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Waste Package Design Methodology Report

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Waste Package Design Methodology Report

TDR-MGR-MD-000006 REV 01

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ACRONYMS

ACI	American Concrete Institute	INEEL	Idaho National Engineering and Environmental Laboratory
ALARA	as low as is reasonably achievable	LWR	light water reactor
ANS	American Nuclear Society		
ANSI	American National Standards Institute	MGR	Monitored Geologic Repository
ASHRAE	American Society of Heating, Refrigerating, and Air-Conditioning Engineers	NNPP	Naval Nuclear Propulsion Program
ASM	American Society for Metals	NRC	U.S. Nuclear Regulatory Commission
ASME	American Society of Mechanical Engineers	NUREG	NRC Regulation
ASTM	American Society for Testing and Materials	ORNL	Oak Ridge National Laboratory
		PWR	pressurized water reactor
B&W	Babcock & Wilcox		
BWR	boiling water reactor	SDD	System Description Document
CFR	Code of Federal Regulations	SNF	spent nuclear fuel
CSCI	Computer Software Configuration Item	SRP	Standard Review Plan
CRWMS M&O	Civilian Radioactive Waste Management System Management and Operating Contractor	STN	Software Tracking Number
		TSPA	Total System Performance Assessment
		UNS	Unified Numbering System
DHLW	defense high-level waste	USGS	U.S. Geological Survey
DIRS	Document Input Reference System		
DOE	U.S. Department of Energy	YMP	Yucca Mountain Project
DTN	Data Tracking Number	YMSCO	Yucca Mountain Site Characterization Office
EPRI	Electric Power Research Institute		
FEP	features, events, and processes		

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1. OBJECTIVE AND SCOPE

The objective of this report is to describe the analytical methods and processes used by the Waste Package Design Section to establish the integrity of the various waste package designs, the emplacement pallet, and the drip shield. The scope of this report shall be the methodology used in criticality, risk-informed, shielding, source term, structural, and thermal analyses. The basic features and appropriateness of the methods are illustrated, and the processes are defined whereby input values and assumptions flow through the application of those methods to obtain designs that ensure defense-in-depth as well as satisfy requirements on system performance. Such requirements include those imposed by federal regulation, from both the U.S. Department of Energy (DOE) and U.S. Nuclear Regulatory Commission (NRC), and those imposed by the Yucca Mountain Project to meet repository performance goals. The report is to be used, in part, to describe the waste package design methods and techniques to be used for producing input to the License Application Report.

2. QUALITY ASSURANCE

All types of waste packages were classified (per QAP-2-3, *Classification of Permanent Items*) as Quality Level-1. *Classification of the MGR Uncanistered Spent Nuclear Fuel Disposal Container System* (CRWMS M&O 1999b, p. 7) provides the classification for waste package designs that will contain uncanistered spent nuclear fuel assemblies. The reference cited here merely serves as an example for waste package classification. The drip shields and emplacement pallets were classified (per QAP-2-3) as Quality Level-1 and Level-2, respectively, in *Classification of the MGR Emplacement Drift System* (CRWMS M&O 2001a).

This technical report has been developed in accordance with AP-3.11Q, *Technical Reports*. The technical work planning that governs the development of this report is *Technical Work Plan for: Waste Package Design Description for LA* (BSC 2001h), which was prepared per AP-2.21Q, *Quality Determinations and Planning for Scientific, Engineering, and Regulatory Compliance Activities*. The results of that evaluation were that this activity is subject to the *Quality Assurance Requirements and Description* (DOE 2000b) requirements.

3. COMPUTER SOFTWARE AND MODEL USAGE

No computer software or models were used in the generation of this report; however, computer software that is used to implement the methodology presented in this report is described in detail in Section 6.

4. WASTE PACKAGE DESIGN METHODOLOGY INPUTS

The following sections list the inputs which are necessary to support the waste package design methodology. None of these inputs were used in this report to produce quality-affecting results in the sense of generating numeric values or defining a specific component design; however, these inputs are quality-affecting in the sense that they define the types of inputs expected by the methodology and provide preferred sources of values. If the methodology used is in consonance with this document to produce quality-affecting results in future analyses, then the quality of these inputs (and whether or not they require further verification) will be determined at that time. It is important to note that applications of the methodology are not restricted to these sources, but that the use of other sources should be appropriate to the design analyses.

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

4.1 DATA AND PARAMETERS

4.1.1 Source Term

The inputs to source term calculations are selected to represent a wide range of waste forms. Differences in the physical forms among the commercial spent nuclear fuel, the DOE spent nuclear fuel, and the high-level waste lead to very different input requirements for generating the source terms for the representative waste forms. Some inputs are equivalent for pressurized water reactor (PWR) and boiling water reactor (BWR) commercial spent nuclear fuel, but due to geometric and operational differences between the two, some inputs are uniquely required by each.

It should be noted that it is not necessary to generate source terms for the naval spent nuclear fuel. This is because, for the naval spent nuclear fuel canister, the thermal output and photon and neutron surface currents are provided by the U.S. Department of the Navy (Naples 1999).

4.1.1.1 Inputs for Commercial Spent Nuclear Fuel Source Term Determinations

The material definitions used in the commercial spent nuclear fuel source term determination are listed in Table 1. For each of these materials, the maximum permissible amount of cobalt is incorporated, except for the stainless steels, where a cobalt impurity of 0.08 weight percent (wt%) is used (Ludwig and Renier, p. 45). For SS-348H, a cobalt impurity of 0.2 wt% is used (ASME 1998, SA-240, Table 1). The remaining elements are representative of the material compositions for each material, but are biased towards the maximum amount of tin, nickel, and niobium, since these lead to larger gamma sources. Elemental impurities in the uranium dioxide of the fuel are given in *Standard- and Extended-Burnup PWR and BWR Reactor Models for the ORIGEN2 Computer Code* (Ludwig and Renier, Table 5.4).

Table 1. Material Compositions Used in Source Term Determinations

Material	Source
UNS ^a R60802 (Zircaloy-2)	<i>Waste Package Materials Properties</i> (CRWMS M&O 1999p, pp. 41-43)
UNS R60804 (Zircaloy-4)	<i>Waste Package Materials Properties</i> (CRWMS M&O 1999p, p. 44)
UNS S30400 (SS-304)	<i>Waste Package Materials Properties</i> (CRWMS M&O 1999p, pp. 20-23)
UNS S30403 (SS-304L)	<i>Waste Package Materials Properties</i> (CRWMS M&O 1999p, pp. 17-19)
UNS S30200 (SS-302)	<i>Specification for Heat-Resisting Chromium and Chromium-Nickel Stainless Steel Plate, Sheet, and Strip for Pressure Vessels</i> , SA-240, ASME 1998 Edition w/2000 Addenda, Section II, Part A (ASME 1998, SA-240, Table 1)
SS-348H	<i>Specification for Heat-Resisting Chromium and Chromium-Nickel Stainless Steel Plate, Sheet, and Strip for Pressure Vessels</i> , SA-240, ASME 1998 Edition w/2000 Addenda, Section II, Part A (ASME 1998, SA-240, Table 1)
Inconel-718	<i>Product Handbook</i> , Inco Alloys International (Inco 1988, p. 11)
Inconel-X-750	<i>Product Handbook</i> , Inco Alloys International (Inco 1988, p. 11)
Stainless Steel CF3M	<i>Metals Handbook Ninth Edition, Volume 3, Properties and Selection: Stainless Steels, Tool Materials and Special-Purpose Metals</i> (ASM 1980, p. 95)

^a Unified Numbering System

^b American Society for Testing and Materials

The isotopic composition of commercially available uranium is provided by the empirical relationships in *Sequoyah Unit 2, Cycle 3 - Volume 2 of Scale-4 Analysis of Pressurized Water Reactor Critical Configurations* (Bowman et al. 1995, p. 20).

Neutron flux scaling factors are also required for regions outside the active fuel in order to determine neutron-activated gamma source terms. These scaling factors are provided by *Spent Fuel Assembly Hardware: Characterization and 10 CFR 61 - Classification for Waste Disposal* (Luskic 1989, p. vi, Table S.1).

The presence of corrosion products ("crud") on the fuel is also accounted for in the source term determination. This is obtained from the following sources:

- *Estimate of CRUD Contribution to Shipping Cask Containment Requirements* (Sandoval et al. 1991, p. 15)
- *Standard Review Plan for Dry Cask Storage Systems* (NRC 1997, Table 7.1)
- *Spent Fuel Corrosion Product and Fuel Cleaning Assessment* (Jones 1992, Table 1).

The half-lives of the radionuclides used in the crud source calculations are provided by *Nuclides and Isotopes, Chart of the Nuclides* (Parrington et al. 1996).

4.1.1.2 Inputs for PWR Source Term Determinations

Selection of PWR Lattice—For the PWR commercial spent nuclear fuel, the Babcock & Wilcox (B&W) Mark B 15x15 PWR fuel assembly is selected as the generic PWR lattice. This lattice has a high initial heavy metal loading and large amounts of stainless steel and Inconel

assembly hardware, maximizing fission product generation and activation of structural hardware. While a typical B&W Mark B assembly has an initial heavy metal loading of 464 kg of uranium, this is increased to 475 kg to provide coverage of the actual waste stream (Assumption 5.1.1.4). Source terms for a generic stainless-steel-clad fuel assembly and for a longer South Texas assembly are also generated. For the longer South Texas assembly, a uranium metal mass of 550 kg is used.

The additional uranium mass of a B&W Mark B assembly is accommodated by increasing the fuel length, rather than by increasing the fuel density. This is consistent with the demonstration of previous calculations that a lower fuel density generates higher gamma and neutron sources (CRWMS M&O 1999a, pp. 48-49). A longer active fuel length and a lower density decrease the fuel self-shielding. This results in a higher flux and consequently higher source intensities.

The physical characteristics of the B&W Mark B 15x15 PWR fuel assembly are obtained from the following sources:

- *Summary Report of Commercial Reactor Criticality Data for Crystal River Unit 3* (Punatar 2001)
- *Operational Data—B&W NSS* (Framatome 1999)
- *Appendix 2A. Physical Descriptions of LWR Fuel Assemblies. Volume 3 of Characteristics of Spent Fuel, High-Level Waste, and Other Radioactive Wastes Which May Require Long-Term Isolation* (DOE 1987).

Both the Mark B and the South Texas assemblies are used in the evaluation of the crud activity on the assembly surface. The larger fuel rod surface area in the South Texas assembly is used as the bounding case, since crud activity is directly proportional to the surface area in the assembly exposed to the coolant.

4.1.1.3 Inputs for BWR Source Term Determinations

Selection of BWR Lattice—For BWR commercial spent nuclear fuel, a General Electric 8x8 BWR fuel assembly is used as the generic fuel design for BWR source term determination. This design has a high initial heavy metal loading and an adequate amount of fuel assembly hardware data. The initial heavy metal loading is conservatively increased from 177 kg to 200 kg to provide coverage of the actual waste stream (Assumption 5.1.1.4). In cases where the hardware for the assembly is not conservative, substitutions and approximations are made to increase conservatism. The stainless-steel-clad fuel assembly is also considered, because it presents higher gamma source intensity due to activation.

As was the case for PWR fuel, the additional fuel mass is added as increased length, rather than as increased density.

The crud activity is directly proportional to the surface area in the assembly components exposed to coolant. Therefore, an assembly that has a higher surface area is used to conservatively evaluate the crud activity. The Advanced Nuclear Fuel 9x9 JP-4 fuel assembly is selected for

crud activity evaluation of a BWR assembly because it has a greater area exposed to coolant than that of the General Electric 8x8 BWR fuel assembly.

The physical characteristics of the General Electric 8x8 fuel assembly are obtained from the following sources:

- *Summary Report of Commercial Reactor Criticality Data for Quad Cities Unit 2*, Rev 00 (CRWMS M&O 1998l, pp. 3, 4, 5, 11, 13, 18 and 333)
- *Summary Report of Commercial Reactor Criticality Data for Quad Cities Unit 2*, Rev 01 (CRWMS M&O 1999n)
- *Core Design and Operating Data for Cycles 1 and 2 of Quad Cities 1* (Larsen et al. 1976, pp. A-1, A-8, and C-12)
- *Appendix 2A. Physical Descriptions of LWR Fuel Assemblies. Volume 3 of Characteristics of Spent Fuel, High-Level Waste, and Other Radioactive Wastes Which May Require Long-Term Isolation* (DOE 1987, p. 2A-16).

Additional information required by the calculation is provided by:

- *CRC Depletion Calculations for Quad Cities Unit 2* (CRWMS M&O 1999c, p. 18)
- *Nuclear Systems I: Thermal Hydraulic Fundamentals* (Todreas and Kazimi 1990, p. 654)
- *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation* (ORNL 1997, Table S2.6.4, p. S2.6.12).

4.1.1.4 Inputs for DOE Spent Nuclear Fuel and High Level Waste Source Term Determinations

The DOE spent nuclear fuel and high level waste source term calculations rely on the input of initial radionuclide inventories and, in the case of high level waste, chemical compositions of the glass waste forms. The initial radionuclide inventories for the DOE spent nuclear fuel are taken from *CD – Design Basis Event Data (DBE), Revision 1, National Spent Nuclear Fuel Program* (INEEL 1999).

The chemical compositions and initial radionuclide inventories for the high level waste are taken from *Draft Environmental Impact Statement for a Geologic Repository for the Disposal of Spent Nuclear Fuel and High-Level Radioactive Waste at Yucca Mountain, Nye County, Nevada* (DOE 1999a, pp. A-36 to A-40, A-45, A-52, and A-53).

The following references provide additional input, and were used in compiling the Draft Environmental Impact Statement:

- "Response to Repository Environmental Impact Statement Data Call for High-Level Waste" (Picha 1997, pp. 6, 7, and 12)

- "Clarification of High-Level Waste and Special Performance Assessment Required Data for Repository Environmental Impact Statement" (Picha 1998a, p. 3)
- *Projected Radionuclide Inventories and Radiogenic Properties of the DWPF Product (U)* (Plodinec and Marra 1994, p. 10)
- *Waste Form Qualification Report (WQR), West Valley Demonstration Project (WVNS 1998, Section WQR-1.1, p. 7 and Section WQR-1.2, pp. AP-1 to AP-3)*
- "Revision to Original INEEL Response to Yucca Mountain Site Characterization Office Data Call for High-Level Waste" (Goff 1998, pp. 3 to 7)
- "Follow Up Response to Repository Environmental Impact Statement Data Call for High-Level Waste" (Picha 1998b, p. 9)
- "Response to Clarification Data for the Repository Environmental Impact Statement (EIS) Data Call Memorandum Dated October 3, 1997" (Taylor 1997, pp. 8 to 10)
- *Plutonium Immobilization Project Input for Yucca Mountain Total Systems Performance Assessment* (Shaw 1999, pp. 3 and 19).

4.1.2 Structural

The external inputs to structural calculations, in addition to those based on higher-tier requirements documents, are the mechanical properties of the design materials and the configuration of the surface facility and engineered barrier system. In addition, the geometry of the waste package, emplacement pallet, and drip shield are used in the process; however, these parameters are varied to obtain designs that comply with the governing requirements.

4.1.2.1 Mechanical Material Properties

The mechanical material properties used in structural analyses are listed in Table 2, along with the sources of the values. Discussions on the use of some of the material properties listed in this table are provided in Sections 4.2.3 and 5.2.

4.1.2.2 Configuration of the Surface Facility Design

Interface control documents that define the design interactions between the surface facility and the waste package currently do not exist. Interface controls that will delineate the design responsibilities of the Waste Package Project and the Surface Facilities Project will be developed as necessary.

4.1.2.3 Configuration of the Engineered Barrier System

Interface control documents that define the design interactions between the engineered barrier system (including the transporter) and the waste package, emplacement pallet, and drip shield currently do not exist. Interface controls that will delineate the design responsibilities of the Waste Package Project and the Subsurface Facilities Project will be developed as necessary.

Table 2. Material Properties and Sources for Structural Analyses

Material Property	Source
SA-240 S31600 (SS 316NG) (Inner Shell – and alternate material for Emplacement Pallet Tubes)	
Density (ρ)	<i>Standard Practice for Preparing, Cleaning, and Evaluating Corrosion Test Specimens</i> . ASTM G 1-90 (ASTM G 1-90 1990, Table X1.1)
Yield Strength (S_y)	<i>ASME Boiler and Pressure Vessel Code</i> , 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table Y-1) <i>Metals Handbook</i> , Ninth Edition, Volume 13, <i>Corrosion</i> (ASM International 1987, p. 931) (used to determine chemical composition of 316NG SS)
Ultimate Tensile Strength (S_u)	<i>ASME Boiler and Pressure Vessel Code</i> , 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table U) <i>Metals Handbook</i> , Ninth Edition, Volume 13, <i>Corrosion</i> (ASM International 1987, p. 931) (used to determine chemical composition of 316NG SS)
Percentage Elongation	<i>Specification for Heat-Resisting Chromium and Chromium-Nickel Stainless Steel Plate, Sheet, and Strip for Pressure Vessels</i> . SA-240, ASME 1998 Edition w/2000 Addenda, Section II, Part A (ASME 1998, SA-240, Table 2) Technical Data Blue Sheet, Stainless Steels, Chromium – Nickel – Molybdenum, Types 316, 316L, 317, and 317L. (Allegheny Ludlum 1999, p. 8)
Elastic Modulus (E)	<i>ASME Boiler and Pressure Vessel Code</i> , 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TM-1)
Mean Coefficient of Thermal Expansion	<i>ASME Boiler and Pressure Vessel Code</i> , 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TE-1)
Poisson's Ratio (ϵ)	<i>Metals Handbook</i> , Ninth Edition, Volume 3, <i>Properties and Selection: Stainless Steels, Tool Materials and Special-Purpose Metals</i> (ASM 1980, Figure 15, p. 755)
Tsw2 Rock	
Density (ρ)	<i>Reference Information Base Data Item: Rock Geomechanical Properties</i> (DTN: MO9808RIB00041.000, Table 5)
SA-240 S31603 (SS 316L) (Emplacement Pallet Tubes)	
Density (ρ)	<i>Standard Practice for Preparing, Cleaning, and Evaluating Corrosion Test Specimens</i> . ASTM G 1-90 (ASTM G 1-90 1990, Table X1.1)
Yield Strength (S_y)	<i>ASME Boiler and Pressure Vessel Code</i> , 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table Y-1)
Ultimate Tensile Strength (S_u)	<i>ASME Boiler and Pressure Vessel Code</i> , 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table U)
Percentage Elongation	<i>Specification for Heat-Resisting Chromium and Chromium-Nickel Stainless Steel Plate, Sheet, and Strip for Pressure Vessels</i> . SA-240, ASME 1998 Edition w/2000 Addenda, Section II, Part A (ASME 1998, SA-240, Table 2)
Elastic Modulus (E)	<i>ASME Boiler and Pressure Vessel Code</i> , 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TM-1)
Poisson's Ratio (ϵ)	<i>Metals Handbook</i> , Ninth Edition, Volume 3, <i>Properties and Selection: Stainless Steels, Tool Materials and Special-Purpose Metals</i> (ASM 1980, Figure 15, p. 755) – because Poisson's ratio is not available for 316L SS, the Poisson's ratio for 316 SS will be used for 316L SS since they have similar chemical compositions.

Table 2. (continued)

Material Property	Source
SA-240 S30400 (SS 304) (Fuel Assembly Components)	
Yield Strength (S_y)	ASME Boiler and Pressure Vessel Code, 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table Y-1)
Ultimate Tensile Strength (S_u)	ASME Boiler and Pressure Vessel Code, 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table U)
Elastic Modulus (E)	ASME Boiler and Pressure Vessel Code, 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TM-1)
Poisson's Ratio (ϵ)	Metals Handbook, Ninth Edition, Volume 3, <i>Properties and Selection: Stainless Steels, Tool Materials and Special-Purpose Metals</i> (ASM 1980, Figure 15, p. 755)
SA-516 K02700 (A 516, Grade 70) (Fuel Tubes, Structural Plates)	
Density (ρ)	Specification for Pressure Vessel Plates, Carbon Steel, for Moderate- and Lower-Temperature Service. SA-20/SA-20M, ASME 1998 w/2000 Addenda, Section II, Part A, (ASME 1998, SA-20, Section 14.1)
Yield Strength (S_y)	ASME Boiler and Pressure Vessel Code, 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table Y-1)
Ultimate Tensile Strength (S_u)	ASME Boiler and Pressure Vessel Code, 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table U)
Percentage Elongation	Specification for Pressure Vessel Plates, Carbon Steel, for Moderate- and Lower-Temperature Service. SA-516/SA-516M, ASME 1998 w/2000 Addenda, Section II, Part A, (ASME 1998, SA-516, Table 2)
Elastic Modulus (E)	ASME Boiler and Pressure Vessel Code, 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TM-1)
Mean Coefficient of Thermal Expansion	ASME Boiler and Pressure Vessel Code, 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TE-1)
Poisson's Ratio (ϵ)	Metals Handbook, Ninth Edition, Volume 1, <i>Properties and Selection: Irons and Steels</i> (ASM 1978, p. 393) - because Poisson's ratio is not available for SA-516 carbon steel, the Poisson's ratio for cast carbon steel will be used
SB-209 A96061 T4 (Alloy 6061 T4) (Thermal Shunts)	
Density (ρ)	ASME Boiler and Pressure Vessel Code, 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table NF-2)
Yield Strength (S_y)	Specification for Aluminum and Aluminum-Alloy Sheet and Plate. SB-209. ASME 1998 Edition w/2000 Addenda, Section II, Part B (ASME 1998, SB-209, Table 3)
Ultimate Tensile Strength (S_u)	Specification for Aluminum and Aluminum-Alloy Sheet and Plate. SB-209. ASME 1998 Edition w/2000 Addenda, Section II, Part B (ASME 1998, SB-209, Table 3)
Percentage Elongation	Specification for Aluminum and Aluminum-Alloy Sheet and Plate. SB-209. ASME 1998 Edition w/2000 Addenda, Section II, Part B (ASME 1998, SB-209, Table 3)
Elastic Modulus (E)	ASME Boiler and Pressure Vessel Code, 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TM-2)
Mean Coefficient of Thermal Expansion	ASME Boiler and Pressure Vessel Code, 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TE-2)
Poisson's Ratio (ϵ)	ASME Boiler and Pressure Vessel Code, 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table NF-1)

Table 2. (continued)

Material Property	Source
SB-265 R52400 (Ti Grade 7) (Drip Shield)	
Density (ρ)	ASME Boiler and Pressure Vessel Code, 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table NF-2) ASM Metals Handbook, Volume 2, Properties and Selection: Nonferrous Alloys and Special-Purpose Materials (ASM International 1990, Table 20, p. 620)
Yield Strength (S_y)	ASME Boiler and Pressure Vessel Code, 1995 Edition w/1995 Addenda, Section II, Part D (ASME 1995, Table Y-1)
Ultimate Tensile Strength (S_u)	Specification for Titanium and Titanium Alloy Strip, Sheet, and Plate. SB-265. ASME 1998 Edition w/2000 Addenda, Section II, Part B (ASME 1998, SB-265, Table 3)
Percentage Elongation	Specification for Titanium and Titanium Alloy Strip, Sheet, and Plate. SB-265. ASME 1998 Edition w/2000 Addenda, Section II, Part B (ASME 1998, SB-265, Table 3)
Elastic Modulus (E)	ASME Boiler and Pressure Vessel Code, 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TM-5)
Mean Coefficient of Thermal Expansion	ASME Boiler and Pressure Vessel Code, 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TE-5)
Poisson's Ratio (ϵ)	ASME Boiler and Pressure Vessel Code, 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table NF-1) ASM Metals Handbook, Volume 2 Properties and Selection: Nonferrous Alloys and Special-Purpose Materials, Specific Metals and Alloys (ASM International 1990, Table 21, p. 621)
SB-265 R56405 (Ti Grade 24) (Drip Shield Structural Members)	
Density (ρ)	ASM Metals Handbook, Volume 2, Properties and Selection: Nonferrous Alloys and Special-Purpose Materials (ASM International 1990, Table 20, p. 620).
Yield Strength (S_y)	Specification for Titanium and Titanium Alloy Strip, Sheet, and Plate. SB-265. ASME 1998 Edition w/2000 Addenda, Section II, Part B (ASME 1998, SB-265, Table 3)
Ultimate Tensile Strength (S_u)	Specification for Titanium and Titanium Alloy Strip, Sheet, and Plate. SB-265. ASME 1998 Edition w/2000 Addenda, Section II, Part B (ASME 1998, SB-265, Table 3)
Percentage Elongation	Specification for Titanium and Titanium Alloy Strip, Sheet, and Plate. SB-265. ASME 1998 Edition w/2000 Addenda, Section II, Part B (ASME 1998, SB-265, Table 3)
Elastic Modulus (E)	ASM Metals Handbook, Volume 2 Properties and Selection: Nonferrous Alloys and Special-Purpose Materials, Specific Metals and Alloys (ASM International 1990, Table 21, p. 621).
Mean Coefficient of Thermal Expansion	ASM Metals Handbook, Volume 2, Properties and Selection: Nonferrous Alloys and Special-Purpose Materials (ASM International 1990, Table 20, p. 620).
Poisson's Ratio (ϵ)	ASM Metals Handbook, Volume 2 Properties and Selection: Nonferrous Alloys and Special-Purpose Materials, Specific Metals and Alloys (ASM International 1990, Table 21, p. 621).

Table 2. (continued)

Material Property	Source
SB-575 N06022 (Alloy 22) (Outer Shell, Emplacement Pallet Plates)	
Density (ρ)	<i>Specification for Low-Carbon Nickel-Molybdenum-Chromium, Low-Carbon Nickel-Chromium-Molybdenum, Low-Carbon Nickel-Chromium-Molybdenum-Copper, and Low-Carbon Nickel-Chromium-Molybdenum-Tungsten Alloy Plate, Sheet, and Strip.</i> SB-575. ASME 1998 Edition w/2000 Addenda, Section II, Part B (ASME 1998, SB-575, Section 7.1)
Yield Strength (S_y)	<i>ASME Boiler and Pressure Vessel Code</i> , 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table Y-1)
Ultimate Tensile Strength (S_u)	<i>ASME Boiler and Pressure Vessel Code</i> , 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table U)
Percentage Elongation	<i>Specification for Low-Carbon Nickel-Molybdenum-Chromium, Low-Carbon Nickel-Chromium-Molybdenum, Low-Carbon Nickel-Chromium-Molybdenum-Copper, and Low-Carbon Nickel-Chromium-Molybdenum-Tungsten Alloy Plate, Sheet, and Strip.</i> SB-575. ASME 1998 Edition w/2000 Addenda, Section II, Part B (ASME 1998, SB-575, Table 3) <i>Hastelloy C-22 Alloy</i> (Haynes International 1997, p. 15)
Elastic Modulus (E)	<i>Hastelloy C-22 Alloy</i> (Haynes International 1997, p. 14)
Mean Coefficient of Thermal Expansion	<i>Hastelloy C-22 Alloy</i> (Haynes International 1997, p. 13)
Poisson's Ratio (ϵ)	<i>Metals Handbook</i> Ninth Edition, Volume 3, <i>Properties and Selection: Stainless Steels, Tool Materials and Special-Purpose Metals, Specific Metals and Alloys</i> (ASM 1980, p. 143) - because Poisson's ratio of Alloy 22 is not available, the Poisson's ratio of Alloy 625 is used for Alloy 22 since they have similar chemical compositions
Thermal Conductivity (k)	<i>Hastelloy C-22 Alloy</i> (Haynes International 1997, p. 13)
Specific Heat (c_p)	<i>Hastelloy C-22 Alloy</i> (Haynes International 1997, p. 13)
Neutronit A 978 (Neutron Absorber Plates)	
Density (ρ)	<i>Sheet and Plate for Nuclear Engineering, BÖHLER Neutronit A976</i> (Kügler 1997, p. 17) - because the density of Neutronit A 978 is not available, the density of Neutronit A 976 is used for Neutronit A 978 since they have similar chemical compositions.
Yield Strength (S_y)	<i>Sheet and Plate for Nuclear Engineering, BÖHLER Neutronit A976</i> (Kügler 1997, p. 15) - because the yield strength of Neutronit A 978 is not available, the yield strength of Neutronit A 976 is used for Neutronit A 978 since they have similar chemical compositions.
Ultimate Tensile Strength (S_u)	<i>Sheet and Plate for Nuclear Engineering, BÖHLER Neutronit A976</i> (Kügler 1997, p. 15) - because the ultimate tensile strength of Neutronit A 978 is not available, the ultimate tensile strength of Neutronit A 976 is used for Neutronit A 978 since they have similar chemical compositions.
Percentage Elongation	<i>Sheet and Plate for Nuclear Engineering, BÖHLER Neutronit A976</i> (Kügler 1997, p. 15) - because the percentage elongation of Neutronit A 978 is not available, the percentage elongation of Neutronit A 976 is used for Neutronit A 978 since they have similar chemical compositions.
Elastic Modulus (E)	<i>Sheet and Plate for Nuclear Engineering, BÖHLER Neutronit A976</i> (Kügler 1997, p. 17) - because the elastic modulus of Neutronit A 978 is not available, the elastic modulus of Neutronit A 976 is used for Neutronit A 978 since they have similar chemical compositions.
Mean Coefficient of Thermal Expansion	<i>ASME Boiler and Pressure Vessel Code</i> , 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TE-1) - because the thermal expansion coefficient of Neutronit A 978 is not available, the thermal expansion coefficient of 316 SS is used for Neutronit A 978 since they have similar chemical compositions
Poisson's Ratio (ϵ)	<i>Metals Handbook</i> , Ninth Edition, Volume 3, <i>Properties and Selection: Stainless Steels, Tool Materials and Special-Purpose Metals</i> (ASM 1980, Figure 15, p. 755) - because Poisson's ratio of Neutronit A 978 is not available, the Poisson's ratio of 316 SS is used for Neutronit A 978 since they have similar chemical compositions

4.1.3 Thermal

The external inputs to thermal calculations, in addition to those based on higher-tier requirements documents, are the thermal properties for the design materials and the configurations of the surface facility, natural system, and engineered barrier system. As is the case for structural analyses, the geometrical descriptions of the waste package, emplacement pallet, and drip shield are also input to the thermal analyses. Again, these are varied parametrically to ensure that the design requirements are satisfied.

4.1.3.1 Thermal Material Properties

The material properties of the major materials used in thermal analyses are listed in Table 3, along with the sources of the values.

