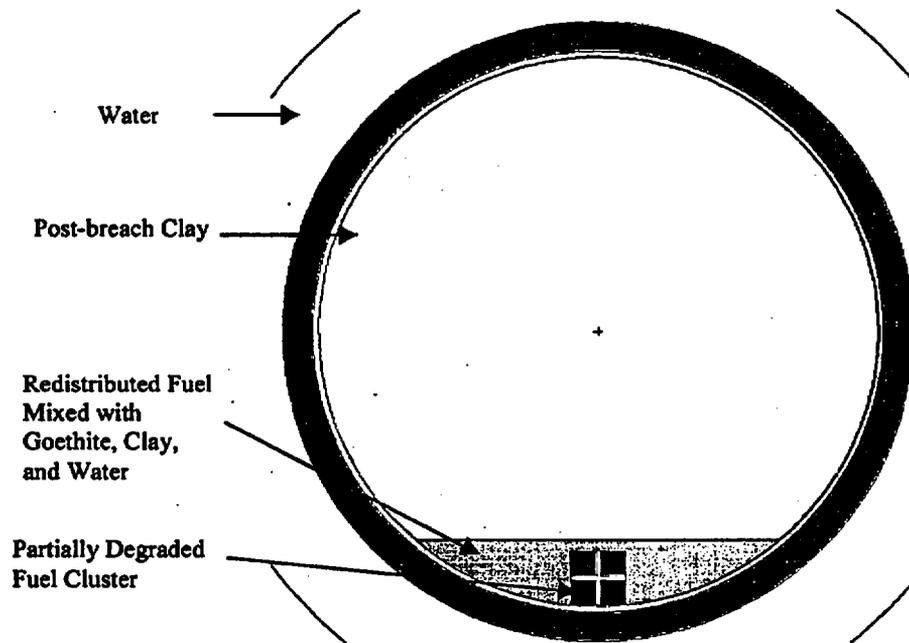


Figure 7-6. Partially Degraded Fuel Cluster in the Degraded Waste Package

7.4.2.4 Fully Degraded Fuel in Degraded Canister and Degraded Waste Package

The fully degraded fuel (UO_2) is mixed with goethite, clay, and water. The degraded fuel contains 20.923 kg uranium with effective enrichment of 93.2 wt%. The fuel, goethite, clay, and water mixture layer is placed on the bottom of the waste package. This configuration is described in Section 6.2.1.7 and corresponds to the configuration class 2. Figure 7-7 gives a representation of this configuration. The fuel and the goethite volume fraction are varied to mix with water and clay. The post-breach clayey material occupies the non-fueled region as shown in Figure 7-7. The results indicate that as the amount of clay in the mixture is increased the k_{eff} decreases. The highest $k_{\text{eff}} + 2\sigma$ of 0.8463 is obtained with no clay or water in the fuel/goethite mixture (CRWMS M&O 2000, Table 6-16).