Table 3. Material Properties and Sources for Thermal Analyses

Material Property	Source
SA-240 S31600 (SS 316NG) (Inner Shell)	
Density (ρ)	<i>Standard Practice for Preparing, Cleaning, and Evaluating Corrosion Test Specimens.</i> ASTM G 1-90 (ASTM G 1-90 1990, Table X1.1)
Emissivity (ϵ)	<i>Marks' Standard Handbook for Mechanical Engineers</i> , 9 th Edition (Avallone and Baumeister 1987, p. 4-68)
Thermal Conductivity (k)	<i>ASME Boiler and Pressure Vessel Code.</i> 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TCD)
Specific Heat (c_p)	<i>ASME Boiler and Pressure Vessel Code.</i> 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TCD)—computed from the thermal diffusivity
SB-575 N06022 (Alloy 22) (Outer Shell)	
Density (ρ)	<i>Specification for Low-Carbon Nickel-Molybdenum-Chromium, Low-Carbon Nickel-Chromium-Molybdenum, Low-Carbon Nickel-Chromium-Molybdenum-Copper, and Low-Carbon Nickel-Chromium-Molybdenum-Tungsten Alloy Plate, Sheet, and Strip.</i> SB-575. ASME 1998 w/2000 Addenda, Section II, Part B (ASME 1998, SB-575, Section 7.1)
Emissivity (ϵ)	<i>CRC Handbook of Chemistry and Physics</i> , 76 th Edition, 1995-1996 (Lide 1995, p. 10-297) for nickel-chromium alloy
Thermal Conductivity (k)	<i>Hastelloy C-22 Alloy</i> (Haynes International 1997, p. 13)
Specific Heat (c_p)	<i>Hastelloy C-22 Alloy</i> (Haynes International 1997, p. 13)
SB-265 R52400 (Ti Grade 7) (Drip Shield)	
Density (ρ)	<i>ASME Boiler and Pressure Vessel Code.</i> 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table NF-2)
Emissivity (ϵ)	<i>CRC Handbook of Chemistry and Physics</i> , 76 th Edition, 1995-1996 (Lide 1995, p. 10-298)
Thermal Conductivity (k)	<i>ASME Boiler and Pressure Vessel Code.</i> 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TCD)
Specific Heat (c_p)	<i>ASME Boiler and Pressure Vessel Code.</i> 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TCD)—computed from the thermal diffusivity

Table 3. (continued)

Material Property	Source
SB-209 A96061 T4 (Alloy 6061 T4) and SB-209 A96061 T451 (Alloy 6061 T451) (Thermal Shunts)	
Density (ρ)	<i>ASME Boiler and Pressure Vessel Code</i> . 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table NF-2)
Emissivity (ϵ)	<i>Marks' Standard Handbook for Mechanical Engineers</i> , 9 th Edition (Avallone and Baumeister 1987, p. 4-68)
Thermal Conductivity (k)	<i>ASME Boiler and Pressure Vessel Code</i> . 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TCD)
Specific Heat (c_p)	<i>ASME Boiler and Pressure Vessel Code</i> . 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TCD)—computed from the thermal diffusivity
Neutronit A 978 (Neutron Absorber Plates)	
Density (ρ)	<i>Sheet and Plate for Nuclear Engineering</i> , BÖHLER Neutronit A976 (Kügler 1997, p. 17)
Emissivity (ϵ)	<i>Marks' Standard Handbook for Mechanical Engineers</i> , 9 th Edition (Avallone and Baumeister 1987, p. 4-68) (the value for stainless steel 316 is used.)
Thermal Conductivity (k)	<i>Sheet and Plate for Nuclear Engineering</i> , BÖHLER Neutronit A976 (Kügler 1997, p. 17)
Specific Heat (c_p)	<i>Sheet and Plate for Nuclear Engineering</i> , BÖHLER Neutronit A976 (Kügler 1997, p. 17)
SA-516 K02700 (A 516, Grade 70) (Fuel Assembly Tubes, Basket Guides)	
Density (ρ)	<i>Specification for General Requirements for Steel Plates for Pressure Vessels</i> . SA-20/SA-20M. ASME 1998 Edition w/2000 Addenda, Section II, Part A (ASME 1998, SA-20, Section 14.1)
Emissivity (ϵ)	<i>Marks' Standard Handbook for Mechanical Engineers</i> , 9 th Edition (Avallone and Baumeister 1987, Table 4.3.2)
Thermal Conductivity (k)	<i>ASME Boiler and Pressure Vessel Code</i> . 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TCD)
Specific Heat (c_p)	<i>ASME Boiler and Pressure Vessel Code</i> . 1998 Edition w/2000 Addenda, Section II, Part D (ASME 1998, Table TCD)
Uranium Dioxide (Fuel)	
Density (ρ)	<i>Nuclear Systems I: Thermal Hydraulic Fundamentals</i> (Todreas and Kazimi 1990, p. 296)
Emissivity (ϵ)	<i>MATPRO – Version 11</i> (Hagman et al. 1981, Equation A-3.2, p. 48)
Thermal Conductivity (k)	<i>Nuclear Systems I: Thermal Hydraulic Fundamentals</i> (Todreas and Kazimi 1990, pp. 302-303, calculated for 95% theoretical density)
Specific Heat (c_p)	<i>Nuclear Systems I: Thermal Hydraulic Fundamentals</i> (Todreas and Kazimi 1990, p. 296)
Zircaloy-2 (Fuel Rod Cladding)	
Density (ρ)	<i>ASM Metals Handbook</i> , Volume 2 <i>Properties and Selection: Nonferrous Alloys and Special-Purpose Materials</i> , Specific Metals and Alloys (ASM International 1990, p. 666)
Emissivity (ϵ)	<i>MATPRO – Version 11</i> (Hagman et al. 1981, Equation B-3.1b, p. 230, calculated as a function of zirconium oxide layer thickness)
Thermal Conductivity (k)	<i>MATPRO – Version 11</i> (Hagman et al. 1981, Equation B-2.1, p. 217)
Specific Heat (c_p)	<i>Nuclear Systems I: Thermal Hydraulic Fundamentals</i> (Todreas and Kazimi 1990, p. 296)
Helium (Fuel Rod and Waste Package Fill Gas)	
Density (ρ)	<i>Handbook Fundamentals. Inch-Pound Edition</i> (ASHRAE 1997, p. 19.71)
Thermal Conductivity (k)	<i>Handbook Fundamentals. Inch-Pound Edition</i> (ASHRAE 1997, p. 19.71)
Specific Heat (c_p)	<i>Handbook Fundamentals. Inch-Pound Edition</i> (ASHRAE 1997, p. 19.71)

Table 3. (continued)

Material Property	Source
Quartz Sand (Invert Ballast)	
Density (ρ)	<i>Introduction to Heat Transfer</i> . 3 rd Edition (Incropera and DeWitt 1996, p. 756)
Emissivity (ϵ)	<i>Introduction to Heat Transfer</i> . 3 rd Edition (Incropera and DeWitt 1996, p. 768)
Thermal Conductivity (k)	<i>Introduction to Heat Transfer</i> . 3 rd Edition (Incropera and DeWitt 1996, p. 756)
Specific Heat (c_p)	<i>Introduction to Heat Transfer</i> . 3 rd Edition (Incropera and DeWitt 1996, p. 756)

4.1.3.2 Configuration of the Natural System and Thermal Transport Properties Thereof

The stratigraphy of the major geologic units near the center of the potential repository, and the corresponding thermal transport properties of the rock comprising those strata, are provided by the Science and Analysis Project. The rock layer thicknesses are measured at the location of N233,760 m and E170,750 m; the ground surface elevation is 4,663 feet (1421.3 m). Examples of such values are presented in Table 4 (CRWMS M&O 2000v). While these values are illustrative of the type of data required for the thermal analyses, they should not be construed as the definitive values for these parameters. Future evaluations by the Science and Analysis Project may result in changes to these values.

4.1.3.3 Configuration of the Surface Facility Design

Interface control documents that define the design interactions between the surface facility and the waste package currently do not exist. Interface controls that will delineate the design responsibilities of the Waste Package Project and the Surface Facilities Project will be developed as necessary.

4.1.3.4 Configuration of the Engineered Barrier System

Interface control documents that define the design interactions between the engineered barrier system (including the transporter) and the waste package, emplacement pallet, and drip shield currently do not exist. Interface controls that will delineate the design responsibilities of the Waste Package Project and the Subsurface Facilities Project will be developed as necessary.

4.1.4 Shielding

Shielding calculations determine radiation dose rates on waste package surfaces and in the vicinity of these surfaces. Radiation dose rate is a function of the radiation type, radiation energy spectrum and intensity, radiation interaction information, material compositions and densities, system geometry, and flux-to-dose rate conversion factors. In addition, calculation of radiation dose rates is dependent on the assumed location of the detector.

Table 4. Illustrative Stratigraphic Thermal Transport Information

T/M ^a Unit	USGS ^b Unit		Integrated Site Model 3.0	Thickness (m)	Grain Density (kg/m ³)	Thermal Conductivity		Specific Heat		
						T≤ 100 °C (W/m·K)	T> 100 °C (W/m·K)	T≤ 95 °C (J/kg·K)	95 °C<T ≤114 °C (J/kg·K)	T> 114 °C (J/kg·K)
TCw	Tpcrv		N.D. ^c	N.D.	2550	2.00	1.60	823	3879	823
	Tpcrn		N.D.	N.D.	2550	2.00	1.60	823	3879	823
	Tpcrl		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
	Tpcpul		N.D.	N.D.	2520	1.67	1.23	882	4352	882
	Tpcpmn		N.D.	N.D.	2510	1.94	1.53	837	4010	837
	Tpcpll		N.D.	N.D.	2510	1.76	1.02	847	4019	847
	Tpcpln		N.D.	N.D.	2510	1.88	1.28	837	4010	837
	Tpcplnc		N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.	N.D.
	Tpcpv		3	Tcpv3	0.0	2470	0.98	0.54	857	4570
Tpcpv		2	Tcpv2	5.49						
PTn	Tpcpv1		Tcpv1	4.69	2380	1.07	0.50	1037	6048	1037
	Tpbt4		Tcbt4	0.53	2340	0.50	0.35	1077	21976	1077
	Tpy		Yucca	7.05	2400	0.97	0.44	849	16172	849
	Tpbt3		Tpbt3_dc	4.58	2370	1.02	0.46	1016	20669	1016
	Tpp		Pah	14.09	2260	0.82	0.35	1330	25560	1330
	Tpbt2		Tpbt2	9.69	2370	0.67	0.23	1224	23878	1224
	Tptrv3		Tptrv3	4.58	2510	1.00	0.37	834	5137	834
	Tptrv2		Tptrv2	0.53						
	Tptrv1		Tptrv1	1.06						
TSw1	Tptrn		Tptrn	46.85	2550	1.62	1.06	866	5629	866
	Tptrl		Tptrl	8.98	2510	1.58	0.89	882	5693	882
	Tptpul		Tptpul	77.68	2510	1.80	0.71	883	5694	883
	Tptpmn		Tptpmn	29.94	2530	2.33	1.56	948	4568	948
TSw2	Tptpll		Tptpll	106.21	2540	2.02	1.20	900	4663	900
	Tptpln		Tptpln	47.73	2560	1.84	1.42	865	4523	865
	Tptpv3		Tptpv3	20.61	2360	2.08	1.69	984	1958	984
Tptpv2		Tptpv2	2.99							
Tptpv1		Tptpv1	11.27							
Tpbt1		Tpbt1	3.35							
CHn1	Tac 5	Tac(v)	Calico	84.37	2240	1.17	0.58	1201	23863	1201
	Tac 4									
	Tac 3									
	Tac 2	Tac(z)			2350	1.2	0.61	1154	22086	1154
	Tac 1									
CHn2	Tacbt				2440	1.35	0.73	1174	13561	1174

^a T/M: Thermal-Mechanical^b USGS: U.S. Geological Survey^c N.D.: No data

4.1.4.1 Radiation Source Terms

The radiation source terms of the waste forms are an important input to shielding calculations. The radiation source terms consist of neutron and photon intensities as functions of their energies. The radiation source terms for commercial spent nuclear fuel have been generated for both PWR and BWR fuel designs. These are documented in the following:

- *PWR Source Term Generation and Evaluation* (CRWMS M&O 1999g)
- *BWR Source Term Generation and Evaluation* (CRWMS M&O 1999a).

For the high level waste glass, conservative photon and neutron source terms are generated using the design basis glass developed at the Savannah River Site Defense Waste Processing Facility, and are provided in *Source Terms for DHLW Canisters for Waste Package Design* (CRWMS M&O 1999m, Attachment VIII, p. VIII-1, and Attachment IX, p. IX-1). These source terms are used in shielding evaluations for all other high level waste glass canisters, which contain less intense radiation sources than the Savannah River Site canister.

To facilitate criticality analysis, DOE spent nuclear fuels (excluding the naval fuels) have been categorized into nine fuel groups. Out of each group, a representative fuel type is chosen as a bounding case for the group. Generally, burnup, fissile enrichments, and total fuel mass determine the selection of the representative fuel used for the criticality analysis. For shielding calculations, the bounding photon and neutron source terms for these criticality analyses are also used. Currently, DOE has completed six of the nine criticality analyses and thus has identified six bounding shielding source terms for the six fuel groups. The bounding source terms for each fuel group are provided in the following documents.

- *Shippingport LWBR (Th/U Oxide) Fuel Characteristics for Disposal Criticality Analysis* (DOE 1999c)
- *FFTF (MOX) Fuel Characteristics for Disposal Criticality Analysis* (DOE 1998)
- *Fermi (U-Mo) Fuel Characteristics for Disposal Criticality Analysis* (DOE 1999b)
- *Shippingport PWR (HEU Oxide) Fuel Characteristics for Disposal Criticality Analysis* (DOE 1999d)
- *TRIGA (UZrH) Fuel Characteristics for Disposal Criticality Analysis* (DOE 1999e)
- *N Reactor (U-metal) Fuel Characteristics for Disposal Criticality Analysis* (DOE 2000a).

Shielding evaluations for waste packages containing the naval spent nuclear fuel use the photon and neutron currents exiting the surfaces of a naval canister. The currents are provided by the U.S. Department of the Navy (Naples 1999, Enclosure 2).

4.1.4.2 Radiation Interaction Information

Radiation interaction information is available in the computer code packages used in shielding calculations (see Sections 6.4.1.3 and 6.4.1.4). This information is derived from evaluated

nuclear data libraries by processing it into formats suitable for the individual codes. An evaluated nuclear data library is produced by combining experimentally-measured cross sections with results predicted by theoretical nuclear calculations, in an attempt to extract the most accurate cross-section information. The radiation transport codes as well as the associated cross-section data have been subject to software qualification (CRWMS M&O 1998h and CRWMS M&O 2000n). However, the user has the responsibility of selecting the appropriate cross-section data set for the problem being solved.

4.1.4.3 Material Chemical Compositions and Densities

Radiation interaction information contains microscopic cross sections of individual nuclides. A microscopic cross section may be interpreted as the effective cross-sectional area presented by the target atom or electron to the incident particle for a given interaction. Although microscopic cross sections deal with probabilities of the interaction of radiation with individual targets (nuclei or electrons), macroscopic cross sections are related to probabilities for interaction with the aggregate of targets that compose the medium through which the radiation is passing. Macroscopic cross sections have units of reciprocal length (cm^{-1}), and they act as linear attenuation coefficients in the photon transport. Shielding analyses require macroscopic cross sections in order to determine interactions of radiation with the materials of the system. The codes calculate the macroscopic cross sections based on material compositions and densities, and, in the case of a Monte Carlo radiation transport code, they select the target element. The chemical compositions and densities of the materials in a waste package shielding calculation are available in the American Society for Testing and Materials (ASTM) standards database.

4.1.4.4 Flux-to-Dose Rate Conversion Factors

Flux-to-dose rate conversion factors are contained in the computer code packages used in shielding calculations (see Sections 6.4.1.3 and 6.4.1.4). The codes and the conversion factors have been subject to software qualification for shielding applications (CRWMS M&O 1998h and CRWMS M&O 2000n).

4.1.5 Criticality

The inputs for the criticality calculation differ between the commercial spent nuclear fuel waste forms and DOE spent nuclear fuel waste forms.

4.1.5.1 Criticality Inputs for Commercial Spent Nuclear Fuel Analysis

For the commercial spent nuclear fuel waste forms, the inputs for criticality calculations are the compositions and geometries of the spent fuel assemblies.

Assembly Geometries and Compositions—For a loading curve evaluation, detailed information is necessary regarding the geometries of fuel assembly components and the material composition of those components. As of this writing, the following sources are used for such pre-irradiated data:

- Babcock & Wilcox 15x15 Mark B2 PWR Fuel Assembly: *Summary Report of Commercial Reactor Criticality Data for Crystal River Unit 3* (Punatar 2001)

- General Electric 7x7 BWR Fuel Assembly: *Core Design and Operating Data for Cycles 1 and 2 of Quad Cities 1* (Larsen et al. 1976).

Source for Axial Burnup Profiles—During reactor operation, the composition of nuclear fuel undergoes changes in its inventory of fission product and actinide isotopes. The reactivity of spent PWR or BWR fuel in a waste package is, in part, a function of the isotopic inventory of the spent fuel. The reactor operating history describes depletion parameters such as local power, fuel temperature, moderator density, burnable absorber rods, and other parameters. The integrated effect of these depletion parameters is usually described as burnup. Burnup is used as the principal measure of the isotopic inventory, and its axial distribution along the fuel can affect its reactivity. To ensure that the axial burnup profiles selected for evaluation appropriately reflect those resulting from reactor operations, a database of actual PWR and BWR fuel depletion histories will be compiled.

4.1.5.2 Criticality Inputs for DOE Spent Nuclear Fuel Analysis

As indicated in Section 4.1.4.1, the DOE spent nuclear fuels (with the exception of naval spent nuclear fuel, which is discussed below) have been categorized into nine fuel groups to facilitate criticality analysis. Generally, burnup, fissile enrichments, and total fuel mass determine the selection of the representative fuel used for the criticality analysis. Each of the nine DOE spent nuclear fuel groups (representing more than 250 fuel types) has been or will be analyzed to determine the appropriateness of the proposed waste package loading configuration. The nine DOE spent nuclear fuel groups are as follows:

1. Uranium Metal Fuels (N-Reactor fuel)
2. Uranium-Zirconium/Uranium-Molybdenum Fuels (Fermi Liquid Metal Reactor fuel)
3. Uranium Oxide Fuels (high enriched uranium fuels – Shippingport PWR fuel)
4. Uranium Oxide Fuels (low enriched uranium fuels – Three Mile Island-2 PWR fuel)
5. Uranium-Aluminum Fuels (foreign research reactor fuel)
6. Uranium/Thorium/Plutonium Carbide Fuels (Ft. St. Vrain Gas Cooled Reactor fuel)
7. Mixed Oxide Fuels (Fast Flux Test Facility Reactor fuel)
8. Uranium/Thorium Oxide Fuels (Shippingport Light Water Breeder Reactor fuel)
9. Uranium-Zirconium-Hydride Fuels (TRIGA fuel)

The parameters important to limiting the performance risk from criticality (e.g., fissile loading, initial enrichment, initial configuration of the basket, initial configuration of the spent nuclear fuel, neutron absorber loading in the canister, etc.) are identified through the evaluation of these analyses. Based on these evaluations, criteria are developed to establish the acceptance of fissile species, fissile mass, initial enrichment, and linear loading for each of the DOE nine spent nuclear fuel groups.

DOE spent nuclear fuel will be placed in standardized canisters and packaged in a manner that will limit the performance risk from criticality. This differs from commercial spent nuclear fuel, in which the waste package basket structure design is used to limit the performance risk from criticality.

The inputs for criticality calculations for naval spent nuclear fuel are described in an Addendum (Mowbray 1999) to the *Disposal Criticality Analysis Methodology Topical Report* (YMP 2000). The Naval Nuclear Propulsion Program (NNPP) is responsible for the performance of preclosure and post-closure criticality calculations for intact naval spent nuclear fuel.

4.1.6 Risk-Informed Processes

In order to identify the type of design analysis that must be performed to evaluate the effects of a given design basis event, the waste package function that may be affected by the event must be identified. The *Monitored Geologic Repository Project Description Document* (Curry 2001, Section 2.6.1) provides a description of the waste package and its functions. The functions listed in this document are hierarchical in nature, and consist of high-level functions.

Details on the systems, structures, and components involved in the design basis events during the fabrication, loading, closure, transport, and emplacement of the waste package are obtained from the specific documents related to those systems, structures, and components, such as the System Description Documents.

4.1.6.1 Waste Package-Related External Events

The *MGR External Events Hazards Analysis* (CRWMS M&O 2000h) identifies a generic list of external events, and eliminates from further consideration those events that are not applicable to the Yucca Mountain site, or which are the result of long-term processes not applicable to the preclosure phase of repository operations.

4.1.6.2 Waste Package-Related Internal Events

The *Monitored Geologic Repository Internal Hazards Analysis* (CRWMS M&O 2000i) identifies a list of waste package-related internal events resulting from failures of handling equipment and/or operator error.

4.1.6.3 Human Error Probabilities

Human error probabilities for performing various tasks may be approximated from anticipated operator actions in the *Handbook of Human Reliability Analysis with Emphasis on Nuclear Power Plant Applications Final Report* (NUREG/CR-1278) (Swain and Guttman 1983). The use of NUREG/CR-1278 is applicable to the Monitored Geologic Repository (MGR) since this will be a NRC regulated facility that will have equipment reliability and procedural requirements similar to those implemented at nuclear power plants.

4.1.6.4 Equipment Failure Rates

Equipment failure rates are obtained from *IEEE Guide to the Collection and Presentation of Electrical, Electronic, Sensing Component, and Mechanical Equipment Reliability Data for Nuclear-Power Generating Stations* (IEEE Std 500-1984).

4.1.6.5 Waste Form Loading Events

The probability of misloading an uncanistered spent nuclear fuel assembly into a disposal container in the Waste Handling Building's Transfer Cell is based on commercial nuclear utility operations information compiled in *Commercial Nuclear Fuel Assembly Damage/Misload Study – 1985-1999* (Framatome ANP 2001). This misload probability is expected to be utilized in the estimation of the frequency for a waste package thermal or criticality misload design basis event.

4.1.6.6 Waste Package Closure and Inspection Events

Weld Flaw Frequency, Size Distribution, Depth, and Orientation – Information on the frequency of occurrence of weld flaws and their size distribution and depth may be obtained from "Flaw Size Distribution and Flaw Existence Frequencies in Nuclear Piping," in *Probabilistic and Environmental Aspects of Fracture and Fatigue: The 1999 ASME Pressure Vessels and Piping Conference*. PVP-386 (Khaleel et al. 1999).

Information on the orientation of weld flaws may be obtained from *RR-PRODIGAL - A Model for Estimating the Probabilities of Defects in Reactor Pressure Vessel Welds* (Chapman and Simonen 1998).

Information on flaw aspect ratios, and the causes and frequency of base metal flaws relative to weld flaws, may be obtained from "Fabrication Flaws in Reactor Pressure Vessels," in *Transactions of the Twenty-Sixth Water Reactor Safety Information Meeting* (Doctor et al. 1998).

Reliability of Ultrasonic Examination – Information on the reliability of ultrasound examination for detection of size flaws may be obtained from the following:

- *Reliability of Nondestructive Examination* (NUREG/CR-3110) (Bush 1983)
- *Piping Inspection Round Robin* (Heasler and Doctor 1996).

4.1.6.7 Waste Package Transport and Emplacement Events

Information on the transporter and on transporter design basis events may be obtained from the following:

- *DBE/Scenario Analysis for Preclosure Repository Subsurface Facilities* (CRWMS M&O 1997c)
- *Subsurface Transporter Safety Systems Analysis* (CRWMS M&O 2000t)
- *Waste Package Transport and Transfer Alternatives* (CRWMS M&O 2000z).

Information on the emplacement gantry may be obtained from *Bottom/Side Lift Gantry Conceptual Design* (CRWMS M&O 2000b).

4.1.6.8 Ground Support Failure and Rock Fall Events

A description of the ground control units used in the emplacement drifts is obtained from BSC 2001c. A constant annual failure rate for the steel sets and rock bolts that are used for ground support is based on an estimate by CRWMS M&O 1999o.

The key block size distribution and number of key blocks per unit drift length are provided in CRWMS M&O 2000d (pp. 40-49).

4.2 CRITERIA

Criteria are derived from two sources: those imposed by the NRC for disposal of waste in a potential geologic repository, and additional requirements necessitated by the design of the repository and waste package.

4.2.1 Nuclear Regulatory Commission Requirements

The requirements for a potential geologic repository at Yucca Mountain are still in a draft form. Regulatory guidance pending the issuance of the new requirements is taken from "Revised Interim Guidance Pending Issuance of New U.S. Nuclear Regulatory Commission (NRC) Regulations (Revision 01, July 22, 1999), for Yucca Mountain, Nevada" (Dyer 1999). In particular, this document provides guidance for the performance of risk-informed analyses for the design basis events of the waste package.

The applicable requirements are to ensure that radioactive exposure to onsite and offsite personnel is maintained below stated limits during Category 1 and Category 2 design basis events. In addition, a requirement is made that analyses are to be performed on systems, structures, and components to ensure that they are able to perform their stated safety functions.

A Category 1 design basis event is defined in Dyer 1999 as "those natural events and human-induced event sequences that are expected to occur one or more times before permanent closure of the geologic repository operations area." Dyer 1999 defines a Category 2 design basis event as "(a) other human-induced event sequences that have at least one chance in 10,000 of occurring before permanent closure of the geologic repository, and (b) appropriate consideration of natural events (phenomena) that have been historically reported for the site and the geologic setting."

Additionally, the proposed regulatory requirements of Dyer 1999 state that "the features, events and processes considered in the performance assessment should represent a wide range of both beneficial and potentially adverse effects on performance [. . .]. Those features, events, and processes expected to materially affect compliance with Sec. 113(b) or be potentially adverse to performance are included, while events of very low probability of occurrence (less than one chance in 10,000 over 10,000 years) can be excluded from the analysis."

Additional requirements on waste package design may be derived from regulations governing other nuclear installations or devices. These are discussed in depth in Section 4.3.

4.2.2 Monitored Geologic Repository Requirements

The designs of the waste packages, emplacement pallets, and drip shields must satisfy the fundamental requirements for a potential geologic repository. These are embodied in the *Yucca Mountain Site Characterization Project Requirements Document* (YMP 2001). These upper-tier requirements are reflected in greater detail in the *Monitored Geologic Repository Project Description Document* (Curry 2001, Section 5). At the system level, requirements and constraints are taken from the System Description Documents (SDDs). The applicable SDDs for evaluations for Site Recommendation are:

- *Uncanistered Spent Nuclear Fuel Disposal Container System Description Document* (BSC 2001i)
- *Defense High Level Waste Disposal Container System Description Document* (BSC 2001a)
- *Naval Spent Nuclear Fuel Disposal Container System Description Document* (BSC 2001e)
- *Emplacement Drift System Description Document* (BSC 2001b)
- *Subsurface Facility System Description Document* (BSC 2001g).

For the formulation of a particular waste package design, the SDD requirements define, in part, the performance requirements of the design. Thus, a conceptual design for a waste package is created on the basis of previous studies and physical insight, then the design methodology is applied to determine the response of the design to the various challenges implied by the SDD requirements and constraints. If the contemplated design cannot meet one or more of those requirements and constraints, then the design is adjusted and the applicable parts of the design methodology exercised again. When all requirements and constraints are satisfied, an acceptable design is achieved.

4.2.3 Waste Package Design Stress Criteria for Material Failure

In the case of analyses that consider the effects of material nonlinear behavior, the maximum-shear-stress or Tresca criterion is assumed to be applicable in determining the threshold for material failure. In general this criterion assumes that failure occurs when stress intensity (defined as the difference between maximum and minimum principal stress) exceeds a certain limit. In particular, the acceptance criteria for plastic analysis as outlined in Appendix F-1341.2 of ASME 1995 (Section III, Division 1) suggest the following stress intensity limits.

- (a) The general primary membrane stress intensity shall not exceed $0.7 \cdot S_u$ for ferritic steel materials, and the greater of $0.7 \cdot S_u$ and $S_y + (S_u - S_y)/3$ for austenitic steel, high-nickel alloy, and copper-nickel alloy materials. Where S_u and S_y are tensile strength and yield strength (engineering definition), respectively.
- (b) The maximum primary stress intensity at any location shall not exceed $0.9 \cdot S_u$.

In the case of lifting analyses, the acceptance criteria are outlined in ANSI N14.6-1993, *American National Standard for Radioactive Materials – Special Lifting Devices for Shipping Containers Weighing 10000 Pounds (4500 kg) or More*. The load-bearing members of the lifting device shall be capable of lifting three times the combined weight of the shipping container, plus the weight of the intervening components of the lifting device, without generating a combined shear stress or maximum principal stress at any point in the device in excess of S_y , and shall also be capable of lifting five times the weight without exceeding S_u .

Finally, in the case of analyses that consider only material linear (elastic) behavior during the postclosure event simulations, the acceptance criterion is based on stress-corrosion-cracking considerations. It is generally assumed that crack initiation will not occur if the stress is below a certain threshold value. Thus, the first principal stress at any location exposed to an aggressive environment shall not exceed the lower bound of $S_y/10$ as suggested by *Waste Package Degradation Process Model Report* (CRWMS M&O 2000y).

Note that the material properties in engineering handbooks (e.g., *ASME Boiler and Pressure Vessel Code*) refer to engineering stress and strain definitions: $S = P/A_0$ and $e = L/L_0 - 1$. Where P stands for the force applied during a static tensile test, L is the length of the deformed specimen, and L_0 and A_0 are the original length and cross-sectional area of the specimen, respectively. The engineering stress-strain curve does not give a true indication of the deformation characteristics of a material during the plastic deformation, since it is based entirely on the original dimensions of the specimen. In addition, ductile metal that is pulled in tension becomes unstable and necks down during the course of the test. Hence, for nonlinear analyses, finite element codes require input in terms of true stress and strain definitions: $\sigma = P/A$ and $\epsilon = \ln(L/L_0)$. The relationships between the true stress and strain definitions and the engineering stress and strain definitions, $\sigma = S \cdot (1 + e)$ and $\epsilon = \ln(1 + e)$, can be readily derived based on constancy of volume ($A_0 \cdot L_0 = A \cdot L$) and strain homogeneity during plastic deformation. Thus, these expressions are applicable only in the hardening region of the stress-strain curve that is limited by the onset of necking (see Figure 1). Since finite element analyses that consider the effects of material nonlinear behavior require the input data in terms of the true stress and strain definitions, the acceptance criteria has to be accordingly modified. Contrary to the yield strength where the difference between two stress definitions is negligible ($\sigma_y \approx S_y$), the true tensile strength can be significantly larger than the engineering counterpart ($\sigma_u > S_u$). Therefore, whenever material nonlinear behavior is considered, both the input data and stress criteria have to be interpreted in terms of the true stress and strain definitions.

4.3 CODES AND STANDARDS

The rules and regulations of the United States Government, as expressed in 10 Code of Federal Regulations (CFR) Part 60 (10 CFR 60), Part 71 (10 CFR 71), and Part 72 (10 CFR 72), are the highest-level requirements for the waste package design. The handling and transport of radioactive materials is also governed by 49 CFR Parts 171-177 (49 CFR 1998), which are the U.S. Department of Transportation rules for transportation of radioactive materials and provide criteria such as contamination limits. 10 CFR Part 51 (10 CFR 51) is also applicable since it

Figure 1. Key Attributes of Bilinear Stress-Strain Curve

describes spent fuel limitations. In addition, 10 CFR 60 will be displaced by 10 CFR 63 (64 FR 8640), which is in draft form. Pending the issuance of this new regulation, guidance is taken from "Revised Interim Guidance Pending Issuance of New U.S. Nuclear Regulatory Commission (NRC) Regulations (Revision 01, July 22, 1999), for Yucca Mountain, Nevada" (Dyer 1999) (see Section 4.2.1).

In addition to the applicable CFRs, documents are published by the NRC to provide more details of the regulations. These documents include the Standard Review Plans (SRPs) for the review of storage (NRC 1997) or transportation packages (NRC 2000), Regulatory Guides, Nuclear Regulations (NUREGs), and Interim Staff Guidance papers.

Standards relevant to the waste package include those published by the ASME, which provide structural engineering guidance, and radioactive materials standards published by the American Nuclear Society (ANS), generally in cooperation with the American National Standards Institute (ANSI). Material specifications and gas properties are provided by ASME, ASTM, and the American Society of Heating, Refrigerating, and Air-Conditioning Engineers (ASHRAE).

Standards exist for the engineering of the waste package in the areas of:

- Structural
- Thermal
- Shielding
- Criticality
- Fabrication.