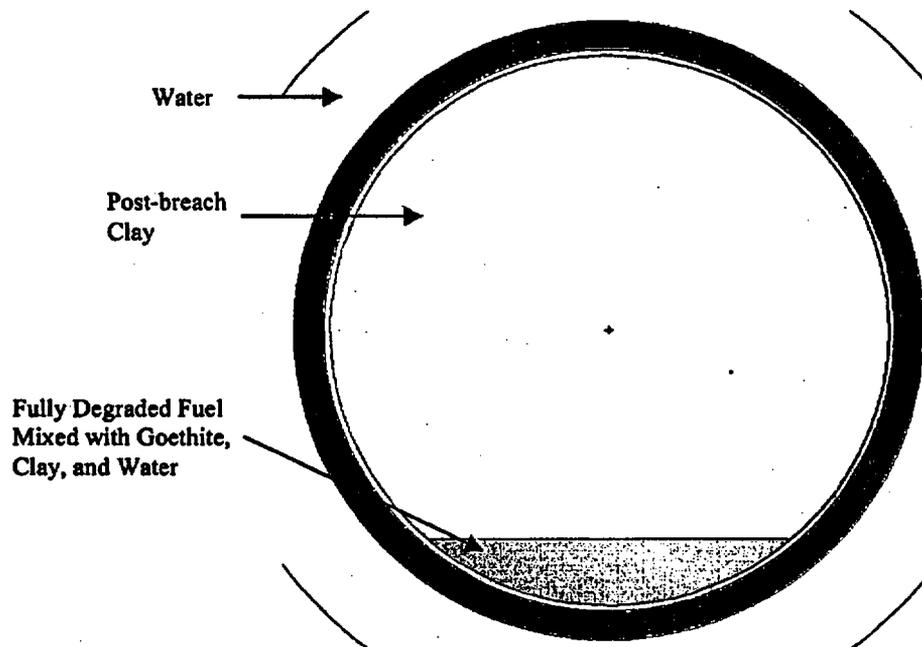


Figure 7-7. Fully Degraded Fuel Cluster Configuration

7.5 SUMMARY

The results of three-dimensional (3-D) Monte Carlo calculations from the intact and degraded component criticality analyses show that the requirement of $k_{eff} + 2\sigma$ less than or equal to 0.93 is satisfied for one Shippingport PWR fuel assembly in the DOE SNF canister. This configuration does not need any neutron absorber in the basket or elsewhere in the waste package to meet this requirement.

8. CONCLUSIONS

This document and its conclusions may be affected by technical product input information that requires confirmation. Any changes to the document or its conclusions that may occur as a result of completing the confirmation activities will be reflected in subsequent revisions. The status of the input information quality may be confirmed by review of the Document Input Reference System database.

8.1 STRUCTURAL ANALYSIS

The results from the 2-D FEA calculations given in Section 3.3 show that there is sufficient clearance between the inner diameter of the support tube and the outer diameter of the DOE SNF canister for the DOE SNF canister to be removed from the waste package after a tipover DBE, which results in the bounding dynamic load.

The maximum deformations in each component of the waste package are acceptable. The outer barrier is directly exposed to a dynamic impact with an essentially unyielding surface. Therefore, local plastic deformations are unavoidable on the outer surface. Similarly, the basket support structure receives the direct impacts of the pour canisters, which result in limited permanent deformations of the basket plates.

The results given in Section 3.3.2 show that there would be no interference between the fuel assembly and the basket structure inside the DOE SNF canister. Thus, the waste package will be able to be unloaded after a tipover DBE.

In the light of the above discussions, it is concluded that the performance of the 5-DHLW/DOE Spent Fuel-Long waste package design is structurally acceptable when exposed to a tipover event, which is the bounding DBE within the criteria specified in the SDD, as long as the 2,721 kg mass limit for the loaded DOE SNF canister is not exceeded.

The SDD criteria for structural calculations (SDD 1.2.2.1.3, SDD 1.2.2.1.4, and SDD 1.2.2.1.6), cited in Section 2.2.1, have TBV-245. The analysis of the results indicates that the waste package will withstand the events mentioned in the structural criteria by meeting the limits by a margin of more than a factor of two. Therefore, the TBV-245 is non-critical and is not carried through the conclusions in this section.

8.2 THERMAL ANALYSIS

Based on the 2-D FEA calculations given in Section 4, the Shippingport PWR waste package satisfies all relevant governing criteria, as listed in Table 8-1. The maximum temperatures are shown in Table 8-1. The HLW glass dominates the thermal heat output of the waste package.

Table 8-1. Shippingport PWR Codisposal Waste Package Thermal Results and Governing Criteria

Waste Package Metric	SDD Criterion	Shippingport PWR Codisposal Waste Package Value
Maximum waste package heat output	< 18,000 W	12828.8 W ^a
Maximum HLW temperature	< 400 °C ^a	252.3 °C
Maximum DOE SNF cladding temperature in codisposal waste package	< 350 °C	249.2 °C

NOTES: ^a This summary report does not specifically report the results for HLW glass canisters. SDD criterion (SDD 1.2.1.6) from CRWMS M&O (1999j) for maximum HLW temperature is listed for information only.

^b See Table 2-5 for elapsed time of zero years.

The SDD criteria for thermal calculations (SDD 1.2.1.8 and SDD 1.2.4.9), cited in Section 2.2.2, have TBV-241 and TBV-251. As shown in Table 8-1, the analysis of the results indicates that the cladding temperature criterion is met by more than 100 °C, and the heat output limit is met by more than 5,000 W. The maximum waste package heat output limit affects the repository performance. Since the actual heat output of 5-DHLW/DOE Spent Fuel Long waste package with the DOE SNF canister containing Shippingport PWR fuel will not increase, an increase in the limit will have no effect on the conclusions presented here. A decrease in the maximum heat output limit, on the other hand, will decrease total heat generated in the waste package and therefore result in lower temperatures throughout the waste package. Hence, the maximum DOE SNF cladding temperature limit will not be exceeded. Therefore, the TBV-241 and TBV-251 are non-critical and are not carried through the conclusions in this section. Note that TBD-179 in SDD 1.2.1.8 does not apply, since it is a temperature criteria for DOE fuels with cladding other than zircaloy or stainless steel.

8.3 SHIELDING ANALYSIS

The results of 3-D Monte Carlo dose rate calculation show that maximum dose rate on the outer surfaces of waste package is below 355 rem/h design limit by a factor of approximately 34. The highest dose rate is only 10.32 ± 0.36 rem/h. The primary gamma dose rate dominates the neutron dose rate by approximately three orders of magnitude.

The SDD criterion for shielding calculations (SDD 1.2.4.7), cited in Section 2.2.3, has TBV-248. The analysis of the results indicates that the dose rate at all external surfaces of a loaded and sealed disposal container is below the criterion limit by a margin of more than a factor of 34. Therefore, the TBV-248 is non-critical and is not carried through the conclusions in this section.

8.4 GEOCHEMISTRY ANALYSIS

The degradation analyses followed the general methodology developed for application to all waste forms containing fissile material that evaluates potential critical configurations from intact through degraded. Sequences of events and/or processes of component degradation were developed. Standard scenarios from the master scenario list in the topical report (CRWMS M&O 1998a) were refined using unique fuel characteristics. Potentially critical configurations were identified and analyzed.

When the glass is allowed to degrade rapidly, the alkaline conditions produce high uranium loss (up to 100%), reducing the chances of internal criticality.

8.5 INTACT AND DEGRADED COMPONENT CRITICALITY ANALYSES

All aspects of intact and degraded configurations, including optimum moderation conditions, water intrusion into the fuel plates, and positioning of the fuel assembly were investigated. The results of 3-D Monte Carlo calculations from the intact and degraded component criticality analyses show that the requirement of $k_{eff} + 2\sigma$ less than or equal to 0.93 is satisfied for one Shippingport PWR fuel assembly in the DOE SNF canister. This configuration does not need any neutron absorber in the basket or elsewhere in the waste package to meet this requirement. With this design, there will be approximately 20 DOE SNF canisters with Shippingport PWR SNF (C2 S2), which corresponds to 20 waste packages.

A number of parametric analyses were run to address or bound the configuration classes discussed in Section 6.2.1. These parametric analyses addressed identification of optimum moderation, optimum spacing, and optimum fissile concentration.

The results from the criticality analysis for the degraded DOE SNF canister (fissile material distributed in the waste package) indicate that the highest k_{eff} is achieved if the fuel and clay layers do not mix. Therefore, the amount of clay in the waste package has no effect on the bounding case, which is a layer of optimally moderated fuel not mixed with any clay. Although varying the amount of water mixed with the fuel changes the k_{eff} , the peak $k_{eff} + 2\sigma$ of the system is less than 0.85, which is well below the interim critical limit.