In addition, guidance for these areas is also provided for transportation casks by the DOE publication generally termed the "Packaging Handbook" (Shappert 1998). The on-site handling of radioactive materials at the potential repository is governed by 10 CFR 60 (10 CFR 60); however, sufficient detail to cover all aspects of on-site handling is not provided, and 10 CFR 72 (10 CFR 72) and 10 CFR 71 (10 CFR 71), and their supporting standards, may be applied as appropriate. In effect, the radiation protection and safety goals of 10 CFR 72 and 10 CFR 71 may be applied to the repository activities, with the evaluation scenarios adjusted to repository conditions. The basic approach used at some DOE facilities for on-site radioactive materials transfers is to provide protection that is the same as, or equivalent to, that provided during off-site shipments under 10 CFR 71. This principal of "equivalency" may be applied to any condition for which explicit guidance is not provided in 64 FR 8640 (10 CFR 63 or 10 CFR 60, as indirect guidance) or by an NRC Interim Staff Guidance. An example of the use of equivalency to relate on-site scenarios to those defined in 10 CFR 71 is presented in Table 5.

4.3.1 Structural Codes and Standards

The applicable codes for structural engineering design and analysis, materials, and fabrication issues are from the *ASME Boiler and Pressure Vessel Code*, Section III, Division 3 (ASME 1998), which is a relatively recent addition to the ASME Code, and as such may not be complete for all aspects of the waste package. If Section III, Division 3, does not adequately define parameters needed for the waste package, Section III, Division 1, Subsections NB and NG (ASME 1995), may be applied instead. It should be noted that Section III, Division 3, is the preferred portion of the ASME Code for the design of the waste package, but it cannot be applied to accident condition analyses as it does not permit plastic deformation. Material allowable stress limits and material compositions and properties are provided by the ASME code for a wide variety of structural alloys. Such materials are commonly termed "code materials."

Table 5. Comparison of Packaging Design Requirements for On-site Alternative Packaging and Off-site Packaging

Condition		Off-site	On-site
Impact		30-foot fall onto unyielding surface	Four-foot fall onto reinforced concrete
Puncture		40-inch fall onto six-inch diameter steel bar	Six-inch fall onto six-inch diameter steel bar
Fire		800°C for 30 minutes	800 °C for 15 minutes or for five minutes if escort by a fire truck is provided
Radiation Dose Rates	Normal Operation	200 mrem/hour at any point on the external surface of the package	As low as is reasonably achievable (ALARA)
	Hypothetical Accident	One rem/hour at one meter from the external surface of the package	ALARA
Radiological Releases		None	Radiological effects on-site not to overexpose personnel, off-site not to exceed site release limits

The boron/stainless alloy employed by the waste package fuel basket is not a code material, but is the subject of ASME Code Case N-510-1 (ASME 1998) that describes the allowable compositions and material properties. ASME Code Case N-510-1 is for 304 stainless steel with boron, whereas the waste package fuel basket design utilizes 316 stainless steel with boron.

Specific standards, code cases, and regulatory guides used in the design of the waste package include the following:

- ASTM A 887-89, (ASTM A 887-89 [Reapproved 2000] 1990). "Standard Specification for Borated Stainless Steel Plate, Sheet, and Strip for Nuclear Application"
- ASME Code Case N-510-1 (ASME 1998). "Borated Stainless Steel for Class CS Core Support Structures and Class I Component Supports Section III, Division 1"
- ASME Code Case N-284-1 (ASME 1998), which specifies a methodology for evaluating buckling stresses in a cylindrical body
- Regulatory Guides 7.6 (Regulatory Guide 7.6 1978) and 7.8 (Regulatory Guide 7.8 1989), which describe the load combinations and stresses that must be evaluated for a transportation package
- NUREG-0612 (NRC 1980), which describes the requirements for lifting and handling of large packages such as the waste package
- ANSI-N14.6 (ANSI N14.6-1993), which addresses lifting devices for large packages
- NUREG/CR-1815 (Holman and Langland 1981) and Regulatory Guide 7.11 (Regulatory Guide 7.11 1991), which address the fracture toughness requirements of cylindrical shells for packages
- NUREG/CR-0481 (Rack and Knorovsky 1978), which addresses elastic plastic data for structural analyses
- NUREG/CR-6608 (Witte et al. 1998), which addresses the impact of large packages during a drop event
- NUREG/CR-6322 (Lee and Bumpas 1995), which provides a methodology for evaluating the buckling stresses in spent nuclear fuel baskets
- NUREG/CR-4554 (Gerhard et al. 1992), which contains information regarding the structural stresses for large packages during a drop event.

A de facto standard for the ability of spent fuel to withstand the effects of high g-loads in an impact, *Dynamic Impact Effects on Spent Fuel Assemblies* (Chun et al. 1987), was developed by Lawrence Livermore National Laboratory for the NRC.

The following are specific applications of structural standards used in the waste package design:

ASTM A 887-89

The ASTM A 887-89 (ASTM A 887-89 [Reapproved 2000] 1990), "Standard Specification for Borated Stainless Steel Plate, Sheet, and Strip for Nuclear Application," prescribes a range of boron-10 contents that are approved for the specification, as well as two metallurgical processes which may be used to manufacture the borated stainless steel. Plate, sheet, and strip are the approved borated stainless steel forms because the manufacturing process assures an even distribution of boron in the resulting steel. Local increases in boron content are undesirable because boron acts as a hardener of stainless steel and reduces the ductility of the alloy. Extrusions and castings would require different metal production processes, and control of the distribution of the boron in the stainless steel alloy would have to be assured. Boron contents in ranges from 0.20-0.29 (Type 304B) up to 1.75-2.25 percent (Type 304B7) are approved by the specification. To this date, a boron range of 1.50-1.74 (Type 304B6) has been applied to waste package spent nuclear fuel baskets.

The two metallurgical processes used to produce borated stainless steel are a traditional metal melt technology (Grade B) and a more modern powder metallurgy process (Grade A). The powder metallurgy process results in a more even distribution of boron in the alloy, and the ductility is improved compared to the wrought (metal melt) process. Since the borated stainless steel is not a load-carrying structural component in existing waste package spent nuclear fuel basket designs, the Grade B alloy is acceptable.

ASME Code Case N-510-1

ASME Code Case N-510-1 (ASME 1998) specifies the code material properties for evaluating 304 stainless steels with boron to allow structural credit to be taken for this material under construction of Section III, Subsections NF and NG components. This code case describes the mathematical combination of principal stresses in these stainless steels to determine the effective stress that could cause failure of the structure, and it also provides the limits and limitations on the use of these materials.

ASME Code Case N-284-1

ASME Code Case N-284-1 (ASME 1998) specifies a methodology for evaluating buckling stresses in a cylindrical body. This code case describes the mathematical combination of principal stresses in a cylindrical shell to determine the effective stress that could cause buckling collapse of the cylinder. Code Case N-284 provides Factors of Safety that are used in the calculation, but it should be noted that these factors only apply when the ASME Code Case N-284 methodology is used. It is inappropriate to use these Factors of Safety if buckling is evaluated using classical crippling and buckling analysis techniques. This is because the Code Case N-284 calculation methodology contains an imbedded measure of conservatism that is not necessarily present in classical methods.

Regulatory Guides 7.6 and 7.8

Regulatory Guides 7.6 and 7.8 describe the load combinations and stresses that must be evaluated for a transportation package. The waste package is not intended as a transportation package; however, the selection and presentation of the various stresses specified in these regulatory guides can be applied to the waste package. The regulatory guides are very prescriptive, and a detailed plan for the stresses and stress combinations is provided. It should be noted that for transport cask baskets, the thermal stress is not considered a secondary stress because the geometry of the spent nuclear fuel basket is not cylindrical, and uneven thermal stresses can thus cause distortion of the basket.

NUREG-0612

NUREG-0612 (NRC 1980) describes the requirements for lifting and handling of large packages such as the waste package. The standard explicitly applies to heavy loads lifted near or over spent fuel pools at nuclear reactor facilities, but is also applied to storage and transport cask lifting devices. Thus, the standard can be applied to the waste package. NUREG-0612 specifies that all components which participate in the load path must be designed to a safety factor of six against yield and a factor of ten against ultimate. The standard implicitly includes a dynamic factor to account for "bounce" when lifting and lowering large objects. The standard permits load-splitting between redundant load paths, so that if a redundant lifting yoke is used, a factor of three against yield is used for each separate yoke and a factor of five against ultimate is applied. These factors ensure that structural failure of lifting components will not occur in normal conditions, but it is the responsibility of the facility personnel to ensure that the lifting attachments are securely engaged to the large package. A positive means of verification of lifting fixture engagement is necessary and, in general, it is necessary to provide a flat surface to set the package on. Guide plates to center a waste package in a specific location in a pool or dry location are not recommended, as such guide devices have caused disengagement of the lifting fixtures for storage cask systems. The particular form of engagement of the lifting fixtures and the waste package is not specified by the standard; only the structural load path requirements are specified.

ANSI-N14.6

ANSI-N14.6 (ANSI N14.6-1993) provides a standard for the crane and lifting devices for large packages. This standard provides guidance on seismic requirements for the crane and lift fixtures and is normally applied in conjunction with NUREG-0612 (NRC 1980); thus N14.6 should be used as supplemental information for lifting device and waste package design.

NUREG/CR-1815 and Regulatory Guide 7.11

NUREG/CR-1815 (Holman and Langland 1981) and Regulatory Guide 7.11 provide a methodology to determine the fracture toughness requirements of cylindrical shells for packages with a thickness less than four inches. The methodology allows the steel type used in the design of a package to be evaluated to ensure that sufficient ductility exists over the operating temperature range of the package. Cold temperatures reduce the ductility of steel alloys, and a substantial temperature margin is provided through the use of these documents to prevent brittle

fracture. Metals that do not comply with the methodology should not be used for structural components of the waste package. (Note: Regulatory Guide 7.12 [Regulatory Guide 7.12 1991] modifies this methodology for cylindrical shells greater than four inches thick.)

NUREG/CR-0481

NUREG/CR-0481 (Rack and Knorovsky 1978) addresses elastic/plastic data for structural analyses and attempts to provide a methodology for evaluating the effects of temperature and strain-rate upon metals such as stainless steel. This approach is useful because strain-rate data are normally measured at room temperature, and the waste package is operated over a range of temperatures below room temperature to significantly higher than room temperature. The methodology can be used to evaluate the data provided by finite-element structural analysis tools to ensure that the data used by the analysis system is appropriate. The waste package could experience significant plastic deformation of the package ends in some drop accident scenarios, and a rock fall could similarly cause substantial deformation of the waste package at any location along its length. Since these accident scenarios would occur at quite different temperatures, the structural parameters over the elastic/plastic regime must be evaluated. One effect noted by NUREG/CR-0481 is that the shape of the stress-strain curve is essentially the same at different temperatures, but it was also noted that dynamic strain-aging might occur at elevated temperatures (over 200°C), even in austenitic stainless steels. Also, a significant variation in material properties was observed in different heats of stainless steel.

NUREG/CR-6608

NUREG/CR-6608 (Witte et al. 1998) discusses the impact of large packages during a drop event, especially with respect to the modeling of the impact target. Waste package drop analyses have previously used an unyielding surface to model the impact target, but NUREG/CR-6608 describes acceptable methods of describing a crushable/breakable impact pad such as a reinforced concrete pad. This model is much more realistic than an unyielding surface, and reduces the g-loads applied to the waste package and spent nuclear fuel basket substantially while providing a conservative calculation. This methodology is now being applied to storage cask safety analyses at the NRC's suggestion.

NUREG/CR-6322

NUREG/CR-6322 (Lee and Bumpas 1995) provides a methodology for evaluating the buckling stresses in spent nuclear fuel baskets by determining the stability capacity of the basket based upon analysis of the individual structural components of the basket. The individual components are treated as columns, beam-columns, and plates. The methodology required for determining buckling stresses and comparing these stresses to the acceptance criteria of the ASME Boiler and Pressure Vessel code is presented in NUREG/CR-6322. The resulting methodology is acceptable to the NRC for transport casks, and is thus applicable to waste packages for handling drop accident scenarios.

NUREG/CR-4554

NUREG/CR-4554 (Gerhard et al. 1992) provides information regarding the structural stresses for large packages during a drop event, and is applicable to the waste package. It is useful for

comparison of stresses calculated for the waste package to those calculated for a commercial cask.

4.3.2 Thermal Codes and Standards

Thermal analysis methodologies are discussed in the SRPs for storage and transportation. Other relevant standards are the following:

- Section III, Division 1, Subsection NB of the ASME code (ASME 1995, NB-1120), in which the temperature limit for containment structural alloys is set. This section states that the code is not applicable to materials subjected to temperatures outside the range presented in Tables 2A, 2B, and 4 of Section II, Part D, Subpart 1 of ASME 1995. Essentially, this sets a temperature limit for alloys used for reactor vessels to 800°F.
- ACI-349 (ACI 1986, Articles A.4.1 and A.4.2), in which bulk temperature limits for concrete are set to 150°F. The NRC has also accepted for storage casks the off-normal bulk temperature limit of 200°F and accident (fire) temperature limit of 350°F mentioned in articles A.4.1 and A.4.2. While concrete is not presently anticipated for use in the drifts, concrete is used in the surface facility and these limits support evaluations of waste package temperature distribution within the surface facility.

A de facto standard accepted by the NRC for the storage of spent fuel, which would be relevant to any temporary storage of spent fuel in the repository surface facility, is *Recommended Temperature Limits for Dry Storage of Spent Light Water Reactor Zircaloy-Clad Fuel Rods in Inert Gas*, PNL-6189 (Levy et al. 1987). This publication provides methods for evaluation of fuel rod pressure at elevated temperatures, and provides temperature limits for a desired forty-year storage period. The ability of irradiated zircaloy cladding to provide a barrier against the release of radioactive material is evaluated as a function of thermal damage to the cladding. Damage is expressed in terms of diffusion-controlled cavity growth of micro-flaws in the zircaloy matrix.

4.3.3 Shielding and Source Term Codes and Standards

Shielding analysis methodologies are discussed in the SRPs for storage and transportation. Shielding analysis methodologies are often validated along with criticality safety software systems. Specific standards include the following:

- NUREG/CR-6484 (Broadhead et al. 1996), which describes verification and validation of the shielding sequences of the SCALE analysis systems
- NUREG/CR-5625 (Hermann et al. 1994), which provides technical support for the NRC decay heat guide using the SAS2H/ORIGEN-S analysis sequence of the SCALE-4 system
- ANSI/ANS-6.1.1 (ANSI/ANS-6.1.1-1977), which contains the flux-to-dose rate conversion factors for neutron and gamma radiation
- NUREG-1536 (NRC 1997) and NUREG-1617 (NRC 2000), which provide guidance for evaluating shielding features of spent nuclear fuel packages.

The following are specific applications of shielding standards to the waste package design:

NUREG/CR-6484

NUREG/CR-6484 (Broadhead et al. 1996) describes the verification and validation of the shielding sequences of the SCALE analysis systems. Example problems are provided to verify the proper installation of the SCALE software on a given computer system. These verification problems exercise the input options of the computer software and demonstrate that the system is working properly, including the scripts that tie the various computer programs together. A second set of problems verifies the functionality of the code system to solve various types of problems, and a comparison of results from different code systems is provided. Validation consists of problems spanning a range of spent nuclear fuel burnups and enrichments and different material types for typical spent nuclear fuel casks. This document has been used in the qualification of the SCALE system for the waste package design analyses.

NUREG/CR-5625

NUREG/CR-5625 (Hermann et al. 1994) provides technical support for major revisions to the NRC decay heat guide, using a data base computed by the SAS2H/ORIGEN-S analysis sequence of the SCALE-4 system. Using generic PWR and BWR assembly models, calculations were performed with each model for six different burnups at each of three separate specific powers to produce heat rates at cooling time in the range of 1 to 110 years. The calculated decay heat results have been verified by comparison with the existing data base of experimentally measured decay heat rates for PWR and BWR spent fuel. The range of parameter values is considered to lie in the mainstream of typical burnup, specific power, enrichment, and cooling time for spent nuclear fuel storage. The decay heat results, calculated and measured, in this guide are valuable for the validation of source term generation of commercial spent nuclear fuel for waste package design.

ANSI/ANS-6.1.1

ANSI/ANS-6.1.1-1977 presents data recommended for computing biological dose rates due to neutron and gamma-ray radiation fields. The standard provides neutron flux-to-dose-rate conversion factors for energies from 2.5E-8 to 20 MeV, and gamma ray factors for energies from 0.01 to 15 MeV. This standard is used to calculate whole-body dose rates to workers in the vicinity of waste packages.

NUREG-1536 and NUGEG-1617

NUREG-1536 (NRC 1997) and NUREG-1617 (NRC 2000) are specifically applicable to dry cask storage systems and transportation packages for spent nuclear fuel, respectively. They provide guidance for evaluating radiation source terms and shielding features of spent nuclear fuel packages. The methodologies recommended by these two documents include: selection of appropriate computer codes, which include the SAS2 sequence in SCALE for source term and SCALE or MCNP for shielding; selection of the fuel that provides the bounding source, specification of gamma source terms as a function of energy for both the spent fuel and the activated hardware materials, representation of the source term locations for the spent fuel and structural support regions, application of an axial peaking factor to account for the axial burnup

profile, proper specification of material densities and compositions, and the use of ANSI/ANS-6.1.1-1977 to perform flux-to-dose rate conversion. The shielding and source term methodologies for the waste package design follow the recommendations of these two NUREGs to assure that the proposed waste package designs meet both preclosure and postclosure shielding design criteria.

4.3.4 Criticality Safety Codes and Standards

The standards for criticality safety analysis are principally NUREGs published by the NRC and ANSI/ANS standards. The storage and transportation SRPs also contain data regarding criticality safety analyses for packages, mainly in the form of checks for compliance with the following standards.

- NUREG-1520 (NRC 1998), which is the SRP for a license application for a fuel cycle facility.
- NUREG/CR-2300 (NRC 1983), which provides methods and data for performing a probabilistic risk assessment.
- NUREG/CR-6483 (Emmett and Jordan 1996), which provides guidance regarding verification and validation of criticality safety software.
- NUREG/CR-6361 (Lichtenwalter et al. 1997), which provides information regarding benchmarks for light water reactor fuel in storage and transportation packages. This publication employs the "fresh fuel assumption," and does not address burnup credit.
- NUREG/CR-6328 (Parks et al. 1995), which documents failures of criticality analysis systems for light water reactor fuel with U-235 enrichments from five to 20 wt%.
- ANSI/ANS-8.1 (ANSI/ANS-1998), which provides information on criticality safety outside of nuclear reactors.
- ANSI/ANS-8.7 (ANS-8.7/ANSI N16.5-1975 [R1987] 1975), which provides further information on criticality with storage of fissile materials.
- ANSI/ANS-8.10 (ANSI/ANS-8.10-1983), which provides criteria for nuclear criticality safety controls in operations with shielding and confinement.
- ANSI/ANS-8.15 (ANSI/ANS-8.15-1981), which provides criteria for nuclear criticality safety controls for special actinide elements.
- ANSI/ANS-8.17 (ANSI/ANS-8.17-1984), which contains guidance for the calculation of bias and uncertainty for criticality systems.
- ANSI/ANS-8.21 (ANSI/ANS-8.21-1995), a standard for fixed neutron absorbers such as the boron/stainless material contained in waste package fuel baskets.

- Regulatory Guide 1.13 (Regulatory Guide 1.13 1981), which provides guidance regarding criticality calculations for packages during handling operations in spent fuel pools.
- Regulatory Guide 3.71 (Regulatory Guide 3.71 1998), which provides nuclear criticality safety standards for fuels and material facilities.

The following are specific applications of criticality safety standards to the waste package design:

NUREG-1520

NUREG-1520 (NRC 1998) is the SRP for a license application for a fuel cycle facility, and provides information relevant to criticality control in the surface facility. This SRP discusses fissile mass limits and various mechanisms for criticality safety including mass limits, spacing, and establishment of neutron absorbers between zones of fissile materials.

NUREG/CR-2300

NUREG/CR-2300 (NRC 1983) provides methods and data for performing a probabilistic risk assessment. The waste package criticality safety analysis for the preclosure time period is deterministic, but NUREG/CR-2300 can be useful in determining the scenarios that must be evaluated. During the postclosure time period, a probabilistic analysis is required, and the NUREG provides guidance regarding methodologies acceptable to the NRC.

NUREG/CR-6483

NUREG/CR-6483 (Emmett and Jordan 1996) provides guidance regarding verification and validation of criticality safety software. Test problems for installation verification, and verification of code functionality are provided for the SCALE-4 criticality safety sequence. These test problems are also applicable to other codes such as MCNP if desired (MCNP is distributed with a set of installation verification test problems which also exercise the features of the code, and these problems may be used). A set of validation problems are provided for U-233, U-235, and Pu-239 fissile systems with a significant range of geometries and fuel forms. The experimental bias and statistical analysis of the uncertainties are described. The methodology can be applied directly to the MCNP computer code typically used to analyze the packages.

NUREG/CR-6361

NUREG/CR-6361 (Lichtenwalter et al. 1997) provides information regarding 180 experimental benchmarks for light water reactor fuel in conditions similar to those present in storage and transportation packages. This document employs the "fresh fuel assumption," and does not address burnup credit. The range of experimental geometries and variety of fissile materials is extensive, and experiments are provided with and without criticality control devices such as water gaps and neutron absorber plates. This benchmark document provides an example of the statistical uncertainty and calculational bias. The light water reactor experiments are applicable to the waste package PWR and BWR spent nuclear fuel designs. NUREG/CR-6361 provides a

computer program named USLSTATS which implements the upper safety limit approach in a manner favored by the NRC.

NUREG/CR-6328

NUREG/CR-6328 (Parks et al. 1995) documents failures of criticality analysis systems for light water reactor fuel with U-235 enrichments from five to twenty weight percent. The particular cross-section data set which exhibits difficulties in the five to twenty weight percent U-235 range is the 123-energy group GAM/THERMOS data set. This data set is relatively old but is still in use because of the extensive experience base and historical record which users have established. This data set was superseded by the ENDF/B-IV data set and the later ENDF/B-V data set, and should not be used for waste package criticality safety evaluations. The technical difficulty with this data set is that the cross-sections have been weighted in a fashion which is appropriate for light water reactor spent nuclear fuel with enrichments from 1.8 to 5.0 weight percent, and for research reactor spent nuclear fuel types which are highly enriched (93 weight percent). In the intermediate enrichment range, very little experimental work has been performed. The problems with the GAM/THERMOS data set were not noticed until a comparison of a transport cask analysis against the United Kingdom's MONK computer code system was performed. It is important to note that the point energy data set provided for MCNP is not sensitive to the technical difficulties experienced by the energy-group format GAM/THERMOS data set, but experimental benchmark verification in the five to twenty weight percent enrichment range is highly desirable for waste package calculations.

ANSI/ANS-8.1

ANSI/ANS-8.1-1998 provides information on criticality safety outside of nuclear reactors. This ANSI standard forms the basis for much of the criticality safety standards expressed in more detailed standards. The overall goals of a criticality safety program are established.

ANSI/ANS-8.7

ANSI/ANS-8.7-1975 provides further information on criticality with storage of fissile materials and is applicable to the preclosure time period for the waste package.

ANSI/ANS-8.10

ANSI/ANS-8.10-1983 provides criteria for nuclear criticality safety controls in operations with shielding and confinement, and is applicable to the surface facility evaluations of the waste package.

ANSI/ANS-8.15

ANSI/ANS-8.15-1981 provides criteria for nuclear criticality safety controls for special actinide elements. This standard can be helpful for DOE-owned spent fuel that contains quantities of actinides not usually found in light water reactor spent nuclear fuel, such as plutonium spent nuclear fuel assemblies.

ANSI/ANS-8.17

ANSI/ANS-8.17-1984 contains guidance for the calculation of bias and uncertainty for criticality systems. This standard is used in conjunction with the guidance in NUREG/CR-6361 (Lichtenwalter et al. 1997). The ANSI/ANS-8.17 standard is more general than the statistical approach described in NUREG/CR-6361 and may be more applicable to postclosure criticality safety evaluations of the waste package.

ANSI/ANS-8.21

ANSI/ANS-8.21-1995 provides guidance for criticality safety using fixed neutron absorbers. This standard explicitly applies to spent nuclear fuel baskets containing strong neutron absorbers for criticality control. The standard is general enough to encompass all versions of the waste package.

Regulatory Guide 1.13

Regulatory Guide 1.13 provides guidance regarding criticality calculations for packages during handling operations in spent fuel pools. This standard is particularly applicable to water pool operations at the surface facility, but is also important to an understanding of the NRC's approval of burnup credit at nuclear power plant spent fuel pools.

Regulatory Guide 3.71

Regulatory Guide 3.71 provides nuclear criticality safety standards for fuels and material facilities, and is applicable to the loading of the waste package within the surface facility.

4.3.5 Fabrication Codes and Standards

Specifications for the fabrication of transportation packages can also be applied to disposal containers. Fabrication of disposal containers typically involves the use of a less restrictive section of the ASME code, due to the less-demanding environment present in a controlled storage facility. Guidance for the fabrication of radioactive materials packaging is provided in the storage and transportation SRPs. In addition, there are several specific publications that apply:

- NUREG/CR-3854 (Fischer and Lai 1985), which provides fabrication criteria for shipping packages
- NUREG/CR-3019 (Monroe et al. 1985), which provides welding criteria for shipping packages
- ANSI N14.5-97 (ANSI N14.5-97 1998), which provides a methodology to calculate leakage rates of gaseous materials
- Regulatory Guide 1.31 (Regulatory Guide 1.31 1978), which provides further information on welding

- Regulatory Guide 1.44 (Regulatory Guide 1.44 1973), which provides information on weld metal sensitization
- Regulatory Guide 7.4 (Regulatory Guide 7.4 1975), which provides information on leak testing of shipping packages
- 10 CFR 21 (10 CFR 21), which defines the process for the reporting of defects and noncompliance of fabrication processes
- ASME, Section II, Part C (ASME 1998), which specifies the conformance criteria of the filler material used by the fabricator of the disposal container during the welding process
- ASME, Section III, Division 1, Subsection NB (ASME 1995), which is to be used as a standard for fabrication and inspection
- ASME, Section V (ASME 1998), which is used to develop the non-destructive examination processes to be used in the fabrication of the disposal container.
- ASME, Section IX (ASME 1998), which is used to develop the welding processes to be used in the fabrication of the disposal container.

The following are specific applications of fabrication standards to the waste package design:

NUREG/CR-3854

NUREG/CR-3854 (Fischer and Lai 1985) provides fabrication criteria for shipping packages, including identification of the ASME service level for various package components, and the applicable part of the ASME code Section III. NUREG/CR-3854 predates the much more recent Division III, which applies to spent nuclear fuel canisters, but it can be applied directly to the waste package for uncanistered spent nuclear fuel.

NUREG/CR-3019

NUREG/CR-3019 (Monroe et al. 1985) provides welding criteria for shipping packages. Tables of ASME categories are provided for various container components, and the welds of these components are evaluated to determine if welds are containment-related welds, criticality-related welds, or other safety-related welds. Specific paragraphs of the ASME code are referenced depending upon the component and classification of weld.

ANSI N14.5-97

ANSI N14.5-97-1998 provides a methodology to calculate leakage rates of gaseous materials from a transport package. The methodology is applicable to waste package seal weld testing in the surface facility. The waste package should not leak during handling and emplacement operations. Leak test procedures are specified that ensure that the leakage is within allowable limits. The leakage rates are expressed in terms of curies of radioactive gas mixture released per second, and can be compared to the allowable limits for normal operation and accident

conditions. This standard is accepted by the NRC for use with the storage and transport of packages, and would also apply to waste packages.

Regulatory Guide 1.31

Regulatory Guide 1.31 provides further information on the ferrite content in stainless steel weld metal. This guide specifies either a chemical analysis or magnetic measurement to confirm the absence of excessive ferrite content, which causes microfissures in the weld metal. Regulatory Guide 1.31 can be used as an example of the concern that must be shown to filler materials during welding, and can be extended to similar controls for the welding of waste packages.

Regulatory Guide 1.44

Regulatory Guide 1.44 provides information on weld metal sensitization at various temperatures. Embrittlement of austenitic stainless steel has been observed and can be avoided by proper pre-heat and cooling techniques. Similar techniques can be applied to the waste package to accommodate the different metals used in the waste package.

Regulatory Guide 7.4

Regulatory Guide 7.4 provides information on leak testing of shipping packages, and basically endorses the use of ANSI N14.5-97. This regulatory guide is thus applicable to testing of the seals provided by the closure welds for the waste package lids.

10 CFR 21

10 CFR 21 describes the process for reporting defects and noncompliance. This regulation will be used by the supplier(s) of the disposal containers to report defects and noncompliance in the fabrication process.

ASME, Section II, Part C

The filler material used by the fabricator of the disposal container shall be specified in the fabricator's approved welding procedures and shall conform to Section II, Part C of ASME 1998.

ASME, Section III, Division 1, Subsection NB

The disposal container shall be fabricated and inspected in accordance with ASME Boiler and Pressure Vessel Code, Section III, Division 1, Subsection NB (Class 1 Components) (ASME 1995) to the maximum extent practicable. Deviations from the ASME Code shall be documented and submitted for approval. It is not the intent that this be an "N" stamped vessel but rather that the ASME Code be used as a standard for fabrication and inspection. Also, rejected defects in materials can be repaired by welding if the ASME Code, Section III, requirements are met and the repair has been approved by the Purchaser. Defective material that cannot be satisfactorily repaired will be rejected and replaced. All material defects and repairs will be appropriately documented on the Supplier's Nonconformance Report that requires the Purchaser's concurrence before implementation.

ASME, Section V

This code section of ASME 1998 is used to develop the non-destructive examination processes to be used by the fabricator for the fabrication process of the disposal container.

ASME, Section IX

This code section of ASME 1998 is used to develop the welding process of the fabricator to be used in the fabrication process of the disposal container.

4.4 INTERFACE CONTROL DOCUMENTS

Currently, there are no documents that define the design interactions between the Waste Package Project and other organizations. Interface controls that will delineate the design responsibilities of the Waste Package Project and other organizations will be developed as necessary.

5. WASTE PACKAGE DESIGN METHODOLOGY ASSUMPTIONS

In every analysis or calculation, the assumptions inherent to the work may be divided into two categories. The first category consists of assumptions that are necessitated either by the calculation process and computational tool employed, or by the particulars of the range of problems at hand. While a particular process or tool may be used to analyze a broad range of configurations, its application to the processing and disposal of waste forms in the potential repository requires that assumptions appropriate to this particular range of application be made. This category of assumptions will be addressed in this report.

The second category of assumptions consists of those specific to a particular analysis or calculation. An example of this category would be a set of assumptions necessary to perform a drop calculation for a particular waste package. This category of assumptions will not be addressed in this report.

None of the assumptions listed in this section were used in this report to produce quality-affecting results in the sense of generating numeric values or defining a specific component design; however, these assumptions are quality-affecting in the sense that they define the assumptions appropriate to the methodology. If the methodology is used in consonance with this document to produce quality-affecting results in future analyses, then the quality of these assumptions (and whether or not they require further verification) will be determined at that time.

5.1 SOURCE TERM GENERATION ASSUMPTIONS

Source term calculations provide heat generation rates, photon and neutron spectra and intensities, and radionuclide inventories of commercial spent nuclear fuel assemblies, DOE spent nuclear fuel, and high level waste. The heat generation rates are used in thermal evaluations of the waste packages and the host rock of the potential repository. The photon and neutron sources are used to determine the radiation level surrounding a waste package. The radionuclide inventories are used to determine dose rates due to the release of radionuclides from the waste packages during the postclosure period. The source terms discussed in this section are not used for criticality calculations.

For the naval spent nuclear fuel canister, the thermal output and photon and neutron surface currents are provided by the U.S. Department of the Navy (Naples 1999).