The SDD criterion for criticality calculations (SDD 1.2.1.5), cited in Section 2.2.5, has TBD-235. Intact and degraded component criticality calculations include variations on moderators and moderator densities, which encompass flooding the waste package. Occurrence of design basis events, including those with the potential for flooding the disposal container prior to disposal container sealing, is considered and analyzed by making very conservative assumptions through many different intact and degraded configurations. Therefore, the TBD-235 is non-critical and is not carried through the conclusions in this section.

8.6 ITEMS IMPORTANT TO SAFETY

As part of the criticality licensing strategy, items that are important to safety will be identified during evaluation of the representative fuel type designated by the NSNFP. As a result of the analyses performed for the evaluation of the codisposal viability of HEU oxide (Shippingport PWR) DOE-owned fuel, several items are identified as important to safety. DOE SNF canister shell is naturally an item that is important to safety since it confines the fissile elements to a specific geometry and location within the waste package. The basket that was designed for the DOE SNF canister containing the Shippingport PWR fuel is also an important safety item since it confines the fissile elements to a specific geometry and location within the DOE SNF canister. The DOE SNF canister basket also provides moderator displacement, and thermal neutron absorption due to its high iron content. The DOE SNF canister loaded weight, which must be less than 2,721 kg, is also an important safety item.

The degraded configurations bound the other types of HEU oxide fuels as long as the limits on mass of uranium and its enrichment, and the linear density are not exceeded. As shown in Section 7, the degraded configurations with a partially degraded fuel assembly bound (more reactive than) the intact configurations. The degraded configurations include varying degrees of degradation resulting in many different geometric configurations and fissile distributions. In addition, Paxton et al. (1987, Fig. 11, Fig. 12 and Fig. 13) indicates that as the density of the fuel region decreases the radius of the fuel region must increase to sustain criticality. For a fixed amount of fuel and constant volume, this implies that as the density of the fuel decreases the fuel region must become shorter and thicker (greater radius), which is a more favorable geometry, to maintain the same k_{eff} . If the amount of fuel also decreases, k_{eff} will decrease. Due to the fissile limit, if the fuel length increases, either the density or the radius or both must decrease. If the density decreases (and the radius is kept constant), according to Paxton et al. (1987) the radius must increase to maintain the same k_{eff} which conflicts with the requirement that the radius is kept constant. Similarly, if the radius decreases (and the density is kept constant), then the density must increase to maintain the same k_{eff} which again conflicts with the requirement that the density is kept constant. If both radius and density decrease, then the system is less reactive. Therefore, longer fuels as well as the fuels with smaller density in this group are bounded by this analysis. If, however, the fuel is shorter than the Shippingport PWR SNF, then the linear density of the fuel (g/cm) must be less than or equal to the linear density of the Shippingport PWR SNF. It is very unlikely that the fuel inventory in the HEU oxide fuel group will have any fuels that will exceed the linear density of the representative HEU oxide fuel, which is the Shippingport PWR SNF.

Hence, the total mass of fissile element (U-235) should not exceed the mass used in deriving the conclusions in this report, which is 19.5 kg of U-235 per DOE SNF canister, with total U-235 to U-238 ratio of 13.7 (93.5% enriched in U-235), or less. In addition, the linear density of the fuel (U-235) should not exceed 79 g/cm, which is calculated by dividing the total fuel mass (19.5 kg U-235) by the active fuel length (246.38 cm).

The shielding source terms and thermal heat output of the fuel assemblies must not exceed the ones used in the analyses. Specifically, the total gamma sources from the HLW glass and the fuel assembly must not exceed $5.6962E+15$ gammas/sec/canister and $1.4434E+15$ gammas/sec/assembly, respectively. HLW glass thermal output should be below the limit required by the applicable SDD, not to exceed 2,540 W per HLW glass canister. Alternatively, it must be demonstrated that HLW glass canisters and/or fuel assemblies with higher shielding source terms or thermal heat outputs will not result in violation of the required criteria.

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