5.1.1 Commercial Spent Nuclear Fuel Waste Forms

5.1.1.1 Generic Fuel Assemblies and Burnup Histories

It is assumed that the commercial spent nuclear fuel waste stream can be approximated by calculating source terms for generic PWR and BWR assemblies at incremental enrichments and burnups, and that a generic burnup history (without the modeling of outages, intermittent down times, etc.) can be used for the depletion calculations. The rationale for this assumption is based on the analysis provided in NUREG/CR-5625 (Hermann et al. 1994), which shows that the heat generation rates of generic PWR and BWR spent nuclear fuel assemblies, in watts per kg U, do not vary significantly for a given burnup and cooling time between 5 and 100 years.

Additionally, the heat generation rate is progressively less sensitive to the irradiation history after a five-year cooling time.

This behavior of the decay heat rates during the repository preclosure period is due to dominance of the radiation generated by the fission products over the radiation generated by the actinides in commercial spent nuclear fuel. Fission product generation is sensitive to the assembly burnup, which is determined by the total number of fissions. It is less sensitive to the neutron spectra or actinide compositions, because the fission yields vary slowly with these variables. While the irradiation history, especially for the last reactor cycle, will significantly influence the short-lived fission products, the dependence of the decay heat rate on the specific power exists only for the first five years of cooling. The mandatory five-year cooling period before waste acceptance, as dictated in 10 CFR 961.11 (10 CFR 961), will progressively decrease the dependence of the heat generation rate on the short-lived fission products and allow for the use of generic burnup histories for the depletion calculations. This assumption is used in Section 6.1.

5.1.1.2 Uniform Specific Power

An average uniform specific power over the entire length of the assembly is assumed, and the total irradiation interval is determined as the ratio of the assembly burnup to the specific power. The rationale for using a uniform power within the assembly volume is that the subsequent shielding and thermal evaluations can conservatively take into account the burnup axial profile through an axial peaking factor (refer to Section 5.4.1). This assumption is used in Section 6.1.

5.1.1.3 Interpolation in Arrays of Results

It is assumed that the source terms can be generated for an array of various enrichments, burnups, and decay times, and that interpolation can then be used to obtain the source terms of any specific assemblies in the waste stream without requiring explicit modeling of the assemblies. The rationale for this assumption is that, as described in Section 5.1.1.1, for a given burnup and cooling time during the repository preclosure period, the decay heat rate, in watts per kg U, is relatively constant for different fuel assembly types. For a sufficiently dense selection of the independent variables (enrichment, burnup, and decay time), the source term error resulting from the use of an appropriate interpolating polynomial is on the order of the fundamental resolution of the calculational methods. This assumption is used in Section 6.1.

5.1.1.4 Assembly Mass Loading

It is assumed that the initial heavy metal loading of a PWR assembly is 475 kg of heavy metal, instead of the 464 kg of a typical B&W Mark B assembly. For a BWR assembly, the initial heavy metal loading is assumed to be 200 kg, instead of the 177 kg of a typical General Electric 8x8 BWR fuel assembly. The rationale for these assumptions is that a higher initial uranium loading leads to a proportionally higher source term, which is generally more conservative for design considerations.

5.1.2 Non- Commercial Spent Nuclear Fuel Waste Forms

5.1.2.1 DOE Spent Nuclear Fuel Waste Forms

For DOE spent nuclear fuel, it is assumed that the total initial radionuclide inventory provided by Idaho National Engineering and Environmental Laboratory (INEEL 1999) is adequate for the analyses of the potential repository at Yucca Mountain. It is also assumed that the inventory for each fuel type can be divided by the number of assemblies of that fuel type to determine the average inventory of that fuel type. The rationale for this assumption is that the Idaho National Engineering and Environmental Laboratory has generated inventories for several representative fuel types in the DOE spent nuclear fuel waste stream, which are used to generate radionuclide inventories for the rest of the waste stream. This assumption is used in Section 6.1.2.2.

5.1.2.2 Defense High-Level Waste

For the defense high-level waste, historical information regarding the inventory at the various sites is used in decay calculations to generate initial radionuclide inventories (DOE 1999a, Appendix A). These inventories are then used in ORIGEN-S decay calculations to obtain source terms over time. The ORIGEN-S code is described in Section 6.1.1.2. It is assumed that the information for the material planned for disposal at Yucca Mountain is accurately represented by the radionuclide inventories provided by the sites. Again, the rationale for this assumption is that the information provided represents an average of the material, not the bounding. This assumption is used in Section 6.1.2.3.

5.2 STRUCTURAL ANALYSIS ASSUMPTIONS

5.2.1 Assumptions for Normal Operations Evaluations

5.2.1.1 Contact Stiffness between Waste Package and Impact Surface

The assumption is made that the contact stiffness between the waste package and the impact surface can be determined iteratively. The rationale for this assumption is explained in the following paragraph.

The magnitude of the contact stiffness (between surfaces used in the simulation) is a parameter that influences the resulting stresses. If the stiffness value is very large, stiffness matrix ill-conditioning and divergence will occur. Similarly, an extremely small stiffness value results in compatibility violations. Therefore, an optimum value for the contact stiffness is one that is between the two, and is arrived at iteratively. For example, for the case of crack initiation on waste package shells, the contact stiffness was doubled from $1.5 \cdot 10^8$ N/m to $3.0 \cdot 10^8$ N/m and the resulting stresses (see CRWMS M&O 1999d, filename: m20s.out, line numbers: 47 and 67) were compared to previous results (see CRWMS M&O 1999h, Table 6.1-1, results for the shell thickness of the 20-mm outer shell and the 50-mm inner shell). The resulting stresses on the outer shell of the waste package showed that the change in stiffness had no significant effect on stress magnitudes. Therefore, an iterative process to determine the value of contact stiffness used in the finite element simulation is deemed acceptable for the subject transient dynamic solution. This assumption is used in Section 6.2.2.2.

5.2.1.2 Treatment of Skirt for Emplacement Loading Evaluation

The exact geometry of the extension of the outer shell (i.e., skirt) is simplified for the purpose of this evaluation in such a way that the total mass of the outer shell is distributed within the cylindrical shell of constant wall thickness. Since the values of the inner and outer shell diameters, essential for the calculation results, must be kept intact, the skirt length is increased to accommodate the outer shell mass. The rationale for this conservative assumption is to provide the set of bounding results, while simplifying the finite element representation. This assumption is used in Section 6.2.2.2.

5.2.1.3 Geometry of Collapsed Drift

Loose rocks from the deterioration of the potential repository emplacement drifts can increase the pressure exerted on top of the drip shield. This additional mass is estimated by assuming that, due to said deterioration, the initially circular cross section of the repository emplacement drift would eventually take the more stable ellipsoidal shape. The extent of this shape change is quantified as the difference between the initial radius of the emplacement drift, R , and the final length of the major semi-axis of the ellipsoid, $3R$. Thus, the change of repository emplacement drift height is estimated to be equal to the width (i.e., initial diameter) of the drift, $2R$. The rationale for this conservative assumption is the bounding value recommended for this category of rocks in the *SME Mining Engineering Handbook* 2nd Edition (Hartman 1992, Table 24.1.7). This assumption is used in Section 6.2.2.2.

5.2.2 Cracks Formed during Design Basis Events

Only one crack is assumed to develop in the waste package shell due to design basis events. The rationale for this assumption is that, in the majority of the design basis events, the stress is highly localized in the vicinity of the impact region on the waste package shells, which are made of highly ductile materials. If the stress exceeds the allowable limit for crack development, it will initiate and cause propagation of only one crack emanating from the impact region. This assumption is conservative because if all of the energy imparted on the waste package is used to create one crack, it will be a more extensive crack than if the energy were divided to create many cracks. Also, since this extensive crack occurs directly at the point of highest stress, it compromises shell integrity the most at the point of highest stress. This assumption is used in Section 6.2.2.4.

5.2.3 First Failure of Inner Lid for Pressurization Design Basis Event

For evaluation of the pressurization design basis event, the inner lid is assumed to fail before the outer lid; however, no structural credit is assumed for the outer lid. The rationale for this assumption is that, despite the ductile nature of the inner shell, the gap between the inner and outer lid at the waste package bottom end is large enough that the inner lid can experience a nonlinear deformation sufficient to develop a through-wall crack. This assumption is used in Section 6.2.2.3.

5.2.4 Use of Static Material Properties

Strain-rate-dependent material properties are not available for all of the materials used; therefore, the material properties obtained under the static loading conditions are assumed for all materials. In general, this is a conservative assumption; nonetheless, in this case, the impact of using material properties obtained under the static loading conditions is anticipated to be small. The rationale for this assumption is that the mechanical properties of subject materials do not significantly change at the peak strain rates in the course of the design basis events. This assumption is used in Sections 6.2.2.4 and 6.2.2.5.

5.2.5 Omission of Structural Damping

No structural damping is used for the material in the evaluation of dynamic analyses. Attenuation of stress waves is not of interest, because the failure criteria is based only on the comparison of maximum stress with the ultimate tensile strength. The rationale for this assumption is that omission of structural damping provides conservative results, since maximum stress values will be higher. This assumption is used in Section 6.2.2.5.

5.2.6 Assumptions for Missile Impact Analysis

5.2.6.1 Application of Empirical Relationships for Impact Analysis

Empirical equations were developed for the perforation of ductile mild steel plates (Jones 1994). These relations are assumed to give conservative results for the waste package shells. The rationale for this assumption is that nickel alloys have higher strength and ductility than mild steels (low-carbon steels), and the ductility of stainless steel is higher than that of mild steel. Therefore, these empirical relations can be conservatively used to approximate behavior of the waste package shells impacted by a pressurized system missile. This assumption is used in Section 6.2.2.4.

5.2.6.2 Assumption of Waste Package Shell as Flat Plate for Impact Analysis

Empirical relations of flat plates are assumed to be applicable to determining the structural response of the waste package shells to missile impact load. The rationale for this assumption is that the effect of shell curvature is small compared to the plate thickness for missile impact loads. Therefore, the structural response of the waste package shells is similar to that of the flat plate in the region of impact. This assumption is used in Section 6.2.2.4.

5.2.6.3 Boundary Conditions for Impact Analysis

The fixed-end boundary conditions of the waste package shells in the localized region of missile impact are assumed to be similar to those of the flat plate shown in the reference (Jones 1994, p. 57, Figure 1). The rationale for this assumption is that the waste package shell in the vicinity of the impact region will resemble a geometric configuration similar to a flat plate with fixed ends. This assumption is used in Section 6.2.2.4.

5.2.7 General Assumptions for Waste Package Drop Analyses

The following assumptions are utilized for the waste package tip-over, swing down, corner drop, horizontal drop, and vertical drop analyses. Assumptions specific to each drop analysis are presented in separate subsections. These drops are defined as follows:

- Waste Package Tip-Over – the waste package is at rest on the ground in a vertical position and an external force (such as a seismic event) causes the waste package to tip over and impact the ground.
- Waste Package Swing Down - the waste package is being lifted in a horizontal orientation at a height of 2.4 m when the lifting device inadvertently releases one end. One end of the waste package remains held by the lifting device while the other end swings down and impacts the ground.
- Waste Package Corner Drop – the waste package is being lifted in a vertical orientation at a height of 2.0 m when the lifting device inadvertently drops it. A corner of the waste package impacts the ground first.
- Waste Package Horizontal Drop – the waste package is being lifted in a horizontal orientation at a height of 2.4 m when the lifting device inadvertently drops it. The waste package impacts the ground squarely on its side.
- Waste Package Vertical Drop – the waste package is being lifted in a vertical orientation at a height of 2.0 m when the lifting device inadvertently drops it. The waste package impacts the ground squarely on its base.
- Waste Package Puncture Drop – the emplacement pallet with waste package is being lifted in a horizontal orientation when the lifting device inadvertently drops it. The emplacement pallet with waste package impacts the ground along its horizontal axis.

5.2.7.1 Unyielding Target Surface

The target surface for the falling or dropped waste package is assumed to be unyielding. The rationale for this assumption is that it maximizes the stress on the falling waste package. This assumption is used in Section 6.2.2.5.

5.2.7.2 Poisson's Ratio for Alloy 22

Poisson's ratio of Alloy 22 is not available in literature. The Poisson's ratio of Alloy 625 (SB-443 N06625) is assumed for Alloy 22. The impact of this assumption is anticipated to be negligible. The rationale for this assumption is that the chemical compositions of Alloy 22 and Alloy 625 are similar (see ASME 1998, Section II, Part B, SB-575, Table 1 and ASM 1980, p. 143, respectively). This assumption is used in Section 6.2.2.5.

5.2.7.3 Poisson's Ratio for SA-516 Carbon Steel

Poisson's ratio is not available for SA-516 carbon steel. Therefore, Poisson's ratio of cast carbon steel is assumed for SA-516 carbon steel. The impact of this assumption is anticipated to be negligible. The rationale for this assumption is that the elastic constants of cast carbon steels are only slightly affected by changes in composition and structure (see ASM 1978, p. 393). This assumption is used in Section 6.2.2.5.

5.2.7.4 Waste Package Temperature-Dependent Material Properties

Some of the temperature-dependent material properties (density, Poisson's ratio, and elongation) are not available for SB-575 N06022 (Alloy 22), SA-516 K02700 (SA-516 carbon steel), SA-240 S31600 (316 stainless steel), and SA-240 S30400 (304 stainless steel) (Poisson's ratio only). The room temperature (20 °C) material properties are assumed for these materials. The impact of using room-temperature material properties is anticipated to be small. The rationale for this assumption is that undetermined mechanical properties of said materials will not significantly impact the results. This assumption is used in Section 6.2.2.5.

5.2.7.5 Waste Package Material Elongation Properties

The elongation of Alloy 22 and 316 stainless steel at elevated temperatures is not available from traditional sources. However, vendor data is available for Alloy 22 and 316 stainless steel (Haynes International 1997, p. 15 and Allegheny Ludlum 1999, p. 8, respectively). For comparison purposes, the percent difference between elongation at room temperature and elevated temperatures can be normalized and applied to the data available from accepted codes, thus ensuring that the bounding case is covered. The rationale for this assumption is to be as reasonably accurate as possible. It would not be logical for the elongation values to remain constant over the range of temperatures under consideration. This assumption is used in Section 6.2.2.5.

5.2.7.6 Uniform Strain of SB-575 N06022 (Alloy 22) and SA-240 S31600 (SS 316NG)

Three-stage deformation characteristics are not observed in the stress-strain curves for Alloy 22 or Type 316 stainless steel (CRWMS M&O 2000r). Therefore, it is conservatively assumed that the uniform strain is 90% of the elongation. The rationale for this assumption is the character of the stress-strain curves for Alloy 22 and Type 316 stainless steel. This assumption is used in Section 6.2.2.5.

5.2.8 Additional Assumptions for Waste Package Tip-Over Analysis

5.2.8.1 Removal of Thermal Shunts

The thermal shunts are removed for the purpose of this calculation. The rationale for this assumption is that the purpose of the thermal shunts is not to provide structural support. Their removal provides a bounding set of results, while simplifying the finite element representation. This assumption is used in Section 6.2.2.5.

5.2.8.2 Geometrical Arrangement of Waste Package Loaded Internals

The exact geometry of the waste form is simplified for the purpose of this calculation in such a way that its total mass is assumed to be distributed within a 304 stainless steel bar of square cross section with uniform mass density. The rationale for this assumption is to provide the set of bounding results, while simplifying the finite element representation. This assumption is used in Section 6.2.2.5.

5.2.8.3 Geometry of Lid Lifting Features

The geometry of the lid lifting features is simplified for the purpose of this calculation in such a way that the total mass of each lifting feature is assumed to be distributed within a disc with uniform mass density and constructed of the same material as the lid to which it is attached. The rationale for this assumption is that the lid lifting feature design is not finalized, and only the mass has an effect on this calculation. The bounding mass of each lifting feature is assumed to be 30 kg. This assumption is used in Section 6.2.2.5.

5.2.9 Additional Assumptions for Waste Package Swing Down Analysis

5.2.9.1 Geometrical Arrangement of Waste Package Loaded Internals

The exact geometry of the loaded internals is simplified for the purpose of this calculation. The spent fuel was modeled as 21 separate solid rectangles, but the thermal shunts and dividers between the fuel assemblies were omitted. However, the side guides, corner guides, and stiffeners were included to accurately represent the contact with the inner shell. The rationale for this assumption is to simplify the finite element representation. This assumption is used in Section 6.2.2.5.

5.2.9.2 Uniform Strain of SA-516 K02700 Carbon Steel

The uniform strain of SA-516 K02700 carbon steel is not available in literature. Therefore, it is conservatively assumed that the uniform strain is 50% of the elongation. The rationale for this assumption is the character of the stress-strain curve for SA-36 carbon steel (see Boyer 2000 and Bowles 1980) which has a similar chemical composition as SA-516 K02700 carbon steel (see ASME 1998, Section II, Part A, SA-516/SA-516M, Table 1 and SA-36/SA-36M, Table 2). This assumption is used in Section 6.2.2.5.

5.2.9.3 Waste Package Angular Velocity

For the purposes of analyzing the initial angular velocity of the waste package before impact, the waste package will be assumed to be a solid cylinder. This is necessary to calculate the rotary moment of inertia. The impact of this assumption on the results is negligible. The rationale for this assumption is the overall cylindrical shape of the waste package and the relatively solid packing of the contents. This assumption is used in Section 6.2.2.5.

5.2.10 Additional Assumptions for Waste Package Corner Drop Analysis

5.2.10.1 Geometrical Arrangement of Waste Package During Drop

The waste package is assumed to strike the ground at an angle that puts the center of mass, which is assumed to coincide with the geometric center of the waste package, directly above the point of impact. The rationale for this assumption is that it induces the highest impact load on the waste package outer shell. This assumption is used in Section 6.2.2.5.

5.2.10.2 Geometrical Arrangement of Waste Package Loaded Internals

The exact geometry of the loaded internals is simplified for the purpose of this calculation. The fuel baskets, thermal shunts, spent nuclear fuel, and all other internals are created as a solid cylinder with an appropriate mass value. The rationale for this assumption is to simplify the finite element representation. This assumption is used in Section 6.2.2.5.

5.2.11 Additional Assumptions for Waste Package Horizontal Drop Analysis

5.2.11.1 Geometrical Arrangement of Waste Package Loaded Internals

The exact geometry of the loaded internals is simplified for the purpose of this calculation. The spent fuel was modeled as 21 separate solid rectangles, but the thermal shunts and dividers between the fuel assemblies were omitted. However, the side guides, corner guides, and stiffeners were included to accurately represent the contact with the inner shell. The rationale for this assumption is to simplify the finite element representation. This assumption is used in Section 6.2.2.5.

5.2.11.2 Uniform Strain of SA-516 K02700 Carbon Steel

The uniform strain of SA-516 K02700 carbon steel is not available in literature. Therefore, it is conservatively assumed that the uniform strain is 50% of the elongation. The rationale for this assumption is the character of the stress-strain curve for SA-36 carbon steel (see Boyer 2000 and Bowles 1980) which has a similar chemical composition as SA-516 K02700 carbon steel (see ASME 1998, Section II, Part A, SA-516/SA-516M, Table 1 and SA-36/SA-36M, Table 2). This assumption is used in Section 6.2.2.5.

5.2.12 Additional Assumptions for Waste Package Vertical Drop Analysis

5.2.12.1 Uniform Strain of 304 Stainless Steel

The uniform strain of 304 stainless steel is not available in literature. Therefore, it is conservatively assumed that the uniform strain is 75% of the elongation. The rationale for this assumption is the character of stress-strain curve for 304 stainless steel (see Boyer 2000). This assumption is used in Section 6.2.2.5.

5.2.12.2 Uniform Strain of SA-516 K02700 Carbon Steel

The uniform strain of SA-516 K02700 carbon steel is not available in literature. Therefore, it is conservatively assumed that the uniform strain is 50% of the elongation. The rationale for this assumption is the character of the stress-strain curve for SA-36 carbon steel (see Boyer 2000 and Bowles 1980) that has a similar chemical composition as SA-516 K02700 carbon steel (see ASME 1998, Section II, Part A, SA-516/SA-516M, Table 1 and SA-36/SA-36M, Table 2). This assumption is used in Section 6.2.2.5.

5.2.12.3 Friction Coefficients of Alloy 22

The friction coefficients for contacts involving Alloy 22 are not available in literature. It is, therefore, assumed that the dynamic (sliding) friction coefficient for all contacts is 0.4. The rationale for this assumption is that this friction coefficient represents the lower bound for most dry contacts involving steel and nickel (see Meriam & Kraige 1987 and Avallone & Baumeister 1987), nickel being the dominant component in Alloy 22 (ASME 1998, Section II, Part B, SB-575, Table 1). This assumption is used in Section 6.2.2.5.

5.2.12.4 Variation of Functional Friction Coefficient

The variation of functional friction coefficient between the static and dynamic values as a function of relative velocity between the contact surfaces is not available in literature for the materials used in this calculation. Therefore, the effect of relative velocity of the surfaces in contact is neglected in these calculations by assuming that the functional friction coefficient and static friction coefficient are both equal to the dynamic friction coefficient. The impact of this assumption is anticipated to be negligible. The rationale for this conservative assumption is that it provides the bounding set of results by minimizing the friction coefficient within the given finite element analysis framework. This assumption is used in Section 6.2.2.5.

5.2.12.5 Waste Package Design Parameters

The following design parameters are assumed for a PWR spent nuclear fuel assembly to be loaded into a 21-PWR waste package: mass = 773.4 kg, width = 216.9 mm, and length = 4407 mm. The rationale for this assumption is that these parameters correspond to the B&W 15x15 fuel assembly, which is the heaviest PWR fuel assembly available (BSC 2001i, Table 2). The mass of the B&W 15x15 fuel assembly has been increased by 11.4 kg (25 lbs) to account for variations in fuel assembly mass. It should be noted that South Texas PWR fuel assemblies will not be disposed in the 21-PWR waste package, and are therefore excluded from this assumption. This assumption is used in Section 6.2.2.5.

5.2.13 Additional Assumptions for Waste Package Puncture Drop Analysis

5.2.13.1 Contact Stiffness Between the Waste Package and the Emplacement Pallet

The magnitudes of the contact stiffness between (1) the waste package and the emplacement pallet and (2) the emplacement pallet and unyielding surface is assumed to be $1 \cdot 10^9$ N/m. The rationale for this assumption is that this magnitude of contact stiffness between surfaces results in simulation convergence and provides results that satisfy compatibility requirements. If the

contact stiffness value is too large, stiffness matrix ill-conditioning and divergence occur. On the other hand, a contact stiffness that is too small will result in compatibility violations. Therefore, an optimum value for the contact stiffness is one that is in between the extremes and is derived by iteration. The iterative process is based on engineering judgement and is supported by the ANSYS V5.4 on-line help. It should be noted that the contact stiffness is neither a measurable nor an intrinsic property of the materials in contact. This assumption is used in Section 6.2.2.5.

5.2.13.2 Poisson's Ratio of 316L Stainless Steel

The Poisson's ratio of 316L SS is not available in literature. The Poisson's ratio of 316 SS (SA-240 S31600) is assumed for 316L SS. The impact of this assumption is anticipated to be negligible. The rationale for this assumption is the similar chemical compositions of these two stainless steels (ASME 1998, SA-240, Table 1). This assumption is used in Section 6.2.2.5.

5.2.13.3 Bending Stiffness of the Inner and Outer Waste Package Shells

The bending stiffness (plate constant) of the inner and outer waste package shells is calculated by assuming that the expression for the bending stiffness of a flat plate is also valid for the waste package shells. The rationale for this assumption is that the diameters of the waste package shells are much larger than their respective thickness. This assumption is used in Section 6.2.2.5.

5.2.14 Assumptions for Rock Fall Upon Both Waste Package and Drip Shield

5.2.14.1 Friction Coefficients for Rock Fall Analysis

The following numbers are specified in order to meet the computational requirements:

Coefficient of static friction = 0.6 (Mariam and Kraige 1987)

Coefficient of kinetic friction = 0.4 (Mariam and Kraige 1987).

This assumption is used in Section 6.2.2.5, in which the rationale for using these values is discussed.

5.2.14.2 Rock Geometry for Rock Fall Analysis

In earlier rock fall analyses, a spherical geometry was assumed for the rock. The rationale for this assumption was that the pointed tip of a rock would crush upon impact before any failure would be observed on the waste package. Therefore, the rock's initial point contact would break up, forming a substantial surface area. Current rock fall evaluations assume a more realistic geometry for the falling rock (CRWMS M&O 2000d, Attachment IX). The finite element solution inherently includes the calculation of an initial point of contact turning into the intersection between a sphere (rock) and a cylinder (waste package) as the impact occurs. Considering that the tensile strength of metals is significantly larger than that of rock, this is a conservative assumption. This assumption is used in Section 6.2.2.4.

5.2.14.3 Deformation of Drip Shield Vertical Section

The vertical section of the drip shield is assumed to deform like a cantilever beam with the free edge at the bottom and the fixed edge connected to the curved section at the top. The rationale for this assumption is that the drip shield bottom end has similar boundary conditions to the free end of a cantilever beam, while the connection between the curved section and the vertical section of the drip shield has enough stiffness to prevent excessive deformation. Although the curved section will deform towards the center of its curvature, the effect of this deformation on the results is small compared to the deflection on the vertical section caused by the lateral active pressure. This assumption is used in Section 6.2.2.4.

5.2.15 Assumptions for Final Closure Weld Stress Reduction

5.2.15.1 De-Coupling of Inner and Outer Shells

The finite-element representations include the outer shell of the waste package. For the purpose of design evaluations for the induction coil heating process, the inner shell is assumed not to make contact with the outer shell, and therefore not transfer any mechanical load due to thermal expansion. The rationale for this assumption is that the region of induction coil heating is localized past the end of the inner shell, having much less thermal effect on the inner shell than the outer shell; and, that there is a significant clearance between the inner and outer shells, prohibiting contact. This assumption is used in Section 6.2.2.7.

5.2.15.2 Thermal Boundary Conditions for Outer Shell

The outer shell boundaries, excluding the region of induction annealing heat-treatment, are assumed to be initially at room temperature and insulated throughout the simulation. The rationale for this assumption is that the effect of increased temperature on the outer shell due to the decay heat of the spent nuclear fuel is anticipated to be small compared to the temperature change due to the induction coil heating process. Additionally, lower temperatures of the outer shell result in slightly conservative results in terms of residual stresses. For the insulated surfaces, no significant convective heat transfer is anticipated to take place between the outer shell and the air; therefore, this assumption has no significant effect on the results. This assumption is used in Section 6.2.2.7.

5.3 THERMAL ANALYSIS ASSUMPTIONS

5.3.1 Assumptions for Repository-scale Thermal Analysis

5.3.1.1 Pillar Representation of Repository

In the pillar representation of the potential repository, the problem domain is represented as a rectangular parallelepiped. Vertically, it ranges downward from the top of the mountain to well into the saturated zone. Laterally, the representation is bounded by planes parallel to the drifts and centered at the midpoint between the drifts. The thermal boundary conditions at these locations are adiabatic surfaces. For the three-dimensional pillar representation, the axial boundaries are placed perpendicular to the drift axis, either between waste packages or axially bisecting one or both waste packages at the end of the drift segment. Again, the thermal

boundary conditions at these planes are adiabatic surfaces. The rationale for this assumption is that it approximates a drift segment at or near the geometric center of the potential repository. The assumption of no lateral heat transfer is appropriate, since it maximizes the temperatures within the pillar; however, it is a very good assumption only from emplacement to about 1,000 years after, at which time appreciable cooling begins from the edges of the repository (CRWMS M&O 1994, p. 7). This assumption is used in Sections 6.3.2.2 and 6.3.2.3.

5.3.1.2 Omission of Gross Water Movement

The effect of water mobilization into the repository from the surrounding rock matrix, as well as that from percolation flux that reaches the repository horizon from the surface, is neglected in these evaluations. The rationale for this assumption is that it is conservative, since it neglects thermal energy transport away from the drifts by the gross movement of this water. While this may be an important effect for long time periods, it is not very important for short periods during which the waste form temperature reaches a peak value. Due to the exponential decrease in waste form heat generation rates, the waste form temperatures peak within a few decades after repository closure. For these time periods, and in conjunction with the low thermal diffusivity of the host rock, the thermal pulse penetrates only a few meters into the host rock. The water mobilized during this time period has a small effect on the peak waste form temperature.

While gross water movement within the host rock fracture network is not represented, the thermal transport constants used in the evaluations are implicitly included. For instance, even though rock strata specific heats are represented as constant values for temperatures below boiling (CRWMS M&O 2000v, Item 1), they are higher than any of the constituents, and hence, include the effect of local water phase change. Near the boiling temperature in the host rock, the specific heat is adjusted upward to account for the latent heat of vaporization of water in the host rock [refer to Figure 2 (a)]. The thermal conductivity is also reduced at rock temperatures above boiling to represent the loss of aqueous water [refer to Figure 2 (b)].

This assumption is used in Sections 6.3.2.2 and 6.3.2.3.

Figure 2. Adjustments to Host Rock Thermal Transport Properties

5.3.1.3 Treatment of Waste Package Internals

The waste form, basket, and basket support structure within the waste package are represented in repository-scale calculations as a homogeneous, smeared-property, heat-generating cylinder. The length of the cylinder corresponds to the inside length of the inner shell, and the diameter of the cylinder corresponds to the inner diameter of the inner shell. The rationale for this assumption is that the internal temperatures are not of immediate interest in repository-scale calculations, provided that the thermal transport properties for the internals are correct in an average sense. This assumption is used in Sections 6.3.2.2 and 6.3.2.3.

5.3.1.4 Fixed Temperature at the Surface of the Mountain

The boundary condition at the top of both two- and three-dimensional repository representations is a fixed temperature, the value of which will be taken from the Technical Data Management System. The rationale for this assumption is that while climatic changes affect the temperature distribution a few meters into the mountain, the rock acts as a thermal capacitor, and the annual averaged surface temperature is adequate for determining temperatures at the repository horizon. This assumption is used in Sections 6.3.2.2 and 6.3.2.3.

5.3.1.5 Initial Temperature Gradient in the Mountain

The initial thermal gradient in the host rock is assumed to be that listed in Table 6. The last row of the table is modified to reflect the assumption that the last gradient reported in the reference extends to the lower bound of the ANSYS representation (a depth of 1300 m, corresponding to the water table depth). The rationale for this assumption is that this gradient is based on a representation gradient profile obtained from the USW G-4 bore hole and is typical for Yucca Mountain (Sass et al. 1988). Also, the temperature gradient below 541 m depth is not known, and is therefore conservatively assumed as stated above. Also the temperature gradient below 541-m depth is not known, and is therefore assumed as stated above. Choosing the lower boundary with a depth of 1300 m, which is far enough from the heat source and the areas of concern, will not significantly affect the repository temperature calculation. This assumption is used in Sections 6.3.2.2 and 6.3.2.3.

Table 6. Initial Temperature Gradient in Host Rock

Depth Range (m)	Gradient (°C/m)
0-150	0.020 ^a
150-400	0.018 ^b
400-1300	0.030 ^b

^a value obtained from interpretation of Figure 1-12 of Sass et al. 1988.

^b value obtained from Table 6 of DTN: MO0007RIB00077.000 which is based on interpretation of Figure 1-12 of Sass et al. 1988.

5.3.1.6 Modes of Heat Transfer within the Drift

Within the drift and the near-field rock, during the repository postclosure period, heat transfer is represented by radiation and conduction only. Convective heat transfer is neglected. The rationale for this assumption is that neglecting convective heat transfer will result in a conservative calculation of waste form peak temperatures. Calculations in a drift above borehole-emplaced waste packages have shown that radiative heat transfer is an order of magnitude greater than the convective heat transfer (Gartling et al. 1981, p. 59); therefore, radiation is the dominant heat transfer mechanism, and convection may conservatively be neglected. Note that forced-convection effects are calculated for the repository preclosure period, as indicated in Section 5.3.1.7.

In addition, the conductive heat transfer between the waste package and the emplacement pallet, and hence through the pallet into the invert, is omitted. The rationale for this assumption is that the emplacement pallet contacts the waste package in only a few places (an indeterminate number due to the evolving design), and conduction is necessarily limited.

The modes of heat transfer in each portion of the repository-scale, two-dimensional representation of the drift and near-field rock are presented in Figure 3, for designs that include or omit backfill. The extension to the three-dimensional analyses is obvious.

This assumption is used in Sections 6.3.2.2 and 6.3.2.3.

Figure 3. Modes of Heat Transfer In and Near Drift

5.3.1.7 Approximation of Heat-Removal by Ventilation

Forced-convection heat transfer is not explicitly represented in the drift; rather, a reduction in heat generation is used as a proxy for this mode of heat transfer (i.e., the ventilation efficiency). The rationale for this assumption is that, while it may be slightly non-conservative since it reduces the surface temperature of the waste package and diminishes radiative heat transfer, it is a reasonable approximation to determine the amount of thermal energy transferred to the near-field rock during the repository preclosure ventilation period. This assumption is used in Sections 6.3.2.2 and 6.3.2.3.

5.3.2 Assumptions for Waste Package-scale Thermal Analysis

5.3.2.1 Two-dimensional Representation of Waste Package Internals

Two-dimensional representations of the waste form, and waste package basket and shells, are representative for the purpose of defining the peak-fuel cladding temperatures. Inherent to this assumption is that axial heat transfer does not significantly affect the solution. The rationale for this assumption is that the metal thermal conductivities and heat generation rate distributions are such that axial heat transfer is negligible. This characteristic behavior is shown in *The TN-24P PWR Spent-Fuel Storage Cask: Testing and Analyses* (Creer et al. 1987) and *Emplacement Scale Thermal Evaluations of Large and Small WP Designs* (CRWMS M&O 1995). This assumption is used in Section 6.3.2.1.

5.3.2.2 Omission of Convection within the Waste Package

Convective heat transfer through the waste package fill gas (within the basket gaps and all other waste package vacancies) is neglected. Considering only conduction and radiation heat transfer is assumed to provide conservative results for peak fuel cladding temperature. The rationale for this assumption is as follows: some convective heat transfer will occur in the waste package fill gas; however, in a horizontal emplacement configuration, convection is minor compared to thermal radiation (at the expected temperatures), and stable convection cells either do not develop or are difficult to predict. Also, some fill gases, such as helium, have poor buoyancy relative to their thermal conductivity (unlike air, for example), and natural convection has a negligible contribution to total heat transfer. An extensive discussion of natural convection heat transfer is contained in *Introduction to Heat Transfer*, 3rd Edition (Incropera and DeWitt 1996, Section 9.2 through Section 9.8, pp. 448-478). This assumption is used in Section 6.3.2.1.

5.3.3 Assumptions for Fuel Assembly-scale Thermal Analysis

5.3.3.1 Boundary Conditions for Fuel Assembly Calculations

The temperatures applied as boundary conditions for the determination of commercial spent nuclear fuel assembly effective properties are assumed to be uniform around the perimeter of the assembly, such that a quarter-symmetric representation of the assembly is adequate. The rationale for this assumption is that the hottest commercial spent nuclear fuel assemblies are in the center of a waste package where the temperature gradients are lowest. This assumption is used in Section 6.3.2.1.

5.3.3.2 Generation of All Decay Heat in UO_2

Heat generation due to the decay of commercial spent nuclear fuel fission products and actinides is assumed to be evenly distributed throughout all of the UO_2 pellets. Radial power profiles within the pellets and within the assembly are neglected, and heat generation in the cladding (and other non-fuel hardware) due to activation and radiation energy is ignored. The rationale for this assumption is that it is conservative to assume that all of the heat produced by the commercial spent nuclear fuel assembly is produced in the UO_2 pellet and not the cladding. The temperature distribution within the pellet and cladding is discussed in *Determination of PWR SNF Effective Conductivity* (CRWMS M&O 1996d, Attachment II), and it is demonstrated that the highest cladding temperatures result when all the heat is generated in the pellet. This assumption is used in Section 6.3.2.1.

5.3.3.3 Geometry of Commercial Spent Nuclear Fuel Assembly

Components of the commercial spent nuclear fuel assembly (cladding, guide tubes, etc.) are assumed not to touch the basket wall or each other. Some spent fuel rods may have bowed such that they contact each other or the basket (or the channel for BWR fuel). The rationale for this assumption is that it is conservative, since the only heat transfer is through the fill gas by thermal radiation and conduction. This assumption is used in Section 6.3.2.1.

5.3.3.4 Omission of Fuel Irradiation Effects

Fuel irradiation effects are neglected for the purpose of determining material properties in the commercial spent nuclear fuel assembly representations. The irradiation of UO_2 pellets induces several changes in the porosity, composition, and stoichiometry of the fuel. These changes, however, are generally small in light water reactors. Introduction of fission products, burnup, and material cracking under thermal cycling lead to a slight decrease in the thermal conductivity of the fuel; however, these effects are neglected. Also neglected are the effects of fuel densification, swelling, restructuring, and plutonium content; and the oxygen-to-metal ratio of the uranium fuel is assumed to be the theoretical value of two. Zircaloy thermal conductivity is primarily a function of temperature; however, other characteristics, such as residual stress levels, crystal orientation, and minor composition differences (i.e., zircaloy-2 versus zircaloy-4 as cladding material) may have secondary influences on conductivity. These effects, as well as cladding dimensional changes (e.g., creepdown, thermal expansion, elastic deformation, and stress irradiation growth) are neglected. The rationale for these assumptions is that while these neglected effects may affect temperatures within the pellet, they have little or no impact on the cladding temperature, the parameter for which margin must be demonstrated. This assumption is used in Section 6.3.2.1.

5.3.3.5 Omission of Cladding Crud

Appropriate emissivity values for light water fuel cladding without layers of "crud" are assumed. The rationale for using these values is that crud generally increases emissivity values, and crud-free oxide thicknesses provide appropriately conservative cladding temperatures. This assumption is used in Section 6.3.2.1.

5.4 SHIELDING ANALYSIS ASSUMPTIONS

5.4.1 Use of an Axial Peaking Factor

Since the radiation source terms are generated with the assumption that the burnup is uniformly distributed within a spent nuclear fuel assembly, an axial peaking factor is used for neutron and photon source strengths in the active fuel region. The rationale for this assumption is to conservatively account for the maximum values of the actual axial source distributions. The axial peaking factor of a PWR spent nuclear fuel assembly is 1.25. This value is based on the predicted axial decay heat rate profile of a PWR spent nuclear fuel assembly provided in *Testing and Analyses of the TN-24P PWR Spent-Fuel Dry Storage Cask Loaded with Consolidated Fuel* (EPRI 1989, p. 3-26). The axial peaking factor of a BWR spent nuclear fuel assembly is 1.4. This peaking factor has been determined from the axial burnup profile of a BWR spent nuclear fuel assembly at lower burnup values (CRWMS M&O 1999a, p. 47). The rationale for using this value is that an axial peaking factor at a lower burnup conservatively bounds the axial profile of a radiation source generated at higher burnup (as shown in CRWMS M&O 1999a [p. 47]). This assumption is used in Section 6.4.2.

5.4.2 Homogenization of the Radiation Source Region

In a three-dimensional shielding analysis for the waste packages containing commercial spent nuclear fuel, the contents and radiation sources of each spent nuclear fuel assembly region are uniformly homogenized. The rationale for this assumption is based upon a study of the effect of source geometry on the waste package surface dose rates (CRWMS M&O 1999a, pp. 22-26). The results of the study indicate that identical dose rates on the external surfaces of a waste package are obtained for two different source geometry representations: a detailed geometric representation, and a representation in which the contents and radiation sources are homogenized inside region dimensions. This assumption is used in Section 6.4.2.

5.4.3 Homogenization of the DOE Spent Nuclear Fuel Canister

The contents and radiation source of the DOE spent nuclear fuel canisters are homogenized inside the cavity of the DOE spent nuclear fuel canister. However, if the DOE spent nuclear fuel canister contains one intact spent nuclear fuel assembly (e.g., Shippingport Light Water Breeder Reactor spent nuclear fuel), the assembly contents and radiation sources are homogenized inside the assembly dimensions. The rationale for this assumption is that the homogenization process decreases the fuel self-shielding and moves the radiation source closer to the outer surfaces of the waste package, allowing more particles to reach the outer surface and, hence, increasing the dose rate. This assumption is used in Section 6.4.2.

5.4.4 Omission of Waste Package Internals

For the one-dimensional shielding analysis of waste package radial dose rates, the fuel region of the waste package, which consists of the waste form, neutron absorber plates, thermal shunts, and other structural members, is radially homogenized inside the waste package cavity with some internal components omitted. The rationale for this assumption is that it is conservative for calculating dose rates on the surfaces of the waste package, since the structure components that

would otherwise attenuate neutrons and photons are not represented. This assumption is used in Section 6.4.2.

5.4.5 Use of a Watt Fission Spectrum

A Watt fission spectrum (Briesmeister 1997, Appendix H, pp. H-5 and H-6) is used for the neutron source energy distribution of the DOE spent nuclear fuel, since the actual neutron spectra are not available for most of the DOE fuels. The rationale for this assumption is that the dose rate evaluation is not sensitive to the neutron spectrum because the neutron dose rate contribution to the total dose rate outside of the waste package is negligible for the repository preclosure period. This assumption is used in Section 6.4.2.

5.4.6 Fresh Fuel Assumption

The composition of fresh fuel is used to represent the attenuation properties of spent fuel in the shielding calculations. The rationale for this assumption is that, while photon attenuation properties of spent fuel and fresh fuel are similar, fresh fuel has a conservatively higher neutron dose rate, due to greater production of fission neutrons. This is not due to the fission yield for neutrons, but rather to the greater abundance of fissile constituents. The neutron and gamma ray sources in the actinides and fission products are derived from the spent fuel composition, and are represented as fixed sources in the shielding calculations. Therefore, the radiation sources are not affected by this assumption. This assumption is used in Section 6.4.2.

5.4.7 Treatment of Trace Elements

For material compositions having elements with specified ranges (i.e., weight percentages of each constituent), the midpoint value is used and the abundance of the most abundant element is adjusted upward to maintain the material density. The rationale for this assumption is that small weight percentage variations of each element constituent do not affect the accuracy of dose results, as long as the density is maintained. This assumption is used in Section 6.4.2.

5.4.8 High Level Waste Glass Source Terms

The source terms for the design basis glass developed at the Savannah River Site Defense Waste Processing Facility are assumed for all other high level waste glass forms. The rationale for this assumption is that these source terms provide conservative (higher) dose rates for the co-disposal waste packages, since the source terms for the rest of the high level waste glass forms are less intense (CRWMS M&O 2000q, Attachments V and VI). This assumption is used in Section 6.4.2.

5.4.9 Infinite Cylinder Representation of a Waste Package in SAS1 Analyses

For waste package shielding analysis, SAS1 is an effective tool for evaluating the radiation levels on and beyond the radial outer surface of a waste package. SAS1 assumes a waste package to be an infinite cylinder with a homogenized fuel region in the center, enclosed by the two shells. The rationale for this assumption is that, since the length of a waste package is approximately three times the diameter, the infinite cylinder representation of the waste package

has been shown to yield accurate dose results for the radial direction. This assumption is used in Section 6.4.2.

5.5 CRITICALITY ANALYSIS ASSUMPTIONS

5.5.1 Assumptions for Depletion Calculations for Commercial Spent Nuclear Fuel

As introduced in Section 4.1.5.1, there are a number of fuel depletion parameters that can be selected to conservatively represent the criticality potential of commercial spent nuclear fuel. Sensitivity studies in *Sensitivity and Parametric Evaluations of Significant Aspects of Burnup Credit for PWR Spent Fuel Packages* (DeHart 1996) have identified those depletion parameters to which waste package reactivity calculations are most sensitive. Waste package design criticality calculations will use a conservative combination of these depletion parameters in the development of waste package loading curves. Each of these parameters is separately discussed in the following sections.

5.5.1.1 Assembly Burnup and Axial Burnup Distribution

For commercial spent nuclear fuel, burnup is used as the principal measure of the isotopic inventory, and its axial distribution along the fuel can affect its reactivity. To ensure that the axial burnup profiles selected for evaluation appropriately reflect those resulting from reactor operations, a database of actual PWR and BWR fuel depletion histories will be compiled. It is assumed that this database will be suitable for determining bounding axial burnup distributions or assembly average values, suitable for waste package criticality calculations. The rationale for this assumption is that modeling spent nuclear fuel with burnup values lower than their true values will increase their reactivity. This assumption is used in Section 6.5.1.1.

5.5.1.2 Assembly Average Moderator Density and Axial Distribution

During fuel depletion, the moderator density and its axial distribution along the fuel can have a significant effect on the reactivity of spent nuclear fuel. To ensure that the axial moderator density profiles selected for evaluation appropriately reflect those resulting from reactor operations, a database of actual PWR and BWR fuel depletion histories will be compiled. It is assumed that this database will be suitable for determining bounding axial moderator density distributions or assembly average values, suitable for waste package criticality calculations. The rationale for this assumption is that modeling spent nuclear fuel with moderator density values lower than their true values will increase their reactivity by hardening the depletion spectrum and thereby increase the rate of plutonium isotope production. This assumption is used in Section 6.5.1.1.

5.5.1.3 Peak Soluble Boron Concentration

It is assumed that the use of the maximum cycle-averaged boron concentration results in conservative generation of commercial PWR spent nuclear fuel isotopes for criticality calculations. The rationale for this assumption comes from the *Sensitivity and Parametric Evaluations of Significant Aspects of Burnup Credit for PWR Spent Fuel Packages* (DeHart 1996). This report indicates that the maximum cycle-averaged boron concentration

used during the depletion process results in isotope inventories that increase the spent nuclear fuel reactivity for criticality calculations. This assumption is used in Section 6.5.1.1.

5.5.1.4 Presence of Burnable Poison Rods

It is assumed that the PWR fuel assemblies contain burnable poison rods that are fully inserted during the complete depletion time period. The rationale for this assumption is that depletion with burnable poison rods inserted hardens the neutron spectrum and increases the rate of fissile plutonium isotope production. This assumption is used in Section 6.5.1.1.

5.5.1.5 Settled Oxide Depth

It is assumed that a 58 volume percent (vol%) settled iron oxide configuration, with intact fuel assembly arrays, is the most limiting fully degraded basket configuration. The rationale for this assumption is that *Criticality Evaluation of Degraded Internal Configurations for the PWR AUCF WP Design* (CRWMS M&O 1997b, p. 48) evaluated various configurations and identified the 58 vol% settled oxide configuration as the bounding case for the fully degraded basket configuration of the Viability Assessment waste package design. The basket materials of the Viability Assessment design are sufficiently similar to those in the Site Recommendation design for use in establishing this rationale. This assumption is used in Section 6.5.1.1.

5.5.1.6 Composition of Degraded Basket Corrosion Product Mixture

It is assumed that the degraded basket corrosion product mixture is similar to that listed on p. 14 of *Supplemental Criticality Evaluation for Degraded Internal Configurations of a 21 PWR Waste Package* (CRWMS M&O 1998m). The rationale for this assumption is that the basket materials of the current waste package design and those of this reference are sufficiently similar. This assumption is used in Section 6.5.1.1.

5.6 RISK-INFORMED ANALYSIS ASSUMPTIONS

The assumptions used in risk-informed analyses may pertain to the uncertainties inherent to the systems, structures, components, events, or conditions that are being evaluated (i.e., the waste package in its environment) or to the modeling method chosen (for example, assumptions related to the modeling of human reliability). The list of assumptions may vary from one study to another, but the assumptions need to be thoroughly described as a part of each study as they have an impact on the resulting estimated frequencies or probabilities. Because the development of the assumptions is a central part of each analysis, it is difficult to compile a comprehensive list of assumptions that will be applicable to all risk-informed analyses. However, some examples of the assumptions used in the waste package risk-informed analyses have been detailed in the following sections.

5.6.1 Assumptions for Assessing Expected Number of Key Blocks

5.6.1.1 Total Waste Package Exposure Length

The cumulative exposed length (of drip shields or waste packages) is assumed to be 60 km. The rationale for this assumption is that it conservatively bounds the 56.222-km estimate of required

drift length for the Site Recommendation inventory (BSC 2001f, Section 6.3.1) and the estimated 59.187 km required for the design-basis inventory (BSC 2001f, Table 29). This assumption is used in Section 6.6.4.

5.6.1.2 Emplacement Drift Orientation

It is assumed that the rock-size distributions that have been estimated for emplacement drifts oriented at 75° azimuth (CRWMS M&O 2000d, p. IX-3) are representative of the planned 72° orientation (or its equivalent, $72^\circ + 180^\circ = 252^\circ$) (BSC 2001f, Section 6.2.2.2). The rationale for this assumption is that the angular difference between the two orientations is small and should only negligibly affect the results. This assumption is used in Section 6.6.4.

5.6.1.3 Density of Repository Rock

The bulk density of the rock in the repository horizon is assumed to be 2.41 MT/m³ for all rock zones under consideration. The saturated bulk density of the Topopah Spring Tuff crystal poor lower nonlithophysal (Tptpln) rock zone has been measured as 2.41 MT/m³; the stated value is the mean of a set of measurements with maximum value of 2.44 MT/m³ and a minimum of 2.34 MT/m³ (DTN: MO9808RIB00041.000, Table 5). For the Topopah Spring Tuff crystal poor middle nonlithophysal (Tptpmn) zone and the Topopah Spring Tuff crystal poor lower lithophysal (Tptpll) zone, the mean measured saturated bulk density is 2.36 MT/m³ for each zone (DTN: MO9808RIB00041.000, Table 5). The rationale for this assumption is that (1) it is convenient for computational purposes to assume a uniform density, (2) it is conservative to use an estimate of saturated (rather than dry) bulk density, (3) it is conservative to use the highest estimated saturated bulk density for the three rock zones under consideration, (4) masses calculated on the basis of the assumed density are linearly proportional to the density and, therefore, are insensitive to a small uncertainty in the density, and (5) this density was used as the density for the key-block simulations that form the basis of this calculation. This assumption is used in Section 6.6.4.

5.6.2 Assumptions for Assessing Waste Package Design Basis Events

5.6.2.1 Repository Preclosure Period

The preclosure period (from beginning of repository operations to permanent closure) is assumed to be 100 y. The rationale for this assumption is as follows. This assumption is based on the performance requirement in the *Yucca Mountain Site Characterization Project Requirements Document* for keeping the repository open for at least 100 y (YMP 2001, Requirement Citation 1.3.2.H). A preclosure operational period of 100 y is conservative because the MGR waste handling and emplacement activities are expected to take less than 40 y. For evaluating events that could occur after emplacement and retrieval are complete (such as rock fall, earthquakes, and early waste package failure), the preclosure period of the applicable preclosure scenario will be assumed (e.g., 325 y). This assumption is used in Section 6.6.4.

5.6.2.2 Maximum Annual Waste Package Emplacement

The maximum number of waste packages emplaced annually is assumed to be 632. The rationale for this assumption is that it reflects the maximum annual waste-transportation cask arrival rate. According to Curry 2001 (Tables 5-1 through 5-4, pp. 5-4 – 5-7), the maximum number of transportation casks arriving in any given year is estimated to occur between 2014 and 2022. The annual waste package emplacement rate corresponding to this transportation cask arrival rate is estimated to be 602. This value has been conservatively increased by five percent. This assumption is used in Section 6.6.4.

5.6.2.3 Emplaced Waste Package Spacing

It is assumed that the waste packages are spaced closely enough in the emplacement drifts that a rock heavier than 6 MT falling in a fully loaded drift would unavoidably strike a waste package. The rationale for this assumption is that the EDA II (Enhanced Design Alternative II) concept indicates that waste packages could have a minimum spacing of 10 cm (BSC 2001b, Criterion 1.2.4.7). At this distance, the ratio of the waste package spacing and the length of a waste package is very small. This assumption is used in Section 6.6.4.

5.6.2.4 Support of Key Blocks

It is assumed that every key block of 6 MT or more in the repository will be supported by at least one steel set and at least one rock bolt during the preclosure period. It is also assumed that the support provided is redundant, in the sense that one of the support units could fail and the rest of the support units would be capable of supporting the block. It is also assumed that the support is independent, in the sense that the failure of one unit will not cause failure of the other units. The rationale for this assumption is as follows:

The ground-control design calls for circular steel sets spaced 1.5 m apart (BSC 2001c, Section 4.1.8) and welded wire fabric throughout the entire length of the emplacement drifts (CRWMS M&O 1999e, p. 5-13). In rock units where large key blocks are likely, that is, the non-lithophysal units Tptpln and Tptpmn, the steel sets will be augmented by fully grouted rock bolts on the upper surfaces of the drifts (BSC 2001c, Section 6.5.2.2). Six rock bolts will be anchored in the centers of the spaces between pairs of steel sets, giving an axial spacing of 1.5 m; the radial spacing will be 1.44 m (BSC 2001c, Figure 6-2). Spot bolts may be applied when evidence of a large key block is observed.

A rock of sufficient size will be supported by more than one support unit, as, for example, the very large blocks greater than 15 MT: the very large key blocks emerging from the key-block simulations tend to be very long along the drift axis, for example, from 14 m for a 15-MT block to 40 m for a 52-MT block (CRWMS M&O 2000d, Table IX-2, p. IX-3). Such blocks are subject to multiple redundant support that easily satisfies the assumption. The smaller rocks would less clearly be redundantly supported, hence the need for this assumption. To get an idea of the maximum size of a singly supported rock, consider the largest hemispherical rock that could be supported by only one ground control unit. A hemisphere centered on a steel set, with its edges just touching four rock bolts, would have a radius of:

$$r = \sqrt{\left(\frac{1.44}{2}\right)^2 + \left(\frac{1.5}{2}\right)^2}$$

$$= 1.04 \text{ m},$$

where the radius is calculated as the hypotenuse of a right triangle whose other sides are half the distance between steel sets and half the distance between rock bolts. The corresponding volume is $2\pi r^3/3 = 2.4 \text{ m}^3$, and the mass is $2.4 \text{ m}^3 \times 2.41 \text{ MT/m}^3 = 5.8 \text{ MT}$. A slight shift in any direction would lead to support by more than one type of ground support. Considering that key blocks are formed by a small number of fracture planes intersecting each other and the surface of the drift, a hemispherical shape is not realistic. Key blocks emerging from the simulations of the key-block analysis tend to be shallow irregular tetrahedrons (except that the drift face is curved). Even the smaller blocks tend to be long enough along the axis of the drift to span two or more steel sets and tend to have large drift-face areas (CRWMS M&O 2000d, Attachment II, files 1mt.weg through 8mt.weg) compared to the roughly $1.44 \times 1.5 = 2 \text{ m}^2$ that is available between supports. For example, a typical block of 5.4 MT has a length projected onto the axis of the drift of 5.4 m and a drift-face area of 8.2 m^2 (CRWMS M&O 2000d, Attachment II, file 5mt.weg). Such a block would span 3 or 4 steel sets and the rock bolts between them. Therefore, even key blocks as small as 6 MT would almost certainly be supported by multiple ground-control units. For the smaller blocks (6 to 15 MT), the question of the ability of individual ground-control units to withstand the required loads may arise. Of the two types of ground control, only the strength of the rock bolts is likely to be questioned in this context. The rock bolts have an allowable axial load of 16 MT and a yield strength of 27 MT. Therefore, considering the smaller key blocks, for which the degree of redundancy in support may be a concern, a single well placed rock bolt is strong enough to support a block alone.

It is assumed that, during the preclosure period, the ground control in the emplacement drifts will be inspected at an interval of at most three years and that all failures will be detected and repaired if necessary. The rationale for this assumption is that operational plans have not yet been developed, and a three year interval is conservative compared to a prescription for monthly inspection before emplacement and annual inspection after emplacement (CRWMS M&O 1997a, p. 102). Operational plans yet to be developed may propose annual inspections by remote-inspection gantry (CRWMS M&O 1997e, Section 7.6.5) during the early years, with the expectation that the inspection schedule would be relaxed if annual inspections indicate few problems. Presumably, a decision to increase the inspection interval would be made with due consideration of the risks involved in light of accumulated experience with ground-control reliability. This assumption is used in Section 6.6.4.

5.6.2.5 Ground Control Annual Failure Rate

A constant annual failure rate of 10^{-4} y^{-1} (CRWMS M&O 1999o, p. 37) is assumed for the steel sets and for fully grouted rock bolts that have been proposed for ground control in the emplacement drifts. The assumed failure rate applies separately to the failure of a single steel set alone and to the failure of a rock bolt alone. Although, as it pertains to rock bolts, the estimated failure rate was derived for rock-bolt channels, and not individual rock bolts, it is applied here to individual rock bolts because channels may not be installed. If individual rock bolts had been considered in the derivation of the failure rate, there would have been several times more

ground-control unit-years and a correspondingly lower failure rate. Therefore, applying the assumed rate to single rock bolts is conservative. The rationale for the assumed failure rate is that it is a conservative assumption made in the absence of precise information about random failure of the proposed ground control units. The rationale for assuming a constant failure rate is that very little is known about the reliability over time, and there is no justification for assuming a particular time dependence. A mechanism for the accelerated corrosion of rock bolts due to the decomposition of the grouting material can be conceived. However, it is expected that the grout material chosen will be long lived in the emplacement drift environment during the preclosure period (BSC 2001d, Section 7.3). This assumption is used in Section 6.6.4.

5.6.2.6 Access Mains and Ramps Ground Control Reliability

It is assumed that the ground control in the access mains and ramps is at least as reliable as the assumed reliability of the ground control in the emplacement drifts. The rationale for this assumption is as follows. The access mains and ramps will be subject to personnel access throughout the preclosure period. Therefore, the designers of the ground control system will regard preventing personnel injury due to rock fall in the access mains and ramps as a very important objective. Furthermore, the reliability of the ground control depends on the frequency of inspections. With personnel access, such inspections could easily be done more frequently than has been assumed for the emplacement drifts, where inspections will have to be conducted remotely if waste packages are present. This assumption is used in Section 6.6.4.

5.6.2.7 Collapse of Surface Structures and Emplacement Drifts During Earthquakes

It is assumed that the structures whose collapse could lead to a waste package failure, such as surface structures and ground control for the emplacement drifts, will be designed to withstand the fault displacement and vibratory ground motion corresponding to a Frequency Category 2 earthquake. The rationale for this assumption is that the waste package is required to be designed to withstand a Frequency Category 2 earthquake, taking credit as appropriate for systems that alter or mitigate the effects of the earthquake (e.g., BSC 2001i, Criterion 1.2.2.1.7). Failure of ground control in the emplacement drifts, and possibly the failure of other structures, could alter the effects of an earthquake and lead to waste package failure. The cited criterion requires the design of the waste package and other structures to prevent waste package failure in the event of a Frequency Category 2 earthquake. This assumption is used in Section 6.6.4.

5.6.2.8 Fault Displacement

For evaluating the direct effects of fault displacement on waste packages, it is assumed that any fault that intersects an emplacement drift will have a Frequency Category 2 seismic displacement of 32 cm or less, which is a recent value given for the Solitario Canyon Fault (USGS 1998, p. ES-12). The rationale for this assumption is the fact that the Solitario Canyon Fault is near the proposed repository (although it will not penetrate any of the underground development) and it is conservative because the other faults near the repository are of much smaller expected displacement. This assumption is used in Section 6.6.4.

5.6.2.9 Maximum Transporter Operating Speed

The transporter is assumed to travel at a maximum operating speed of 8 km/h in the main drifts and 3 km/h (50 m/min) on the surface and in the emplacement drifts. The rationale for this assumption is that it is based on information given by BSC 2001j (Criterion 1.2.2.1.2) and CRWMS M&O 1998d (p. I-34), respectively. This assumption is used in Section 6.6.4.

5.6.2.10 Transporter Derailment Frequency

For the evaluation of transporter derailment frequency, it is assumed that the use of commercial railroad and mining statistics is conservative. The rationale for this assumption is that the use of this data overestimates the probability of derailment because commercial railroad and mining operations are subject to many environmental and operational conditions that will not be present in a highly regulated, nuclear waste repository. This assumption is used in Section 6.6.4.

5.6.3 Assumptions for Assessing the Probability of Occurrence of Waste Package Defects

5.6.3.1 Occurrence Frequency of Weld Flaws

Information on the frequency of occurrence of weld flaws, their location, and their depth (i.e., through-wall extent) distribution was obtained from results of an expert-system-based simulation code, RR-PRODIGAL, developed by the Pacific Northwest National Laboratory and Rolls Royce and Associates. In work sponsored by the NRC, a matrix of cases was run to investigate the effects of weld thickness, material, welding method, and post-weld inspections on flaw density and depth distribution of typical pipe welds of the nuclear industry. It is assumed that the results, gathered by Khaleel et al. 1999, are bounding for predicting the features of the flaws in the welds. The rationale for this assumption is as follows. The results of the weld simulations were used in the pilot application of risk-informed methods for the Surry Power Station (Khaleel et al. 1999, p. 128). Moreover, comparisons of flaw frequencies predicted by RR-PRODIGAL with observed flaws found in actual piping and vessel welds have been performed in an effort to benchmark the code. The results provided by RR-PRODIGAL were found to be consistent with measured flaw data, or conservative by a factor as large as ten (Simonen and Chapman 1999, p. 105). This assumption is used Section 6.6.5.

5.6.3.2 Weld Flaw Repairs

It is assumed that all flaws detected by post-weld inspections are repaired sufficiently to meet any postclosure performance criteria. The rationale for this assumption is that the flaw rejection criteria for waste package welds will likely be based on the minimum flaw size having postclosure performance concerns. This assumption is used in Section 6.6.5.

5.6.3.3 Multi-Pass, Ultrasonic Examination Credit

It is assumed that the credit for multi-ultrasonic inspections (i.e., ultrasonic inspections using several angles of examination) can be taken by evaluating the square of the ultrasonic probability of non-detection obtained from Bush 1983 (pp. 13A.5.6 through 13A.5.9). The rationale for this assumption is that the ultrasonic probability of non-detection applies to a single-angle examination, which does not detect as many defects as a multi-angle examination would. Taking

the square of the ultrasonic probability of non-detection is the same as considering that two independent examinations are performed. This is reasonable when considering that CRWMS M&O 1998n (p. 12) accounts for four different angles to examine the closure welds, which makes it possible to detect flaws that a single-angle ultrasonic inspection would not be able to detect. This assumption is used Section 6.6.5.

5.6.3.4 Weld Defect Configuration

The possible defects present in the welds are either rounded defects that have no direction (such as tungsten inclusion, silicon, porosity), or planar defects (such as lack-of-fusion defects, which occur because of missed sidewall or lack of penetration in the sidewall, and are, by definition, in the direction of the weld bead). It is assumed that 1% of the defects are planar and in a direction normal to the direction of the weld center line, that is, in the case of the lid welds, radially oriented. The rationale for this assumption is that it is supported by a publication of Shcherbinskii and Myakishev 1970, that describes a statistical treatment of weld flaw orientations based on analysis of ultrasonic examination flaw-orientation measurements. It appears that planar-type weld flaws detected ultrasonically tend to be predominately oriented in the direction of the weld centerline. The distribution of the orientation angle is approximated by a centered normal distribution with a maximum standard deviation of 5 degrees. Consulting a table of the cumulative normal distribution indicates that 99% of the flaws are located within about ± 13 degrees. Thus, assuming a proportion of 1% of radially oriented defects in the lid welds (for which the angle would be near ± 90 degrees) is acceptable. This assumption is also supported by experimental results obtained from ultrasonic testing-inspected lid welds related to a 4-inch thick carbon steel cylinder mock-up prepared for the Yucca Mountain Project (CRWMS M&O 1998n). The inspections carried out revealed thirteen flaws on the bottom lid weld, and three on the top lid weld: the orientation of all these flaws was planar with respect to welding direction, (CRWMS M&O 1998n, p. 14). These results are consistent with the assumption. This assumption is used in Section 6.6.5.

6. WASTE PACKAGE DESIGN METHODOLOGY

This section describes the analytical methodology and computational tools used in each of the disciplines within the Waste Package Design Section. For each discipline, reference is made to specific computational tools and their current qualified versions, to demonstrate that qualified computer codes embodying these methodologies exist. However, this should not be construed to limit subsequent analyses and calculations to only these versions. New versions of these computer codes can and will be qualified for future analyses and calculations.

This section contains no discussion of alternate methods, as there are no alternate methods that are considered applicable. This analysis does not provide estimates of any of the factors for the Postclosure Safety Case or Potentially Disruptive Events, and is therefore assigned Level 3 importance.

6.1 SOURCE TERM DETERMINATION

The following describes the generation of source terms for the commercial spent nuclear fuel, DOE spent nuclear fuel, and high level waste. The method for calculating DOE spent nuclear fuel and high level waste source terms differs from that for the commercial spent nuclear fuel, as the information available for these waste streams is significantly different from that for commercial spent nuclear fuel. For a commercial spent nuclear fuel assembly with any given enrichment, burnup, and cooling time, a burnup calculation can be performed that reasonably simulates the irradiation history of the assembly in the reactor core and the subsequent decay after it is removed from the reactor. For the DOE spent nuclear fuel and the high level waste, the chemical composition (in the case of the high level waste) and the estimated radionuclide inventory at a certain year are provided. The source terms for these waste forms can be computed by simply decaying the radionuclides to the desired times. The methodology and computational tools used to generate the source terms are presented in more detail in the following sections.

For the naval spent nuclear fuel canister, the thermal output and photon and neutron surface currents are provided by the U.S. Department of the Navy (Naples 1999).

6.1.1 Computational Tools

Oak Ridge National Laboratory developed the SCALE code system for the NRC to satisfy the need for standardized analysis methods for licensing evaluations of nuclear fuel facilities and package designs. The SCALE system is a collection of well-established functional modules (computer codes) that can be used individually or in combination to perform criticality, shielding, and heat transfer analyses. The system has many control modules, each of which combines several functional modules into analysis sequences to perform a specific analysis. The SAS2H control module and the ORIGEN-S functional module in the SCALE system are the primary computational tools for source term generation.

6.1.1.1 Description of SAS2H for Commercial Spent Nuclear Fuel Source Term Generation

In depletion analyses, the fuel isotopics change with time and are significantly different between fuel cycles. Hence, the fuel isotopics and their macroscopic cross sections must be updated to reflect these changes. For each time-dependent fuel composition, SAS2H performs one-dimensional neutron transport analyses of the fuel assembly using a two-part procedure with two separate lattice-cell representations. The first representation (Path A) is a unit fuel-pin cell from which cell-weighted cross sections are obtained. The cell-weighted cross sections from this calculation are used in a second representation of a larger unit-cell (Path B) that represents the entire assembly within an infinite lattice. The zones in Path B can be structured for different types of BWR or PWR assemblies containing water rods, burnable poison rods, gadolinium fuel rods, etc. The fuel neutron flux spectrum obtained from Path B is used to update the nuclide cross sections for the specified burnup-dependent fuel composition. The updated cross sections are then used in a point-depletion computation to produce the burnup-dependent fuel composition to be used in the next spectrum calculation. This sequence is repeated over the entire irradiated history of the assembly. An example of these representations for a BWR assembly is presented in Figure 4.

The functional modules executed by SAS2H to carry out the depletion analysis are BONAMI-S, NITAWL-II, XSDRNPM-S, COUPLE, and ORIGEN-S. BONAMI-S and NITAWL-II perform resonance self-shielding analyses of the cross sections in each irradiation cycle. XSDRNPM-S performs the one-dimensional neutron transport analyses in Path A and Path B. COUPLE updates the cross-section constants of all nuclides in the ORIGEN-S nuclear information library with the cell-weighted information and the weighting spectrum from XSDRNPM-S. ORIGEN-S calculates the fuel depletion in all cycles and the decay of nuclides at the completion of fuel irradiation. A more detailed description of ORIGEN-S is provided in the next section. The computational flow diagram in SAS2H for commercial spent nuclear fuel source term generation is presented in Figure 5.

Figure 4. SCALE Representation of the Fuel Pin Cell and Assembly for SAS2H Calculations

Figure 5. Calculational Flow for Source Term Generation

The source terms for the DOE spent nuclear fuel and the high level waste are not calculated with the SAS2H control module, because the radionuclide inventories are given for these fuels. The inventories are entered directly into ORIGEN-S to be decayed to the desired times. This is similar to the final ORIGEN-S case for the commercial spent nuclear fuel. In the case of high level waste, the radionuclide inventory is mixed with the glass chemical composition and then decayed.

6.1.1.2 Description of ORIGEN-S

ORIGEN-S is the main functional module of SAS2H (the control module of the SCALE code system) that carries out the depletion and decay calculations. It can also be used as a stand-alone program. ORIGEN-S computes time-dependent concentrations and source terms of a large number of isotopes, which are simultaneously generated or depleted through neutronic transmutation, fission, radioactive decay, input feed rates, and physical or chemical removal rates.

ORIGEN-S can use three kinds of cross-section libraries. card image libraries with nuclear and photon yield information, binary libraries with nuclear transition and photon yield information, and the Master Photon Data Base containing detailed photon energy and intensity data. The second of these, the binary library, contains the same type of information that the card-image libraries do, but for only one kind of problem. This represents a major advantage over the card image libraries in that these cross sections can be replaced with those determined from the detailed neutronics calculations performed by the functional modules that precede ORIGEN-S in

the SAS2H module. This means that rather than using a previously defined cross-section set, the code can be used in conjunction with the cross-section processing codes of SCALE that create problem-specific libraries. This capability has led to the NRC preference for ORIGEN-S. The following is an excerpt from NUREG-1536 (NRC 1997):

“Generally, the applicant will determine the source terms using ORIGEN-S (e.g., as a SAS2 sequence of SCALE), ORIGEN2, or the DOE Characteristics Data Base. Although the latter two are easy to use, both have energy group structure limitations. If the applicant has used ORIGEN2, verify that the chosen cross-section library is appropriate for the fuel being considered. Many libraries are not appropriate for a burnup that exceeds 33,000 MWd/MtU.”

This statement derives from the fact that previous compilations of source term values used ORIGEN2 and relied on previously calculated cross-section libraries of limited information, which can easily be used outside the applicable range. These libraries are only appropriate for fuels that have undergone certain irradiation histories, and are not as accurate as the problem-specific libraries generated for ORIGEN-S.

6.1.2 Description of Pertinent Analyses

6.1.2.1 Commercial Waste Forms

The thermal output, radionuclide inventories, and radiation spectra for commercial spent nuclear fuel are developed according to the source term methodology in this document. Radiation source terms for commercial spent nuclear fuel have been created for both PWR and BWR fuel designs. These are documented in:

- *PWR Source Term Generation and Evaluation* (CRWMS M&O 1999g)
- *BWR Source Term Generation and Evaluation* (CRWMS M&O 1999a).

The commercial spent nuclear fuel source terms calculated with the representative PWR and BWR assemblies can be interpolated to provide reasonably close approximations for all assemblies in the waste stream. It is assumed that these interpolated source terms are comparable to those that would have been obtained from a detailed calculation for each assembly. The waste stream source terms are documented in the following: *Waste Packages and Source Terms for the Commercial 1999 Design Basis Waste Streams* (CRWMS M&O 2000aa).

6.1.2.2 DOE Spent Nuclear Fuel

The total initial radionuclide inventory provided by Idaho National Engineering and Environmental Laboratory (INEEL 1999) has been used to calculate the total radionuclide inventory and the source terms for the average DOE spent nuclear fuel canisters for the time period out to one million years. The ORIGEN-S program is used to perform the decay calculations. The following two documents provide the results of the calculations:

- *Radionuclide Inventories for DOE SNF Waste Stream and Uranium/Thorium Carbide Fuels* (CRWMS M&O 2000k)

- *Source Terms for Average DOE SNF Canisters* (CRWMS M&O 2000p).

6.1.2.3 Defense High-Level Waste

According to the *Waste Acceptance System Requirements Document* (DOE 1999f, p. 19), the producers of high level waste are required to report the estimated total and individual canister inventory, and the associated uncertainties, of radionuclides (in curies) that have half-lives longer than 10 years and that are, or will be, present in concentrations greater than 0.05 percent of the total radioactive inventory indexed to the years 2010 and 3110. The time-dependent photon and neutron sources, decay heat sources, and radionuclide contents and activities of the high level waste forms are generated in ORIGEN-S decay calculations using the initial radionuclide inventories and chemical compositions of the high level waste forms provided by the producers. These calculations are documented in the following references:

- *Waste Acceptance System Requirements Document* (DOE 1999f)
- *Source Terms for HLW Glass Canisters* (CRWMS M&O 2000q).

6.2 STRUCTURAL DESIGN

6.2.1 Computational Tools

6.2.1.1 ANSYS

ANSYS is a finite-element software package that can be used to solve a variety of problems. The versions of ANSYS used at the time of this writing are Version 5.4 (CRWMS M&O 1998g) and Version 5.6.2 (CRWMS M&O 2000l). Waste packages, drip shields, and pallets can be represented as two-dimensional or three-dimensional finite-element geometries, depending on the symmetry of the design or the loading. ANSYS is widely used for structural evaluations for both static and dynamic problems. Materials can be represented with elastic or elastic-plastic temperature-dependent properties. Dynamic evaluations can be performed, such as real-time events with gravitational acceleration acting on component masses. Interfaces between components are represented with contact elements that incorporate interface stiffness and friction. Seismic evaluations can be performed as frequency domain analyses using a response spectrum, or can be solved as time-domain analyses using time histories (acceleration, velocity, or displacement). Thermal expansion and stress can be calculated by combining thermal and structural representations into a single analysis.

6.2.1.2 LS-DYNA

LS-DYNA is a finite element program for nonlinear dynamic analysis of structures in three dimensions. Livermore Software Technology Corporation is the development source for the LS-DYNA finite element analysis software program. The validated versions of LS-DYNA used at the time of this writing are Version 950.c (CRWMS M&O 2000m) and Version 950.d which was qualified as part of the ANSYS Version 5.6.2 software package (CRWMS M&O 2000l). LS-DYNA is capable of simulating complex real world problems, and is widely accepted as the premier analysis software package for a vast number of engineering applications. LS-DYNA analysis capabilities include, but are not limited to, nonlinear dynamics, rigid multi-body

dynamics, quasi-static simulations, thermal analysis, fluid analysis, fluid-structure interactions, and finite element method-rigid multi-body dynamics coupling. LS-DYNA is well suited for performing dynamic impact analyses of the waste packages, drip shields, and emplacement pallets.

6.2.1.3 Mathcad

Mathcad can solve systems of equations, allowing the user to evaluate the impact of parameter variance quickly.

6.2.2 Description of Pertinent Analyses

Structural calculations demonstrate that the waste packages, drip shield, and emplacement pallet meet the requirements for both normal operations and design basis events. These fall into the following broad groups:

- Normal Operations
- Internal Pressurization
- Impacts on Waste Package or Drip Shield
- Dynamic Impacts on the Waste Package
- Seismic Evaluations
- Residual Stress Reduction.

6.2.2.1 Geometric Design Calculations

Geometric design calculations are primarily sizing calculations to verify that each waste package is designed to accept the waste forms with the dimensions given in the system description documents. Additionally, external features and features that interface with the Surface Facilities Project and the Subsurface Facilities Project are discussed and demonstrated to show compliance with the proper criteria. These calculations are written as sections of the analysis of the appropriate waste package design, rather than as stand-alone calculations.

6.2.2.2 Normal Operations Calculations

Normal operating loads are those associated with expected normal operations, such as loading, maneuvering, and emplacing the waste packages.

Vertical and Horizontal Lifting by Trunnion Ring— Lifting calculations will be performed as three-dimensional, static finite-element analyses for each waste package design, using ANSYS. The geometry of the internal structure of the waste packages will be simplified, and symmetries will be taken into account within the representation of the waste packages. Nevertheless, the features of the problem relevant to the structural calculations (overall dimensions, masses, and mechanical properties of the materials) will be preserved.

In the horizontal lifting calculations, the trunnion ring will be taken into account by applying appropriate boundary conditions to the waste package. As for the vertical lifting calculations, a potential/proposed design of the trunnion ring will be included in the finite element representation.

Lifting by Emplacement Pallet—A lifting calculation is performed for the heaviest waste package design loaded on an emplacement pallet. This calculation is performed as a quarter-symmetric, three-dimensional, static finite-element analysis using ANSYS. This representation includes the internal structure of the waste package as a cylinder of uniform mass density. The overall mass and dimensions of the waste package define this density, and it is appropriately modified to take into account its symmetry within the representation. This approach preserves all features of the problem relevant to the structural calculation.

Static Loading of Waste Package on Emplacement Pallet—The stresses in the emplacement pallet and the outer shell of the heaviest waste package, due to the static loading of the waste package on the pallet, are assessed using a quarter-symmetric, three-dimensional, static, finite-element analysis in ANSYS. The representation is further simplified by replacing the internal structure of the waste package by an equivalent set of forces acting along the line of contact between the inner shell and basket in the direction of the gravitational acceleration. This approach preserves all features of the problem relevant to the structural calculation. The geometry of the skirt is simplified in such a way that the total mass of the outer shell is distributed within the cylindrical shell of constant wall thickness. Since the values of the inner and outer shell diameters, essential for the calculation results, must be kept intact, the skirt length is increased to accommodate the outer shell mass.

Static Load of Collapsed Drift on Drip Shield—The stress and buckling within the drip shield, due to static load of the rock from the collapsed drift, is evaluated using a quarter-symmetric, three-dimensional, static, finite-element ANSYS analysis. The drip shield connector plates, connector plate guides, and lifting plates are not included in this representation. This slightly conservative approach has a negligible effect on calculated results. The overburden pressure, which takes into account the masses of the loose rock, is applied statically on appropriate structural members.

6.2.2.3 Internal Pressurization Calculations

The pressurization of the waste package is assumed to occur due to the rupture of all fuel rod cladding or other primary barriers contained in the waste package, provided the waste form retains an intact pressure boundary before being loaded into the disposal container. The calculation uses a closed-form solution to the problem of a cylindrical shell subject to internal pressure load to determine the maximum stresses in the waste package shells. In this evaluation, the inner lid is assumed to fail before the outer lid; however, no structural credit is assumed for the outer lid. Evaluations are performed over uniform waste package temperatures ranging from 20°C to 600°C. The peak stresses (membrane and bending) at the junction of the shell and lid from these evaluations are obtained and shown to be less than the ultimate tensile stress.

6.2.2.4 Impacts on Waste Package or Drip Shield

Rock Fall on Waste Package—The waste package rock fall is evaluated as a three-dimensional, transient dynamic, elastic-plastic finite-element analysis using LS-DYNA. The interaction of the waste package internals and waste package shells is conservatively assumed to maximize the stress on the shells. A realistic rock geometry is assumed for this evaluation. The rock's shape and dimensions are obtained from the Subsurface Facilities Project, and static material properties

are conservatively used due to the unavailability of dynamic material properties. Further conservatism is included by use of material properties at maximum repository temperatures.

The rock may have an initial velocity due to a seismic event, and then be additionally accelerated due to gravitational forces until it strikes the waste package surface. The simulation is continued throughout the impact until the rock begins to rebound, at which time the induced stresses reach peak values. This approach also provides the results of the rock impact in terms of the residual stresses, since the finite element simulation is continued until the steady state values of stresses are obtained. The resulting residual stresses are subsequently used to assess the susceptibility of the drip shield design to stress corrosion cracking.

Rock Fall on Drip Shield—The fall of rocks onto a drip shield is evaluated as a three-dimensional, transient dynamic, elastic-plastic finite-element analysis using LS-DYNA. A realistic rock geometry is assumed for this evaluation. The rock's shape and dimensions are obtained from the Subsurface Facilities Project and static material properties are conservatively used due to the unavailability of dynamic material properties. Further conservatism is included by use of material properties at maximum repository temperatures.

The relative velocity between the rock and the drip shield includes three different phases prior to impact: initial velocity of the rock toward the drip shield in accordance with the seismic ground motion, the velocity gained by the rock due to gravitational acceleration, and the velocity of the drip shield toward the rock just prior to impact in accordance with the seismic ground motion. The finite element simulation is continued throughout the impact until the rock begins to rebound, at which time the stresses reach peak values and the maximum displacements are obtained. This approach also provides the results of the rock impact in terms of the residual stresses, since the finite element simulation is continued until the steady state values of stresses are obtained. The resulting residual stresses are subsequently used to assess the susceptibility of the drip shield design to stress corrosion cracking.

Equipment Impact on End of Waste Package—The fall of handling equipment onto the end of a waste package will be evaluated as a three-dimensional, transient dynamic, elastic-plastic finite-element analysis using LS-DYNA. Demonstration of the waste package structural margin for this design basis event is not necessary for Site Recommendation, but will be necessary for License Application; therefore, the development of the detailed methodology necessary for performing such calculations will be deferred until after Site Recommendation.

Missile Impact on Waste Package—The calculation for missile impact on a waste package is performed as a dynamic, low-velocity impact analysis using basic strength-of-materials relationships and empirical relationships obtained for the impact of projectiles onto plates. The region of missile impact is represented as a flat plate supported at each end.

6.2.2.5 Dynamic Waste Package Impacts

Vertical Drop—The vertical drop evaluation is performed for a waste package as a three-dimensional, axisymmetric, transient dynamic, elastic-plastic finite-element analysis using LS-DYNA. This representation of the waste package is positioned just above an essentially unyielding surface. The interaction of the waste package internals and waste package shells is

conservatively assumed to maximize the stress on the shells. While both static and kinetic friction have a negligible effect, approximate friction coefficients are used. Static material properties are conservatively used, due to the unavailability of dynamic material properties.

Tip-Over—The tip-over evaluation is performed for a waste package as a three-dimensional, transient dynamic, elastic-plastic finite element analysis using LS-DYNA. A half-symmetric representation of the waste package is oriented with an angle from vertical such that the center of mass is rotated past the pivot point, inducing an overturning moment. The waste package representation is then allowed to rotate and impact an essentially unyielding surface.

Horizontal Drop on Flat Surface—The horizontal drop evaluation is performed for a waste package as a three-dimensional, transient dynamic, elastic-plastic finite element analysis using LS-DYNA. A full representation of the waste package is positioned just above an essentially unyielding surface. The interaction of the waste package internals and waste package shells is conservatively assumed to maximize the stress on the shells. Both static and kinetic friction have a negligible effect. The relationship between stress and strain follows the bilinear stress-strain curve.

Horizontal Drop with Emplacement Pallet—The horizontal drop with emplacement pallet evaluation will be performed as a three-dimensional, transient dynamic, elastic-plastic finite element analysis using LS-DYNA. A half-symmetric representation of the waste package and pallet will be positioned just above an essentially unyielding surface.

Corner Drop – The corner drop evaluation is performed for a waste package as a three-dimensional, transient dynamic, elastic-plastic finite-element analysis using LS-DYNA. A full representation of the waste package is oriented with an angle from vertical such that the center of mass is located directly above the corner of impact. In addition, this representation of the waste package is positioned just above an unyielding surface. The interaction of the waste package internals and waste package shells is conservatively assumed to maximize the stress on the shells. Both static and kinetic friction have a negligible effect. The relationship between stress and strain follows a bilinear stress-strain curve.

Transporter Runaway—The transporter runaway evaluations will be performed as a three-dimensional, transient dynamic, elastic-plastic finite-element analysis using LS-DYNA, in a manner similar to the vertical and horizontal drops. Impact limiters (represented as yielding surfaces) may be required to show compliance with the criteria. Demonstration of waste package structural margin for this design basis event is not necessary for Site Recommendation, but will be necessary for License Application; therefore, the development of the detailed methodology necessary for performing such calculations will be deferred until after Site Recommendation.

6.2.2.6 Seismic Evaluations

Evaluation of Waste Package Movement and Loads on Emplacement Pallet—The movements and stresses of the waste package and pallet due to a seismic event are evaluated using a three-dimensional, transient dynamic, finite element ANSYS representation, with a seismic acceleration time history as input. The details of this aspect of the methodology have not

been established at the time of this writing. LS-DYNA is currently undergoing benchmark testing so that it may be utilized in the performance of these analyses. A detailed discussion of the seismic analysis methodology, including the waste package fragility analysis, will be included in a future revision of this document.

Evaluation of Drip Shield Movement and Loads—The movement, potential separation, and stresses within the interlocked drip shields are evaluated using a three-dimensional, transient dynamic, finite element ANSYS representation, with a seismic time history as input. The details of this aspect of the methodology have not been established at the time of this writing. LS-DYNA is currently undergoing benchmark testing so that it may be utilized in the performance of these analyses. A discussion of the methodology will be included in a future revision of this document.

6.2.2.7 Residual Stress Reduction

The waste package is designed to retain hermeticity for very long periods of time. The chief challenge to maintaining this objective is stress corrosion cracking. Three conditions are simultaneously required to induce stress corrosion cracking: a corrosive environment, a material susceptible to corrosion, and tensile stresses. Removing or reducing the effect of any one of these conditions could eliminate or lessen the potential for stress corrosion cracking. While a non-corrosive environment cannot be assured, Alloy 22 has been chosen as the waste package outer shell material by virtue of its low susceptibility to corrosion, addressing the material requirement. However, residual tensile stresses in the final closure weld of the waste package may make Alloy 22 susceptible to stress corrosion cracking at these weld locations.

Two countermeasures are currently being contemplated for the reduction of residual stresses in the waste package final closure weld. These are to induce compressive stresses in the closure lid weld with laser peening, and to anneal the outer lid weld with induction coil heating. These two processes in conjunction will provide compressive stresses to an adequate depth that would sufficiently reduce the susceptibility of the waste package final closure weld to stress corrosion cracking.

Localized Compressive Stress Creation by Laser Peening—Laser peening is intended to induce compressive stresses in the outer surface of the final closure weld and adjacent material. If this method were used exclusively, it would create compressive stresses to a depth of only a few millimeters from the surface of the lid; however, a residual stress less than 10% of yield strength of the outer barrier material must be maintained for a depth of [TBD-235] to mitigate stress corrosion cracking (BSC 2001a, Criterion 1.2.1.22). The details of this methodology have not been established at the time of this writing. A discussion of the methodology will be included in a future revision of this document.

Weld Annealing by Induction Coil Heating—Induction coil heating is intended to induce compressive stresses at greater depths. This technique involves localized heating of the material by surrounding coils. The material is then quickly cooled to room temperature by quenching. This quick temperature reduction is necessary to ensure that adverse phases do not precipitate out of the alloy. The quenching agent has not yet been decided upon at the time of this report, but is intended to be included in a future revision of this document.

Calculations of the residual stresses produced by induction annealing are performed as transient thermal and thermal-stress evaluations using two-dimensional, axisymmetric, finite-element analysis with ANSYS. Since the closure weld section is the single part of the waste package significantly affected by the heat treatment, and it is far from the bottom end of the waste package, half-symmetry is used in the representation. The outer shell and the lid have position constraints in directions perpendicular to each symmetry plane. The outer shell boundaries, excluding the region of induction heating, are assumed to be initially at room temperature and thermally insulated throughout the simulation. The calculation is performed as a heat-up of the annealed region, followed by rapid quenching of the heated region. Thermal stresses are computed at each step of the process. The results are reported in terms of the residual stress as a function of depth from the surface of the waste package in the region of highest tensile stress.

6.3 THERMAL DESIGN

The purpose of the waste package thermal analyses is to ensure that the waste form temperatures do not exceed levels that are important to maintaining their long-term integrity. For commercial spent nuclear fuel, this involves ensuring that the cladding temperature does not induce rupture, compromising the cladding as a barrier to radionuclide release. For defense high-level waste glass, this involves ensuring that the glass does not reach a transition temperature that would result in an alteration of the glass microstructure, increasing the solubility of the glass and reducing the time required for mobilization of the radionuclides embedded in the glass matrix.

Thermal evaluations may be performed for different levels of detail and accuracy. For survey calculations, two-dimensional calculations are appropriate, while three-dimensional calculations are used for detailed evaluations. The flow of these calculations is presented in Figure 6.

6.3.1 Computational Tools

6.3.1.1 ANSYS

The primary computational tool used to perform thermal analyses is ANSYS. The versions of ANSYS used at the time of this writing are Version 5.4 (CRWMS M&O 1998g) and Version 5.6.2 (CRWMS M&O 2000l). ANSYS solves all three modes of heat transfer: conduction, convection, and radiation. For analyses described here, convection is neglected. This is conservative for problems where high temperatures are limiting. For conduction, the thermal conductivity and specific heats may be both spatially varying and temperature-dependent. For radiation, ANSYS determines an effective thermal conductivity and applies it to Fourier's Law of heat conduction. This effective thermal conductivity is computed from the thermal communication between each element of the surfaces, using gray body diffuse radiation theory. For an enclosed system of finite radiating surfaces, the theory of gray body diffuse radiation heat transfer is appropriate (Siegel and Howell 1992, Equation 7-31, p. 271).

ANSYS allows three types of thermal boundary conditions: temperature, heat flux, and a convection condition. The boundary condition of convection does not imply a detailed convection calculation, but rather a heat flux proportional to the difference between the instantaneous surface temperature and the free-stream temperature (i.e., Newton's Law of Cooling). These boundary conditions are applied at the surfaces of the problem domain.

Figure 6. Thermal Analysis Technique Decision Flowchart

Consistent with finite element analysis, the problem domain is divided into polygons. Within these solids, the thermal transport properties and volumetric heat generation magnitudes (as appropriate) are spatially constant. However, the variation in temperature both within and among the polygons is approximated by one of a number of shape functions. This technique permits larger polygons to be used than would be possible with uniform temperatures within the polygons and a simplistic relationship among the polygons.

6.3.1.2 Mathcad

Mathcad can solve systems of equations, allowing the user to evaluate the impact of parameter variance quickly.

6.3.2 Description of Pertinent Analyses

Thermal analyses supporting the determination of temperature fields within the waste packages, in the drift, and throughout the mountain, utilize a multi-scale representation of the potential repository. In such representations, the detail of each element of the repository is proportionate to the scale of the evaluation. This is illustrated in Figure 7, which presents a three-dimensional pillar representation of the repository.

On the largest scale, this representation approximates the repository as an infinitely repeating series of "pillars," extending from the top of the mountain to a plane well into the saturated zone. The waste packages are represented by effective heat-transfer parameters, but without a detailed representation of the waste package internals or waste form. The time-varying surface temperature for the limiting waste package is obtained from this representation, and it provides the boundary conditions for detailed two-dimensional calculations of the temperature field within the waste package. In the two-dimensional waste package representation, the waste form and disposal container are represented by effective heat-transfer parameters. The 2-D representations correlate average fuel volume temperatures to the peak-cladding temperature for commercial spent nuclear fuel (SNF) waste forms. These effective heat-transfer parameters are determined from even more detailed thermal analyses of individual fuel assemblies and adjacent waste package internals (fuel assembly tubes).

This concept of multi-scale analyses is applied in a number of ways for the thermal evaluation of the waste package. The balance of this section will discuss such applications.

6.3.2.1 Fuel Assembly Effective Thermal Conductivity Correlations

Effective thermal conductivity is used to predict peak cladding temperatures for spent nuclear fuel assemblies. This method, developed in the *Spent Nuclear Fuel Effective Thermal Conductivity Report* (CRWMS M&O 1996g), provides a best estimate of peak cladding temperatures compared to correlations such as "Wooton-Epstein" (Wooton and Epstein 1963), which produces an undetermined degree of conservatism. Such conservatism often leads to over-design. Rather than representing the waste package and every fuel rod in every assembly, this method represents the fuel assemblies as a smeared (distributed) solid volume with uniform volumetric heat generation. The smeared properties represent the combined thermal radiation and conduction heat transfer from the fuel rods to the inner-basket structure.

To determine the appropriate effective thermal conductivities for PWR and BWR commercial spent nuclear fuel assemblies, detailed thermal representations of typical fuel assemblies are developed using a finite-element computer code (refer to Figure 8). Vacuum conditions and fill gases of helium, nitrogen, and argon are evaluated with various rod array sizes (e.g., 8x8 assemblies for BWR commercial spent nuclear fuel or 15x15 assemblies for PWR commercial spent nuclear fuel). For BWR fuel, the evaluation considered the effects of channels between

Figure 7. Multi-scale Thermal Analysis Representation

Figure 8. Finite Element Representation of Fuel Assembly

fuel assemblies, cladding oxidation, locations of guide tubes and water rods, emissivity variation, and inner-basket temperature gradients.

The nominal zirconium-oxide thickness for PWR fuel is 50.8 μm (2 mils), and that for BWR fuel is 101.6 μm (4 mils). These values are typical of fuel that has been exposed in commercial light water reactors. From the *Preliminary Waste Form Characteristics Report, Version 1.0* (Stout and Leider 1994, p. 2.1.3.1-3), 50 μm (~2 mils) is a conservative maximum for PWR commercial spent nuclear fuel with a discharge exposure of about 40 GWd/MtHM (gigawatt-days/metric tons heavy metal). BWR environments induce a significantly thicker cladding oxide layer in the 40 to 50 GWd/MtHM exposure range. The 101.6 μm thickness represents an upper bound based on BWR design experience (CRWMS M&O 1996a; CRWMS M&O 1996b; CRWMS M&O 1996c).

Calculated effective thermal conductivities were found to be highly temperature-dependent due to the contribution of thermal radiation, with little dependence on assembly heat output.

Results from this method were compared to those from previous applications using alternate methods and to actual test results from spent-fuel storage casks (CRWMS M&O 1996g, Sections 7.2 and 7.3). The comparisons to experimental data and test calculations indicate that the effective thermal conductivities provide a best estimate of cladding temperatures within a spent-fuel waste package. Further, the effective thermal conductivities were consistent with single-point values previously published by storage cask vendors (CRWMS M&O 1996g, Section 8.0).

6.3.2.2 Repository-Scale Two-Dimensional Analyses

While detailed repository-scale three-dimensional calculations are necessary to demonstrate margin to the waste form thermal requirements, repository-scale two-dimensional calculations are appropriate to study the sensitivity of the temperature field to changes in the major thermal variables. Such a representation consists of a perpendicular slice through a single waste package, extending from the top of the mountain to well into the saturated zone, and accounting for the thermal transport properties of each stratigraphic unit (refer to Figure 9). Such a representation appropriately calculates the temperature field for a drift located near the center of the potential repository, provided the packages may be approximated as an infinitely-long cylinder with an axially-uniform heat generation rate.

Since such two-dimensional representations have low computational requirements, a large number of such calculations may be performed quickly. This rapidity of computation enables time-dependent temperature field calculations that span the design space (i.e., the range of independent variables). Low-order, multi-variate regressions may then be performed and response surfaces created. The functional form of the response surface selected is based on insight into the heat-transfer physics and the fidelity with which the particular functional form reproduces the calculational results.

This representation is truly applicable only to an infinitely long waste package; however, simple adjustments may be made to approximate three-dimensional effects. The effect of increases in waste package separation is obtained by adjusting the average waste package heat generation rate (and hence the linear power). This functional form is shown in Equation 1.

$$P_{\text{linear}} = \frac{Q_{\text{WP}}}{(\bar{L}_{\text{WP}} + \delta)} \quad (\text{Eq. 1})$$

Here Q_{WP} is the waste package heat generation rate at emplacement, $\bar{L}_{\text{WP}}$ is the average-waste package length, and δ is the skirt-to-skirt gap between waste packages. The appropriateness of this adjustment decreases with increasing waste package spacing, since the localized relatively-high-heat regions of such an arrangement are not accounted for. For the range of waste package spacings currently considered, this adjustment is applicable.

Figure 9. Illustration of Two-dimensional Repository Representation

An operating curve is the locus of values for two independent variables – holding other independent variables constant – which results in a particular temperature value on the response surface. For instance, if the ventilation duration, waste package heat generation rate at emplacement, and backfill effective-thermal conductivity are fixed, a curve may be constructed providing the combinations of skirt-to-skirt separations and ventilation efficiencies necessary to obtain a given peak-drift wall temperature. This process is illustrated in Figure 10.

While these two-dimensional calculations cannot legitimately be used to quantify the effect of non-uniform heat generation rates, the results from just a few previous three-dimensional cases may be used in conjunction with these to estimate the magnitudes of both three-dimensions and non-uniformity. By assuming the nominal heat generation rate for the potential repository, peaking factors may be developed for a range of design basis heat generation rates. For instance, simple linear correlations for incremental temperature increases for non-uniformity may be developed. Such a functional form is shown in Equation 2.

$$\Delta T = a_0 + a_1 \cdot P_{linear} \quad (\text{Eq. 2})$$

Here, a_0 and a_1 are fit coefficients and P_{linear} is that shown in Equation 1.

Such an expression is used to adjust upward the peak waste package-surface temperature and the corresponding peak-cladding temperature for the particular design basis heat generation rate calculated. The waste form limit may then be decremented by the difference between the peak-cladding and waste package surface from the two-dimensional calculation. The resulting waste package-surface temperature is now the target peak waste package-surface temperature. This is illustrated in Figure 11.

Figure 10. Illustration of Response Surface Interrogation

6.3.2.3 Repository-Scale Three-Dimensional Analyses

This representation (refer to Figure 7) approximates the repository as an infinitely repeating series of "pillars," extending from the top of the mountain to a plane well into the saturated zone. Layers corresponding to the stratigraphy of the mountain represent the host rock of the repository. For each of these layers, thermal transport properties (viz., temperature-dependent thermal conductivity and specific heat) appropriate to the local rock properties are used. Laterally, adiabatic surfaces are placed at the center of the rock masses between the drifts. The variability of the waste package heat generation rates is incorporated by representing just a few waste packages within the drift segment. The thermal transport properties of these waste packages are represented by temperature-dependent effective values, but not with an explicit representation of the internals. The time-dependent heat generation rates of the waste packages are adjusted to ensure that the average heat generation rate of the drift segment is the same as that of the repository as a whole.

Once the time-dependent surface temperatures are obtained for the design basis waste package, these serve as boundary conditions for a two-dimensional analysis of the waste package internals. In this representation, the waste form and the adjacent waste package internals are represented by effective heat transfer parameters and correlate average volume temperatures to the peak-cladding temperature for commercial spent nuclear fuel waste forms.

$T_{WP}^{2-D}(q_{average})$ - WP surface temperature from response surface at the emplacement repository thermal load

$T_{WP}^{2-D'}$ - WP surface temperature modified for three-dimensional effects

$T_{PC}(T_{WP}^{2-D'}, q_{DB})$ - Peak-cladding temperature given modified WP surface temperature and design-basis thermal load

*In this process, the locus of points (ϵ, δ) , for which $T_{PC}(T_{WP}^{2-D'}, q_{DB}) = 350^\circ\text{C}$, is determined. This creates the operation curve for peak waste package cladding temperature.

Figure 11. Three-Dimensional Effect Accommodation

6.4 SHIELDING DESIGN

The purpose of shielding analyses is to evaluate the effects of ionizing radiation on personnel, equipment, and materials. For waste package shielding, gamma rays and neutrons emitting from the commercial spent nuclear fuel or defense high level waste are the primary radiation sources. During normal operations at the potential repository, loading and handling of the waste packages will be carried out remotely to avoid exposure of personnel to harmful radiation levels. Shielding analyses for waste package design are performed primarily to assess radiation effects to materials and equipment.

Since the waste packages are required to contain the waste forms for thousands of years, the waste package barriers must reduce radiation levels at the waste package surface such that radiolysis-enhanced corrosion under aqueous conditions is negligible. Shielding analyses are hence carried out to determine radiation dose on the waste package surface, in order to evaluate the consequence of the radiolytically-induced corrosion. Shielding evaluations are also performed for equipment to determine radiation exposure during welding of the waste package closure lids. Monitoring and control equipment, such as the welding heads and cameras, will be relatively close to the radiation sources. The results of the shielding evaluation will be used to quantify the shielding necessary for equipment to function properly at a given location for a required period of time.

In the event of emergency situations, personnel access in the proximity of the waste packages may be required. Shielding analyses provide an evaluation of the radiation environment surrounding the waste packages, assuring safety of the personnel.

6.4.1 Computational Methods and Tools

Shielding analyses concern attenuation of neutrons and gamma rays through materials. The radiation dose rates outside a waste package are determined by solving the Boltzmann equation for radiation transport, which governs the behavior of the radiation particles in a material. Two methods for solving the Boltzmann transport equation for shielding applications have received the most development, and have been used extensively for radiation shielding problems. They are the discrete-ordinates method and the Monte Carlo method. The computational tools used for waste package shielding analyses rely on these two methods.

6.4.1.1 Monte Carlo Method

The Monte Carlo method obtains radiation doses for shielding problems by employing a stochastic process to solve the Boltzmann transport equation. Using random variables, an "analog" Monte Carlo method simulates the histories of individual particles through the geometry (the "random-walk" process) and then analyzes these particle histories to derive the desired responses, such as flux density and dose rate. One particle history includes the birth of a particle at its source, its "random walk" through the transporting medium as it undergoes various scattering interactions, and ultimately the death of the particle, which terminates the history. A death can occur when the particle is absorbed, leaves the system, or loses significance owing to other factors.

For waste package shielding analyses, the analog Monte Carlo method is inadequate and inefficient in calculating radiation responses with acceptable accuracy, because the events of interest are usually very rare. From the shielding point of view, the particles that escape the waste package are of primary interest for radiation dose evaluation. However, the probability of recording such an event in a Monte Carlo calculation is extremely low ($<10^{-5}$), and an unacceptably large number of histories is required to obtain acceptable results. For this reason, variance-reduction techniques must be employed for Monte Carlo shielding analyses of waste package design. Variance-reduction techniques are procedures for altering the analog Monte Carlo process so as to reduce the variance of the calculated results. They are also known as "importance sampling" or "biasing techniques." The natural distributions in the "random walk" are modified by some importance function, and the particle statistical weights are adjusted from the analog value of unity to remove the bias. The purpose of variance-reduction techniques in Monte Carlo shielding analyses is to improve the efficiency of a calculation by reducing the variance of the results without increasing the computing time. The objective is to maintain a reasonable particle population in the primary regions of interest and, at the same time, control the fluctuation of statistical weight of the particles.

6.4.1.2 Discrete-Ordinates Method

The discrete-ordinates, or S_n , method solves the Boltzmann transport equation by using deterministic numerical techniques. The S_n method is based on expressing the continuous form of the Boltzmann transport equation in terms of discrete values of the space, energy, and angle variables. Whereas the continuous transport equation represents particle balance over differential intervals, the discrete-ordinates formulation represents particle balance over finite intervals. The spatial variables are expressed as finite intervals, the angular variables are specified in terms of a finite number of discrete directions and corresponding weights, representing solid angles, and the energy domain is divided into a finite number of ranges called energy groups.

6.4.1.3 MCNP

MCNP (Briesmeister 1997) (version MCNP4B2 at the time of this report [CRWMS M&O 1998h]) is a general-purpose Monte Carlo computer code for neutron, photon, electron, or coupled neutron/photon/electron transport. It is capable of calculating eigenvalues for critical systems and performing fixed-source (shielding) calculations to obtain radiation doses. For waste package design, MCNP is used for criticality and shielding calculations. The code allows a detailed geometric representation of the system being analyzed. MCNP uses continuous-energy nuclear and atomic data libraries. The MCNP package provides nuclear data tables derived from the Evaluated Nuclear Data File system, the Evaluated Nuclear Data Library and the Activation Library from Lawrence Livermore National Laboratory, and evaluations from the Applied Nuclear Science (T-2) Group at Los Alamos (Briesmeister 1997, p. 1-4). MCNP evaluates the secondary gamma radiation in a coupled neutron/photon transport, as well as the Bremsstrahlung radiation produced by the electrons generated in the photon transport.

Because of its versatility, MCNP is extensively used in dose rate evaluations for the waste packages. MCNP also serves to confirm the validity of the homogenized spent nuclear fuel assemblies used in SAS1 calculations (refer to Section 6.4.1.4), and to determine the effect of

source geometry on the waste package surface doses. The input specification in the MCNP dose rate calculations represents a conservative or equivalent treatment of the system being analyzed. MCNP applicability to the dose rate evaluations for the waste packages requires the following code features and calculational approaches:

- Separate photon and neutron transport calculations.
- A coupled neutron/photon transport calculation when capture gamma rays (photons created as a result of a neutron being captured by a nucleus) significantly contribute to the total dose rate.
- Photon or neutron surface flux tally specification.
- Dose function specification, which consists of flux-to-dose conversion factors provided in the MCNP manual (Briesmeister 1997, pp. H-5 and H-6). These flux-to-dose conversion factors are extracted from ANSI/ANS-6.1.1 (ANSI/ANS-6.1.1-1977).
- Photon interaction information.
- Available neutron continuous-energy cross-section tables, preferably those for neutron interaction cross sections with elements of the attenuating medium.
- Contents of the source regions homogenized inside region volumes. The commercial spent nuclear fuel consists of four source regions: bottom end-fitting, active fuel, plenum, and top end-fitting regions. Studies of the effect of source geometry on the waste package surface dose rates have shown that the homogenization of the assembly contents and source inside the assembly regions gives practically the same waste package surface dose rates as does the detailed geometric representation (CRWMS M&O 1998b, pp. 22-26).
- Uniform volume source distribution specifications in each source region of the uncanistered commercial fuel and defense high level waste waste packages. Because the radiation source generation method assumes a uniform burnup within the active fuel region, an axial peaking factor is used for photon and neutron source intensity in the active fuel region to conservatively account for the maximum values of the actual axial source distributions.
- Surface source distribution specifications for the naval spent nuclear fuel waste package.
- The default implicit neutron and photon capture and cell importance based on the MCNP manual recommendations (Briesmeister 1997, p. 2-121), as variance reduction techniques. The shielding analysis for the waste packages does not require extensive use of variance reduction techniques.

6.4.1.4 SAS1

SAS1 is a one-dimensional discrete-ordinates shielding calculation sequence using simplified input. SAS1 is a module of the SCALE computer code system (ORNL 1997) (Version SCALE 4.4A at the time of this report [CRWMS M&O 2000n]) consisting of three processes:

(1) preparation of the multi-group cross-section information and mixing table used for the shielding calculation, (2) execution of a one-dimensional radiation transport analysis, and (3) calculation of dose rates outside the waste package. The default neutron and photon-to-dose rate conversion factors used in SAS1 are extracted from ANSI/ANS-6.1.1 (ANSI/ANS-6.1.1-1977). For waste package shielding analyses, SAS1 provides an effective and efficient tool for evaluating the radiation level on and beyond the radial outer surface of the waste package.

SAS1 represents a waste package as an infinite cylinder with a homogenized fuel region in the center, enclosed by the two shells. The homogenized fuel region consists of the waste form, neutron absorber plates, thermal shunts, and other structural members. Since the length of a waste package is approximately three times the diameter, the infinite cylinder representation of the waste package is assumed (refer to Section 5.4.9), and has been shown to yield accurate dose results for the radial direction. SAS1 can also be used to estimate the radiation dose rate in the emplacement drift, since the internals of the waste package are approximated as an infinite cylinder.

SAS1 has been applied in parametric studies to evaluate the effect of shielding materials on the waste package and to examine the individual dose rates due to neutrons, gamma rays, and capture gamma rays as functions of time for waste forms with different initial enrichment and burnup characteristics.

6.4.2 Description of Pertinent Analyses

For Site Recommendation, shielding analyses are performed for four waste package designs: the 21-PWR waste package, 44-BWR waste package, 5-DHLW/DOE SNF co-disposal waste package, and the naval spent nuclear fuel waste package. For all four waste package designs, radiation dose rates in the axial and radial directions are determined on segments of the waste package surfaces. The results of the shielding calculations allow an estimation of the average operation time of welding equipment, radiolysis-induced corrosion, and the radiation environment outside the waste packages for personnel access.

6.4.2.1 21-PWR and 44-BWR Waste Package Analyses

For the 21-PWR and 44-BWR waste packages, neutrons are present only in the active fuel, but photons emit from the active fuel, plenum, top end-fitting, and bottom end-fitting regions. Shielding calculations for the commercial waste packages must include all sources in order to compute the dose rates of the waste packages. Dose rates due to the representative (average) sources for 21-PWR and 44-BWR waste packages are computed, as well as the dose rates due to the maximum sources.

6.4.2.2 5-DHLW/DOE SNF Waste Package Analyses

The 5-DHLW/DOE SNF waste package contains five high level waste glass canisters and a central DOE spent nuclear fuel canister. The DOE spent nuclear fuel canister holds one of the DOE-owned waste forms, which include Enrico Fermi reactor fuel, TRIGA reactor fuel, Fast Flux Test Facility reactor fuel, Shippingport reactor fuel, and others. The high level waste glass canister from the Savannah River Site is used in the shielding analyses because it has the maximum intensity among the high level waste glass canisters.

6.4.2.3 Naval Fuel Waste Package Analyses

The NNPP provided photon and neutron canister surface currents for the naval spent fuel canister (Naples 1999). Therefore, naval waste package shielding calculations are performed with a surface source rather than the volume sources used in the analysis of other waste package types.

6.5 CRITICALITY DESIGN

The methodology to be used for criticality analysis for the potential repository at Yucca Mountain, Nevada, is detailed for the preclosure period in the *Preclosure Criticality Analysis Process Report* (CRWMS M&O 1999f), and for the postclosure period in the *Disposal Criticality Analysis Methodology Topical Report* (YMP 2000). These reports provide the design requirements; applicable regulations, codes and standards; summary descriptions of the types of computational tools to be used; and the types of analyses to be performed. The preclosure period covers the time period ranging from the time of receipt of the waste forms until the permanent closure of the repository. The *Disposal Criticality Analysis Methodology Topical Report* has been submitted by the DOE to the NRC for review. This section summarizes the criticality methodology detailed in the revised topical report.

6.5.1 Computational Tools

A combination of neutronic computer codes are used to calculate the material (isotopic) composition of commercial spent nuclear fuel and the effective neutron multiplication factor (k_{eff}) of fissile-material configurations. These are utilized for both preclosure and postclosure analyses. Additional tools for modeling geochemistry and transient reactivity are utilized in the postclosure methodology. Brief descriptions of each of these tools follow.

6.5.1.1 Isotopics

A two-step process is used in determining isotopic concentrations for criticality evaluations where burnup credit is to be applied. For commercial spent nuclear fuel, initial isotopic concentrations are calculated using the SAS2H module of the SCALE computer code system using the 44-energy group cross-section library. The SAS2H module performs one-dimensional depletion calculations to represent the changes in isotopic inventories of the commercial spent nuclear fuel during irradiation, and provides isotopic concentrations of the discharged fuel. The ORIGEN-S module of the SCALE system is then used to perform radioactive decay calculations and provide isotopic concentrations for the time frames of interest for both the preclosure and postclosure periods.

The current version of the SCALE computer code system qualified for use is SCALE 4.4A (STN [software tracking number]: 10129-4.4A-00, CRWMS M&O 2000n). Qualification of subsequent releases of SCALE will be performed as they become available and as their use is judged to be necessary.

6.5.1.2 Criticality

The neutronic representation tool used for predicting criticality is MCNP. MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron transport, and has the

capability of calculating effective neutron multiplication factors (k_{eff}) for generalized systems containing fissionable material. MCNP uses the isotopic compositions of the materials, a detailed representation of the geometry, and a set of nuclear information libraries to calculate k_{eff} for the system. The nuclear information libraries used by MCNP are comprised of continuous-energy cross sections of materials. A full set of these material cross sections has been evaluated and is provided through the MCNP code package. From this full set a reduced set of these information libraries has been evaluated for application in the criticality calculations to be performed here (*Selection of MCNP Cross Section Libraries*, CRWMS M&O 1998e).

The current version qualified for use is MCNP4B2 (CSCI: 30033 V4B2LV, CRWMS M&O 1998h). Qualification of subsequent releases of MCNP will be performed as they become available and as their use is judged to be necessary.

6.5.1.3 Corrosion

WAPDEG is the Monte Carlo code used to generate statistics on waste package breach times. It is based on the abstraction of experimental and theoretical data on the corrosion of materials used for waste package barriers, over the range of parameters expected for the repository environment. WAPDEG is run as part of the Total System Performance Assessment (TSPA) process, and the principal output is a distribution of breach times at various locations on the waste package (top, bottom, sides) for a given set of environmental conditions (temperature history, relative humidity history, exposure to drips, etc.). Disposal criticality analyses primarily use the "base case" output distributions from the latest approved version of the TSPA, to determine time range over which degradation, accumulation, and criticality analyses must be performed. Through the analyses the breach time distributions are also incorporated into the calculation of probability of criticality and resulting risk.

The current version qualified for use is WAPDEG V4.0 (STN: 10000-4.0-00, CRWMS M&O 2000o). It is expected that future revisions to this code will occur, and the newly qualified versions will be used.

6.5.1.4 Geochemistry

EQ3/6—EQ3/6 is a software package for geochemical simulation of aqueous systems. The major components of the package include EQ3NR, a speciation-solubility code; EQ6, a reaction path code, which simulates water/rock interaction or fluid mixing in either a pure reaction progress frame or a time frame; EQPT, a data file preprocessor; EQLIB, a supporting software library; and several supporting thermodynamic data files. The software deals with the concepts of thermodynamic equilibrium, thermodynamic dis-equilibrium, and reaction kinetics. One of the thermodynamic data files (data0.ymp.r0) is qualified for use on the Yucca Mountain Project (DTN: MO0009THERMODYN.001).

Of the EQ3/6 components, the primary geochemistry code used for degradation analysis internal to the waste package is EQ6. It is used in a solid-centered, flow-through mode, which automatically incorporates the adjustment of water volume at each time step. This enables the simulation of water inflow and outflow to track the time-step adjustment process exactly. This

code ensures that the chemical changes are accurately resolved in time and that the volume of water in the waste package at any given time is accurately represented.

The software package, EQ3/6, Version 7.2b was approved for Quality Assurance work (CSCI: UCRL-MA-110662, CRWMS M&O 1998f). The solid-centered flow-through mode was added to EQ6 V7.2b by the Software Change Request LSCR198 (CRWMS M&O 1999k) and the Software Qualification Report for Media Number 30084-M04-001 (CRWMS M&O 1998i). The most recent approved version of EQ6 is Version 7.2bLV (STN: 10075-7.2bLV-00, CRWMS M&O 1999l), which added several new capabilities, such as the capability of incorporating radioactive decay into the calculations. Qualification of subsequent releases of EQ3/6 will be performed as they become available and as their use is judged to be necessary.

PHREEQC—PHREEQC, Version 2, is the primary code for geochemistry calculations external to the waste package. It is used to calculate the accumulation of fissile material in the void spaces of the invert and in the host rock. PHREEQC is a geochemical transport code that is designed to perform a wide variety of low-temperature, aqueous, geochemical calculations, based on an ion-association aqueous representation. It has the following capabilities:

1. Speciation and saturation-index calculations
2. Reaction-path and one-dimensional transport calculations involving reversible reactions which include aqueous, mineral, gas, solid-solution, surface-complexation, and ion-exchange equilibria; and irreversible reactions, which include specified mole transfers of reactants, kinetically controlled reactions, mixing of solutions, and temperature changes
3. Inverse modeling, which determines sets of mineral and gas mole transfers that account for differences in composition between waters, within specified compositional uncertainties.

The current version qualified for use is PHREEQC V2.0 (STN: 10068-2.0-00, CRWMS M&O 1999j). Qualification of subsequent releases of PHREEQC will be performed as they become available and as their use is judged to be necessary.

6.5.1.5 Transient Neutronics

Internal transient reactivity calculations supporting the criticality consequence evaluations are performed by the reactor transient code RELAP5/MOD3.2. RELAP5/MOD3.2 is a coupled-neutronic, thermal-hydraulic, time-dependent code designed for light water reactor transient evaluations, including loss-of-coolant-accidents and operational and design basis transient evaluations. This includes reactivity, thermal, and pressure transients. The code uses generic component representations from which general systems for both nuclear and non-nuclear systems involving steam, water, and non-condensable gases may be analyzed. The code consists of a one-dimensional, thermal-hydraulic representation that solves the continuity, momentum, and energy equations for two fluids (or two phases). Limited two-dimensional flow simulation capabilities are accessible with cross-flow junctions in the modeling. It also contains a point-reactor kinetic representation, where coupling to the thermal-hydraulics representation is made through reactivity feedback effects, including fuel and moderator temperature, moderator density, and soluble poison (boric acid) concentration. The application of RELAP5/MOD3.2 is

limited to waste package performance evaluations with intact fuel rods. The validity range for the fluid and mixture property data in RELAP5/MOD3.2 extends to the low temperature and pressure conditions applicable to in-package criticality.

The current version qualified for use is RELAP5/MOD3.2 V1.0 (CSCI: 10091-1.0-00, CRWMS M&O 1999i). Qualification of subsequent releases of RELAP5 will be performed as they become available and as their use is judged to be necessary.

An additional, fully-coupled nuclear thermal-hydraulic code is being developed and will be qualified for use in the evaluation of transient external criticality generally and in those cases of transient internal criticality for which RELAP5 cannot be applied (e.g. the absence of fuel cladding or mixture of fissionable material with moderator).

6.5.2 Preclosure Criticality

The methodology for loading the waste form into the disposal container has been developed such that subcriticality is ensured during the preclosure period and for the period during which the waste package is intact, sealed, and undamaged. This methodology may be referred to as the "criticality loading curve evaluation." This evaluation establishes a simple criterion, in terms of the available waste form information, to determine whether a waste form can be loaded into a given disposal container. Adhering to this process ensures that a subcritical configuration exists. For DOE spent nuclear fuel and other non-commercial waste forms (except naval spent nuclear fuel), where a bounding loading configuration and enrichment are used with no burnup credit (hence, no range of burnup enrichment pairs), the "loading curve" is simplified down to point values for each group. The calculated effective multiplication factor (k_{eff}) for naval spent fuel canisters will be shown to not exceed 0.95 unless at least two unlikely, independent and concurrent or sequential events have occurred in the conditions essential to nuclear criticality safety. The calculated k_{eff} will be sufficiently below unity to show at least a five percent margin after allowance for the bias and the uncertainty in the experiments used to validate the method of calculation.

6.5.2.1 Critical Limit Determination

Criticality is attained when the effective neutron multiplication factor (k_{eff}) of a system of fissionable material in a given geometry becomes equal to or greater than unity. Conversely, subcriticality is defined by an effective neutron multiplication factor less than unity. When designing a system, i.e., a waste package, to be subcritical, it must be demonstrated that the calculated k_{eff} conservatively represents the true neutron multiplication of the system. This is accomplished by choosing a value below unity where nuclear criticality is assumed to occur. This value is known as the critical limit. The critical limit is intended to bound and account for the bias and uncertainty in the calculational method experiments.

For the waste package loading curve evaluations of commercial spent nuclear fuel described in Section 6.5.2.2, the critical limit is determined from three different classes of applicable experiments: laboratory critical experiments, radiochemical assays, and commercial reactor critical measurements. The computational tools used for the loading curve evaluations involving burnup credit are the SAS2H module of the SCALE package for the generation of the isotopic

quantities and MCNP to evaluate the criticality of the systems by determining the k_{eff} for each of the systems.

Laboratory Critical Experiments—Laboratory critical experiments are a set of well-documented, industry-standard, critical measurements. MCNP is used to evaluate these experiments using the same cross-section library set that is used in the loading curve evaluations. These evaluations provide inputs for the bias and uncertainty in the criticality methodology. Laboratory critical experiments are the only data measurements used for the evaluation of criticality of waste forms not utilizing burnup credit.

Radiochemical Assays—Radiochemical assays include a set of isotopic measurements performed on irradiated fuel. These measurements provide the isotopic concentrations of the fuel after a known exposure in a reactor. The SAS2H module uses the known operational history to predict the isotopic concentrations of the fuel, which are compared to the measured quantities. Resulting isotopics from both the measured and calculated isotopic results are used as input for a representative MCNP criticality evaluation. Results of the criticality evaluation provide additional data to be used in the determination of the bias and uncertainty for the criticality methodology. Additionally, code-to-code comparisons between SAS2H and an industry-standard, two-dimensional lattice depletion code used for reactor core design analysis will be performed to provide additional information for establishing the isotopic component of the reactivity bias and uncertainty.

Commercial Reactor Critical Measurements—Commercial reactor critical measurements are performed to provide additional data for establishing the reactivity bias and uncertainty for both PWR and BWR commercial spent nuclear fuel. A commercial reactor critical evaluation consists of using the computer codes and disposal criticality analysis methodology to perform best-estimate predictions of known critical configurations in commercial nuclear reactors. These criticality demonstrations are performed during each reactor core startup and effectively provide benchmark data for comparison to the disposal criticality methods. The goal is to properly predict neutron multiplication for a fuel mass that includes actinides and fission products created during commercial power operation. The commercial reactor critical measurements involve using SAS2H to perform best-estimate modeling of the depletion.

The depletion portion of the analysis uses the best available information to represent the operational in-reactor history of the fuel, which includes time-dependent power, soluble boron concentration (PWRs only), fuel temperature, moderator temperature (or moderator voiding for BWRs), and control rod history. The reactivity portion of the commercial reactor critical measurements consists of an MCNP criticality calculation using the isotopic concentrations of the fuel from the depletion calculations as input to a best-estimate representation of the reactor core, including state conditions existing during the reactor startup criticality demonstration. The resulting k_{eff} values are compared to the measured value obtained during the actual startup criticality demonstration, which is, by definition, a neutron multiplication value of unity (with minor corrections for long reactor periods).

Determination of a critical limit for each waste form is obtained by performing a statistical evaluation of the benchmark data utilized. A summary of the process to be used for estimating the critical limit is provided in Figure 12. The results of the laboratory critical experiments,

radiochemical assays, and commercial reactor critical evaluations will be used as input in the determination of the critical limit, and are different sets of input to the process presented in Figure 12 (top box).

6.5.2.2 Preclosure Loading Curve Determination

Once a critical limit has been determined, a process is necessary which ensures the waste package remains subcritical during the preclosure phase of the repository. The available information used in this determination for commercial spent nuclear fuel (waste form) consists of four components: bundle identification number, initial enrichment, assembly average discharge exposure, and decay time (measured in time since removal from in-reactor operation). With this information, a curve is developed for each commercial waste form (PWR, BWR, and mixed-oxide) that represents the required minimum-average assembly burnup as a function of the initial-average assembly enrichment allowable for loading into a particular type of disposal container (refer to Figure 13). For assemblies that are analyzed to be in the unacceptable region (to the right of the loading curve) of Figure 13, additional means of reactivity control are utilized. Such reactivity control increases the margin to criticality, either by the addition of disposable control rods within the assembly or the loading of these assemblies into an alternate disposal container, which is smaller and possesses a higher negative reactivity component inherent in its design. Note that Figure 13 is a hypothetical loading curve, not applicable to any specific disposal container or waste form.

The loading curve is a locus of burnup/enrichment pairs giving a constant k_{eff} having a value corresponding to the critical limit developed, plus any administrative margin imposed to ensure subcriticality. A value of 5% for the administrative margin is used for preclosure analysis (BSC 2001i, Criterion 1.2.2.1.12), which ensures operations during the loading and emplacement process of the waste package will remain subcritical. No administrative margin requirement will be added for the postclosure phase. Postclosure criticality evaluations are based on the developed critical limit without any margin to ensure subcriticality, since subcriticality during postclosure is not required (Dyer 1999).

The calculations to determine the waste form-specific loading curves are formulated such that conservative values and methods are utilized. Prior to performing these loading curve evaluations, sensitivity studies are performed using SAS2H to determine the depletion methodology that ensures the resulting isotopics are conservative relative to the actual operating history of each fuel assembly. These sensitivity studies include determination of a limiting axial profile, assembly radial variations, control rod insertion fraction, chemical shim control, and fuel and moderator temperature. Using these limiting input values in the bounding representation, fuel isotopic concentrations are then calculated using SAS2H for different average assembly enrichments as a function of burnup, covering the range of commercial fuel enrichments and exposures. (For the entire range of discharge exposures, isotopics are determined for various cooling times, including the minimum required five-year decay time, as dictated in 10 CFR 961.11 [10 CFR 961]).

Figure 12. Process for Estimating a Critical Limit

Figure 13. Hypothetical Loading Curve for a Commercial Disposal Container/Waste Form

Criticality evaluations using MCNP are then performed using the isotopic concentrations from the depletion analysis. The criticality evaluations are performed using the specific waste package, assuming flooded conditions and an isotopic inventory for the fuel that results in a conservative representation of the reactivity. The assumption of flooded conditions is sufficient to cover all design basis events under consideration during the repository preclosure period.

To determine the loading curve, criticality calculations are performed for the waste package fully loaded with identical assemblies of a specific initial average assembly enrichment and average discharge exposure. For a given initial enrichment, the margin to criticality of the waste package increases as the discharge exposure increases. A sufficient number of criticality calculations are performed to determine the discharge exposure at which the waste package, loaded with assemblies of the same initial enrichment, is potentially critical as defined by the upper subcritical limit (which currently is defined as the critical limit minus 5%). For each of these initial enrichment values, waste package criticality calculations are performed as a function of assembly burnup. These calculations are performed for a sufficient range of discharge exposures to have a minimum of two data points on either side of the upper subcritical limit (refer to Figure 14). Determination of the actual burnup corresponding to the upper subcritical limit is effected by linear interpolation between the two nearest points on each constant initial enrichment line. Once curves are developed for each initial enrichment, the enrichment and burnup pairs corresponding to the upper subcritical limit are readily combined to create the loading curve for a specific commercial waste form, as seen in Figure 13.

Figure 14. Typical Criticality Enrichment Curve

It is not envisioned that all commercial spent fuel will be applicable to the predetermined loading curve. For some assemblies, as previously addressed, additional reactivity control will be introduced by means of adding disposable control rods inside the assembly and/or placing them in inherently less-reactive waste packages.

6.5.3 Postclosure Criticality

Postclosure criticality analysis begins with the assumption that the preclosure criticality process has ensured that all waste packages will remain subcritical until the waste package is breached. The preclosure loading curve analysis and criteria ensure this for commercial fuel, as discussed in the previous section. Thus, the essential requirement for postclosure criticality evaluations is that the waste package must be breached by some mechanism, allowing water to enter the waste package and begin the degradation process.

An overview of the postclosure criticality methodology is provided in Figure 15 (YMP 2000, p. 1-10). There are five parts of the postclosure methodology:

1. The Master Scenario List and configuration classes

2. The specific values of parameters and/or parameter ranges characterizing each configuration class (as determined from degradation and accumulation analyses).
3. Identification of whether a configuration class has the potential of becoming critical
4. For those configurations that have a criticality potential, the probability of that occurrence
5. The consequence of such a criticality.

Criteria for each of the last three parts are established for criticality, probability, and consequence as design constraints that will ensure defense-in-depth to criticality for the postclosure phase. The decision points in Figure 15 indicate these criteria. Each of the five areas is addressed separately below.

6.5.3.1 Configuration Classes

As identified above, postclosure criticality assumes the breach of the waste package and then considers the different features, events, and processes (FEPs) that may result in a favorable situation for criticality to occur. To include all of the possible different configurations for consideration, a Master Scenario List has been established. This list defines a comprehensive set of degradation scenarios, which are used to identify a limited set of configurations, to be considered in the criticality analysis of all waste forms. The scenario list was developed considering the range of waste forms, waste package, and engineered barrier system designs, the characteristics of the site, and the degradation characteristics of the waste package materials.

The Master Scenario List divides potentially critical configurations into three regions of occurrence: configurations occurring internal to the waste package; configurations external to the waste package but in the drift, which is considered near-field; and configurations external to the waste package and occurring in the far-field. The individual configurations are then classed into groups, called configuration classes. Each configuration class is defined as a single scenario or a set of related scenarios that result in a common range of material composition and geometry.

This range of parameters thus comprises the class. These parameters may include the amounts of fissionable material, neutron absorber material, corrosion products, and moderator, and may also stipulate the time of occurrence. There are six configuration classes that cover the range of internal scenarios that result in the potential for criticality (YMP 2000):

1. The basket is degraded, but the waste form is relatively intact. For criticality to occur, several additional conditions are required: sufficient moderator is present, neutron absorber is flushed from the waste package, and most of the fissionable material remains in the package.
2. Both basket and waste form are degraded, with the same three additional conditions as in (1) required to effect criticality.

Figure 15. Overview of Disposal Criticality Analysis Methodology

3. The fissionable material from the waste form is mobilized and moved away from the neutron absorber, which remains in the largely intact basket.
4. Fissionable material accumulates at the bottom of the waste package, together with moderator provided either by water trapped in clay or by hydration of metal corrosion products, so that criticality can occur without standing water in the waste package.
5. As with (4) above, the moderator is provided by water trapped in clay, but in this case the fissionable material is distributed throughout a major fraction of the waste package volume.
6. The waste form has degraded in place with other internal components intact. This configuration class is of interest if the degradation of the waste form can distribute the fissionable material into a more reactive geometry than that of the intact waste form.

Scenarios leading to external criticality can arise from the combination of FEPs that breach and degrade the waste package in such a way as to produce a source term (outflow of radioactive materials from the waste package). There are ten configuration classes that cover the range of results of potentially-critical external scenarios:

1. Accumulation, by chemical reduction, of fissionable material by a mass of organic material (reducing zone) located in the unsaturated zone (rock above the water table such that all the pore space is not filled with water) either beneath the repository, at a narrowing of the tuff aquifer, or at the surface outfall of the saturated zone flow. Although the probability of the existence of such a reducing zone at Yucca Mountain is extremely low (CRWMS M&O 1996f, Section 7.6.2), it is important because it has the potential for accumulating a higher mass of fissionable material than any of the other external configuration classes.
2. Accumulation by sorption, onto clay or zeolite.
3. Precipitation of fissionable material in fractures and other void space of the near-field, either from adsorption or from a reducing reaction. The two configurations are considered together because they are both limited by the same buildup of non-fissionable deposits in the fractures of the near-field.
4. Accumulation of fissionable material in a standing water pond in the drift. This scenario involves waste packages that may not have been directly subjected to dripping water, but are located in a local depression so that water flowing from other dripping sites may collect around the bottom of the package during periods of high flow. A variant of this configuration class could have the intact, or nearly intact, waste form in a pond in the drift. Such a configuration would be evaluated for waste forms that could be demonstrated to be more robust, with respect to aqueous corrosion, than the waste package. Since there is no mechanism for completely sealing the fractures in the bottom of the drift, an in-drift pond would be expected to occur only within a short time (weeks or less) following a high infiltration episode. The detailed analyses for the License Application will evaluate the

probability of occurrence for a pond of sufficient depth to cover enough assemblies to result in criticality, while the assemblies are stacked in a geometry favorable to criticality.

5. Accumulation by processes involving the formation, transport, and eventual breakup (or precipitation) of fissionable material containing colloidal particles. It has been suggested that the colloid-forming tendency of plutonium will enhance its transport capability, providing the potential for accumulation at some significant distance from the waste package. Such transport and accumulation could lead to final accumulation in dead-end fractures, clay or zeolite, topographic lows, open fractures, and degraded concrete, respectively.
6. Accumulation at the low point of the emplacement drift (or any connecting drift). The scenario leading to this configuration must have a mechanism for sealing the fractures in the drift floor so that the effluent from individual waste packages can flow to, and accumulate at, a low point in the drift or repository, possibly in combination with effluent from other waste packages. As with (4) above, such a pond would be expected to occur only within a short time (weeks or less) following a high infiltration episode. However, it should be noted that the repository design has been re-evaluated to maintain a zero slope in the emplacement drift. Therefore, there can be no significant accumulation in the drift from effluent that may flow out of multiple waste packages.
7. Accumulation of fissionable material (uranium) by precipitation, in the saturated zone, at the contact between the waste-package plume and a hypothetical up-welling fluid or a redox front (at a boundary between two different groundwater chemistries, flow meets a different chemistry so that an oxidation-reduction reaction can take place). This configuration is considered unimportant because there is no evidence for any such bodies below Yucca Mountain that would have sufficiently different chemical or redox characteristics to significantly concentrate fissionable material from the contaminant plume (CRWMS M&O 1997f).
8. Accumulation at the surface of the invert due to filtration by the degradation products, or remnants, of the waste package and its contents.
9. Accumulation by precipitation from encountering perched water (groundwater deposit isolated from the nominal flow and not draining because of an impermeable layer beneath) having significantly different chemistry from the fissionable material carrier plume. This case will be evaluated for License Application to determine how much fissionable material can be accumulated before the chemistry of the perched water is changed to that of the carrier plume.
10. Accumulation by precipitation from the chemistry changes made possible by carrier plume interaction with the surrounding rock. Preliminary analysis indicates that the amount of material that could be precipitated in this manner is limited by the fact that chemistry changes in the carrier plume itself would precipitate non-fissionable material from the carrier plume before any precipitation of fissionable material from the waste package plume (CRWMS M&O 1997d). The result would be fracture filling with non-fissionable material, as with (3) above.

6.5.3.2 Parameter Ranges

For each configuration class, parameter ranges are established. The parameter ranges are established from degradation analysis using EQ3/6, the configuration generator code, and accumulation analyses with PHREEQC. The degradation analyses provide information on parameters that affect the potential for criticality. The most noteworthy parameters include the amounts of fissionable material, neutron absorber material, corrosion products, and moderator. The parameter ranges established for each configuration class determine the inputs for the criticality representation.

For configuration classes internal to the waste package, ten steps are used to specify the geochemistry related steps necessary to develop a credible range of parameters from the degradation analysis:

1. Identify specific corrosion rates for each internal component, which are representative of the range of degradation rates for those components and the configuration classes defined previously.
2. Identify specific water flow rates, which are representative of the range of water drip rates onto a waste package under a dripping fracture. This information will be obtained from the unsaturated zone flow representation produced by the Performance Assessment Project (CRWMS M&O 2000w, Section 3.2).
3. Identify the range of dripping water chemistry parameters.
4. Estimate the location of potentially reacting materials, to determine whether they are actually reacting, using the information from Steps 1-3 above. This estimation is repeated as the degradation process continues, so that the continuing interaction of physical and chemical processes is captured.
5. Perform parametric EQ3/6 calculations using the solid-centered, flow-through mode and the representative parameter range for each configuration class.
6. Examine results for concentrations of fissionable materials, neutron absorbers in solution and in solids, and insoluble corrosion products of other internal waste package components.
7. Examine results for formation of clay (either from glass in co-disposed waste forms or from the silica and alumina in the in-flowing water).
8. Quantify the possible range of hydration for degradation products if the package could not be flooded.
9. Quantify the amounts of undegraded material and solid degradation products present for each configuration class.
10. Evaluate the potential for adsorption of soluble fissionable material or neutron absorber material on corrosion products.

The repository parameters of interest for potentially critical external configurations include: the physical and chemical degradation properties of materials used in invert; fracture frequency/intensity, distribution of fracture apertures; the location of deposits of zeolites and other adsorbing materials; and the location and characteristics of potential reducing zones.

The identification of external configurations with the potential for criticality starts with the determination of the source term (fissionable material in the solution flowing out of the waste package, or its remnant) as a function of time, by combining the geochemical and physical flow analyses considered in the internal configuration evaluations. The subsequent steps for identifying external configurations with the potential for criticality are:

1. Development of a statistical distribution for flow rate and path, which is a strong function of the characteristic of the fracture network beneath the waste package.
2. Determination of adsorption on fracture walls or in the matrix of highly porous rock or zeolite deposits.
3. Determination of mineral precipitates from reactions of the waste package plume with the host rock fracture walls and from pH change on mixing of waste package effluent with ambient (neutral) groundwater, using PHREEQC. This includes an accounting of both fissile and other materials because they compete for the limited fracture void space.
4. Determination of alternate paths, or spreading, when the primary fractures are filled. This step includes consideration of the possible collection of the source terms from several waste packages.
5. Determination of reaction products from the plume encountering a reducing zone using PHREEQC and EQ3/6. This step includes consideration of the following limiting factors: void space available in the reducing zone for product precipitation, and low flow rate of the waste package plume.

After the initial degradation analyses are performed and parameter ranges for the configurations in each class are defined, the original configuration class definitions are re-evaluated to ensure the ranges of the parameters remain covered by the configuration class. For example, an original (internal configuration) class of "partial basket degradation" may be split into two subclasses, one with the corrosion products fully distributed in the water surrounding the fissionable material, and another with the corrosion products settled to the bottom of the waste package, but still contained within the package.

6.5.3.3 Criticality Criterion

The range of parameters established for each configuration determines the input to be used for the criticality analyses.

A criticality criterion is established to identify the criticality potential of a configuration class. For postclosure degraded criticality calculations, the critical limit as described in Section 6.5.2.1 will be used as the determinant of the criticality criterion, without any additional administrative margin.

MCNP calculations are performed for representative parameter values of each configuration class to establish whether any combination of the parameters that constitute the range can be made such that the calculated k_{eff} value for the configuration meets or exceeds the criticality criterion. Any configuration class that has at least one combination of parameters that produce a k_{eff} value at or above the criticality criterion is then considered potentially critical, and further evaluations are performed for that configuration class.

Configuration classes that have no combination of parameters within their ranges that result in a k_{eff} value at or above the established critical limit, according to MCNP, are considered acceptable for disposal, and no additional calculations are necessary for the configuration classes.

6.5.3.4 Probability

An evaluation is performed for each potentially critical configuration class to determine the probability of occurrence of all criticalities.

For potentially critical configurations, additional criticality calculations are performed to identify the point in each parameter range at which the calculated k_{eff} value of the system meets or exceeds the critical limit. For each configuration class, ranges of each parameter are represented by at least three characteristic points (the minimum, 50% penetration into the range, and the maximum value). Waste form parameters for commercial fuel have points for the enrichment and burnup ranges in increments of 1 wt% and 10 GWd/MtU or less, respectively, throughout their ranges. The entire parameter space is analyzed by evaluating all possible combinations of the characteristic points (varying one parameter at a time, holding the others fixed). The resulting k_{eff} values are tabulated as a function of the parameters. Using linear interpolation on this table, an estimate of the surface of parameters corresponding to the critical limit (the "area of importance") is made.

Due to the large range of k_{eff} values that results from evaluations over the entire range of each parameter, refined criticality calculations covering a narrower range in the area of importance are also performed. These additional criticality calculations are performed to further refine the interpolation. Three additional points are evaluated for each parameter, defined by the estimated parameter value at the critical limit and $\pm 5\%$ of the total range from that point. Burnup and enrichment increments no finer than 0.5 wt% and 5 GWd/MtU are evaluated. For parameter values at the edge of the range, two additional points into the range at 5% increments are evaluated. The individual k_{eff} values for a specific configuration within the class are obtained by linear interpolation of each parameter.

To reflect the uncertainty associated with each parameter, probability distributions are developed over the parameter range for a given configuration.

Criticality criterion and probability calculations are performed with MCNP, using a full waste package. Isotopic concentrations are determined from SAS2H depletion calculations consistent with the preclosure methodology. ORIGEN-S decay calculations are then performed to determine time-dependencies of the depleted waste form. All material compositions are determined from geochemistry calculations using EQ3/6 in a solid-centered, flow-through mode.

Evaluations of external configurations also use the geochemical transport code PHREEQC to account for accumulation by adsorption.

A Monte Carlo technique is used to estimate criticality probability. The process is represented in Figure 16 and Figure 17 for the development of the internal and external criticality probabilities, respectively. Cumulative distribution functions are developed for each parameter over its respective range. Random numbers are sampled from a uniform distribution between zero and unity, and each random number is used to extract a sample parameter value from the cumulative distribution function.

Cumulative distribution functions are performed on parameters affecting criticality potential, as well as those affecting waste package degradation (available as input from the TSPA analyses).

This latter group includes drip rates, barrier lifetimes, and possible locations of significant penetrations of the waste package shells. The number of iterations (or realizations) to be performed is dependent on the level of statistical confidence necessary to determine if the probability criterion, which is described later, has been met, within the range of uncertainty. The critical frequency for the configuration class under evaluation is determined by the number of realizations that ended in a criticality, divided by the total number of realizations performed. The major probabilistic considerations of the individual steps on Figure 16 for internal criticality are as follows:

1. Sample from distribution of drip rates. The distribution of seepage fraction, seepage rate and their temporal variation will be obtained from a drift-scale seepage model, which will include the effects of thermal reflux. In practice, these distributions will be abstracted from the most recent version of the TSPA.
2. Sample from the distribution of barrier lifetimes. This distribution is obtained by (a) first applying the TSPA program WAPDEG to obtain waste package failure distributions under always-dripping and no-dripping conditions, and (b) then combining the WAPDEG output with the value for drip rate sampled in the previous step.
3. Sample from the distribution of possible locations of significant waste package shell penetrations. This distribution of penetration locations is also generated by the WAPDEG program. The lowest penetration on the waste package will determine the depth of water standing in the waste package, which, in turn, determines the number of assemblies covered by water and the potential for the occurrence of a criticality event.
4. Sample from the range of waste form parameters (e.g., burnup and enrichment for commercial spent nuclear fuel), and test their ability to produce a criticality event under the worst-case degradation conditions, if such worst case conditions can be defined (e.g., loss of all neutron absorbers and the time of peak criticality potential). This is done using the tabulated results of k_{eff} values versus the parameter ranges, evaluated at the sampled burnup and enrichment. An independent sampling is performed for each assembly loaded into the disposal container, and the limiting pair of burnup and enrichment values is used to represent all assemblies in the disposal container. If there can be no criticality event

Figure16. Monte Carlo Technique for Informational Flow, Internal

Figure 17. Monte Carlo Technique for Informational Flow, External

occurrence for the waste form characteristics, the realization is ended. This step of the methodology is primarily for commercial spent nuclear fuel, which has a large range of burnup and enrichment, and therefore a large range of criticality potential.

5. Sample from the distribution of degradation parameters for the waste form and other internal components, and calculate the amount of neutronically significant material remaining in the waste package. These calculations are made with the mass-balance equations of the configuration generator code, which uses the sampled degradation parameters as coefficients in the equations. The distributions of the degradation parameters are consistent with those used for the TSPA.
6. Evaluate criticality of the configurations defined by the previous step, using the method described in (4) above. If k_{eff} is greater than the critical limit, increment the internal criticality counter, end the realization, and start another realization (until the desired number of realizations is reached).

For external criticality, the major probabilistic considerations consistent with the individual steps in Figure 17 are as follows:

1. Sample for the source term and environmental parameters from their respective distributions. The former is determined by abstracting the EQ3/6 geochemical analyses, which were based on the distribution of environmental parameters (this is one of the outputs from the degradation calculation as shown in Figure 16). The distribution of environmental parameters is taken to be that used in, or generated by, the TSPA.
2. Randomly select the external path from among those leading to one of the standard set of external criticality locations, with the selection process weighted according to the probability of such a location existing and being encountered. The current standard external locations fall into the following general categories: (1) coating of the fracture walls of the drift invert and nearby host rock, (2) deposits of adsorbing material, and (3) deposits of reducing material (CRWMS M&O 1998c).
3. Sample from the distribution of transport parameters, which are taken to be those used in, or generated by, the TSPA. Calculate the amounts of fissionable material transported through the portion of the external environment that contains little material with the capability of removing fissionable material from the flow. For the near-field, these calculations are performed with EQ3/6, using the transport mass balance equations from the configuration generator code. PHREEQC is used for the far-field. Parameters that have significant uncertainty are selected using the Monte Carlo technique.
4. Sample from the distribution of accumulation parameters, which are taken to be those used in, or generated by, the TSPA.
5. Calculate the amounts of fissionable material removed from the flow, at the portion of the external environment that contains sizeable amounts of material capable of removing fissionable material from the flow. These calculations are performed as stated in (3).
6. Evaluate the k_{eff} value for configurations having a significant accumulation of fissionable material. If this is above the critical limit, a potential external criticality has been identified, and the external criticality counter is incremented (for the specific location), as indicated in Figure 17. Whether the k_{eff} value is above or below the critical limit, the realization is ended and a new one begun.

Probabilistic calculations are performed using the Monte Carlo technique as described above for each waste package/waste form, in each potentially critical configuration class, and results are reported as a probability of criticality per waste package/waste form. A probability of criticality for the entire repository is then taken as the average over the repository, weighted by the relative quantity of each waste package/waste form type. It can then be evaluated against an established probability criterion.

If the probability criterion is exceeded, design options for reducing the probability below the criterion will be explored. One option is to load a higher percentage of commercial spent nuclear fuel with additional reactivity control into inherently less-reactive disposal containers.

6.5.3.5 Consequence

For all potentially critical configuration classes that exceed the probability criterion, a consequence evaluation is performed for such criticalities. The consequence evaluation is necessary in the determination of criticality risk, which is the basis of the criticality methodology consistent with the potential requirements of 64 FR 8640 (10 CFR 63) and 10 CFR 963 (which are both currently in draft form, 64 FR 8640 as described in Section 4.3 and 10 CFR 963 as 64 FR 67054). It also provides input into the TSPA as necessary. The actual inclusion of criticality consequences in the TSPA base case analysis will be determined by whether the criticality probability and consequence magnitude are significant by comparison with other TSPA radionuclide (inventory and release) inputs.

For these analyses, criticality is divided into steady-state and transient evaluations.

Steady-State Criticality Evaluations—Steady-state evaluations involve long-term criticality events in which the generated power is fairly constant or slowly varying over time. This is the type of criticality event evaluated for potentially critical configuration classes. The increase in radionuclide inventory is the primary evaluated consequence of a steady-state criticality – other consequences are evaluated in terms of their feedback effect on radionuclide production. 10 CFR 963 (64 FR 67054) states the primary licensing design criterion as the relative dose impact at the accessible environment, expressed in terms of increased dose experienced by a control group. The inventory increment is the primary evaluated consequence because it has the greatest impact on increasing the established control group dose. Another contributing consequence of a steady-state criticality is usually an increase in temperature, which can increase the corrosion rate of waste package internals.

Radionuclide inventories are determined by the ORIGEN-S module of the SCALE software package. The duration of the criticality is determined by the amount of water present to produce the criticality, which is determined from the probabilistic analysis for the evaluated configuration class. The initial isotopics used for both internal and external configurations are those calculated by ORIGEN-S at the time of criticality origination, consistent with the materials from a single waste package. The radionuclide increase associated with the criticality is determined by performing the ORIGEN-S calculation at a specified power level for the duration of the criticality, then decaying the resulting isotopics for a period of 1,000 years. The radionuclide increment is then determined by comparing these isotopic concentrations to those at the same point in time without any criticality occurrence considered.

The power level used in ORIGEN-S for the criticality period is determined from the drip rate of water into the critical system. For a steady-state criticality, the power generated is such that the evaporation rate (water leaving the system) is in equilibrium with the drip rate (water flowing into the system) after accounting for other heat losses. If the evaporation rate does not equal the drip rate, the system cannot sustain a criticality.

Transient Criticality Evaluations—Transient criticality will occur if the k_{eff} is rapidly increased from sub-critical to critical (rapid reactivity insertion rate). It is much less likely than steady-state criticality because such changes in the space of less than one minute do not usually occur in nature. Nevertheless, such occurrences are possible, so calculations are performed to

determine if standard configurations that are subcritical can be overcome by a reactivity insertion event that will raise the k_{eff} of the system to the critical limit or higher. These configurations are termed predecessor configurations. For internal configurations, the RELAP5/MOD3.2 code is used to establish which configurations can become predecessor configurations. An example of a predecessor configuration is an intact waste package containing stacked intact fuel assemblies and a completely degraded internal basket structure. The water within the waste package covers only half of the assemblies. By some event, an assembly above the waterline falls into the water and becomes submerged, raising the reactivity enough to make the system critical. Seismic events are considered a mechanism by which predecessor configurations can become critical, and the probability of seismic events is included in the calculation.

The probability of the configurations becoming critical within a transient period is then determined. The design probability criterion states that the average criticality frequency will be less than 10^{-4} per year for the entire repository for the first 10,000 years. If any configuration were determined to be capable of supporting criticality events and found to have an estimated probability of occurrence below the design probability criterion, but contribute to a total probability of criticality for the entire repository inventory above the proposed 10 CFR 63 (Dyer 1999) screening probability threshold of 10^{-4} in 10,000 years, consequence analyses would be performed (YMP 2000, Section 3.2.2).

In addition to predecessor configurations, those potentially critical configurations that have a steady-state criticality risk are also evaluated for the transient reactivity impacts of such a criticality, by associating an additional probability of occurrence (i.e., seismic or otherwise) with a modified consequence. The modified consequence may include a higher radionuclide inventory due to increased degradation rates.

The consequences of such transient criticalities are evaluated as a radionuclide increment, as with the steady-state analysis. Other effects of transient criticalities – increased temperature, system pressure, and material degradation – are evaluated in terms of their feedback effect on radionuclide release. These are the principal consequences that are passed to the Performance Assessment Project for inclusion in TSPA as appropriate. Any potential autocatalytic criticality event, which contains positive feedback, is also included in the transient risk evaluation. In addition to the radionuclide inventory increment resulting from the transient criticality, the potential transport of the total radionuclide inventory is evaluated, if credible configurations are identified which can lead to such effects (i.e., a potential autocatalytic criticality of sufficient magnitude to create an explosive force whereby immediate dispersion of radionuclides will occur). As no credible configuration of this type has been identified, nor is it anticipated, the probability evaluations for this event type show that it falls below the 10^{-8} screening criteria, and consequence evaluations will not be performed. If such an autocatalytic configuration is recognized as credible in the future, an analysis will be performed in conjunction with a TSPA evaluation from these transient criticality events.

Criticality consequences are evaluated on a per-waste-package basis. This is necessary in order to calculate a criticality risk, to demonstrate compliance with the criterion of 10 percent radionuclide increase mentioned above. The percentage increase in radionuclide inventory is determined by the sum of the products of probability of criticality occurrence (for a single spent nuclear fuel waste package as a function of time), multiplied by the radionuclide inventory

increment due to that criticality (measured in curies), divided by the radionuclide inventory of a single waste package, with the integral taken over the entire time frame considered for repository performance evaluation. Both the radionuclide inventory and the increment due to criticality are evaluated at 1,000 years following the criticality shutdown.

Criticality evaluations are also performed considering multiple criticality events. The first type of multiple criticality effect considered is that of common mode failures. Mechanisms for common mode failures, such as design and manufacturing defects, are identified and the probability of these mechanisms evaluated. The other type of multiple criticality event is that in which the conditions leading to a critical configuration for a single waste package causes criticalities in other waste packages. The probability of these multiple criticalities for a single realization is determined. This additional probability term is then combined with the probability of the single event, to yield an overall probability for that potentially critical configuration leading to multiple criticalities. If the probability of either of these multiple-criticality events is determined to be above the 10^{-8} -per-year criterion, then a consequence evaluation is performed, in the same manner as for a single criticality. The combination of the probability and consequence of these multiple criticalities is then included in the total criticality risk term.

Criticality evaluations are also performed to determine the potential of a volcanic event to act as a predecessor to a criticality event. The methodology is similar to that of the base criticality, in terms of evaluating the probability and then the consequence (if necessary), but it differs in the potential configurations considered. This analysis consists of the following five steps:

1. Determine the probability of a volcanic event affecting the potential repository site over the evaluation period.
2. Evaluate the potential for waste package breach due to a volcanic event, as a function of the magma temperature and the degree of existing waste package shell degradation. This will include consideration of the probability distributions of all the determining parameters.
3. Evaluate the potential patterns for transport of the fissionable material by magma, considering the probabilities of patterns that confine the magma flow versus patterns that disperse the flow.
4. Evaluate the potential for accumulation of fissionable material from the magma flow, identifying the required geometries and probability of occurrence.
5. Evaluate the criticality of any accumulations identified in (4), using silica moderation, water moderation, or a combination of both, depending on the mechanism of accumulation.

If, at any step in the evaluation, the probability of a criticality from the volcanic event falls below the criterion of 10^{-8} per year for the entire repository, the evaluation is concluded as not being credible. If the probability of occurrence is above 10^{-8} per year, then the consequence of the criticality is evaluated in conjunction with a TSPA analysis considering volcanic events.

Analyses thus far have shown that the probability of criticality from volcanic intrusion within 10,000 years following emplacement is less than 10^{-8} for commercial spent nuclear fuel. Other waste forms will be evaluated.

6.5.4 Criticality Determination for Commercial Spent Nuclear Fuel

In determination of the preclosure loading curve for PWR and BWR commercial spent nuclear fuel, evaluations are performed for initial enrichments ranging from 2 to 6 wt% in 0.5 wt% increments, and assembly average burnups ranging from 20 to 50 GWd/MtU, in 10 GWd/MtU increments.

In the determination of the point at which criticality occurs, to support the postclosure probability analysis, waste form configuration parameters will cover the same range of initial enrichment and burnup as in the preclosure evaluations, but with enrichment increments of 1 wt%. Further refinements of the point at which criticality occurs will be consistent with this general methodology.

6.5.5 Criticality Determination for other DOE Waste Forms (Defense High Level Waste-Glass and DOE Spent Nuclear Fuel)

The analysis methodology for co-disposal waste packages consisting of defense high level waste and DOE spent nuclear fuel is the same as the commercial fuel methodology, with the primary exception being the preclosure loading curve determination. Material compositions of defense high level waste and DOE spent nuclear fuel are evaluated for preclosure criticality using a single bounding material composition. This composition is such that no loading curve is necessary, as all fuel meeting these criteria will be sufficiently below the preclosure criticality threshold. Postclosure analysis will follow the same general methodology addressed above.

6.5.6 Criticality Determination for Naval Fuel

The NNPP is responsible for the performance of preclosure and post-closure criticality calculations for intact naval spent nuclear fuel. The NNPP will perform these calculations in accordance with an Addendum (Mowbray 1999) to the *Disposal Criticality Analysis Methodology Topical Report* (YMP 2000).

6.6 RISK-INFORMED PROCESSES

Waste package risk-informed analyses are intended to assess the occurrence frequency or probability of the different FEPs that can contribute to the degradation of a waste package and lead to its potential breach, during the pre- or postclosure phase of the potential Monitored Geologic Repository. Since the assumptions required for these analyses may be open to interpretation and uncertainty, supplemental uncertainty and sensitivity analyses are performed.

6.6.1 Computational Tools

SAPHIRE—(Systems Analysis Programs for Hands-on Integrated Reliability Evaluations) performs integrated probabilistic risk assessment analyses for complex systems by giving the user the ability to create and analyze both fault trees and event trees (Russell et al. 1994). The version of SAPHIRE used at the time of this writing is Version 6.69 (CRWMS M&O 2001b). This program allows an analyst to perform many of the functions necessary to create, quantify, and evaluate the risk associated with a facility or process being analyzed. This program includes software to define the database structure, to create, analyze, and quantify the data, and to display

results and perform sensitivity analyses. The frequency of waste package design basis events can be readily calculated through the evaluation of fault trees and event trees constructed using this software package.

6.6.2 General Methodology

As a general rule, waste package risk-informed analyses start with a preliminary study. The purpose of this study is to compile a comprehensive list of factors that may affect the FEP to be examined. For example, in the analysis intended to evaluate mechanisms that might lead to an early failure of a waste package, a literature review was performed to obtain information on defect-related failures in various types of welded metallic containers, the types of defects that produce these failures, and the mechanisms that cause defects to propagate to failure.

Next, based on this comprehensive list, a screening phase eliminates from further consideration the FEPs that are not critical, according to various criteria. A FEP may be eliminated because it is not applicable (for example, a defect mechanism identified in the preliminary study may not be applicable to the waste package because the manufacturing processes involved are different), or because its occurrence frequency or probability is judged improbable (below an NRC regulatory limit, for instance). The screening criteria are listed as input to each risk-informed analysis.

To evaluate the occurrence frequency or probability of a FEP, probabilistic safety assessment methods such as fault-tree and event-tree modeling may be applied. For quantifying fault trees and event trees, several tools may be used, from Microsoft Excel to specific reliability tools such as the SAPHIRE software program described above.

Fault Trees—Fault trees account for every relevant combination of elementary failure modes contributing to the global occurrence frequency or probability of the studied FEP, including common mode failures and potential human errors. The failure rates associated with elementary failure modes are taken from the most relevant database available, and human error probabilities are assessed with a relevant evaluation method (such as *Handbook of Human Reliability Analysis with Emphasis on Nuclear Power Plant Applications Final Report*, Swain and Guttman 1983).

Event Trees—Event trees may be used when the studied FEP is the result of an accident sequence (scenario), i.e., an initiating event followed by other subsequent events. The frequency of the studied FEP is determined from the frequency of the initiating event and the conditional probabilities of the other events in the sequence. For example, when assessing the probability of a waste package being accidentally loaded with fuel outside its thermal design basis, different accident sequences are taken into consideration, each developing a particular scenario (for instance, in a given accident sequence, the operator performs a task correctly but fails to perform the following one).

6.6.3 Uncertainty and Sensitivity Analysis

The range of uncertainty in the results of the waste package risk-informed processes can be evaluated by means of uncertainty and sensitivity analyses. Uncertainty analyses are performed on the basis of the probability distributions of the various parameters used in the risk-informed calculations. They provide a confidence interval associated with the mean probability or occurrence frequency of the studied FEP. When dealing with complex or numerous probability

distributions, a Monte Carlo method may be used to perform the uncertainty evaluations. Sensitivity analyses are intended to identify the key factors whose variability has the most significant impact on the resulting FEP occurrence frequency or probability. Sensitivity analyses therefore make it possible to determine the most critical factors related to the studied FEP.

6.6.4 Waste Package Design Basis Events Considered

The following external design basis events for the waste package are considered:

- Vibratory ground motion due to seismic activity
- Fault displacement due to seismic activity
- Industrial-activity-induced accident
- Military-activity-induced accident.

The following internal design basis events for the waste package, associated with normal operations, are considered:

- Dead loads (load on a component produced by its own weight)
- Live loads (loads associated with the actions of handling, transportation, or emplacement)
- Internal pressure loads
- Thermal loads.

The following internal design basis events for the waste package, associated with equipment failure or operator error, are considered:

- Falling objects strike the waste package (these include a rock or handling equipment falling onto the waste package)
- Waste package drop events (these include a vertical drop from a Disposal Container Handling System bridge crane, horizontal drop from a Waste Handling Building horizontal lifting system, vertical or horizontal drop onto a sharp object, waste package on pallet falling out of a transporter, and an emplacement drift gantry dropping a waste package)
- Waste package tip-over
- Collisions and transporter accidents (these include the collision or bumping of a waste package into another waste package while being placed in a Disposal Container Cell lag storage area, transporter collisions, transporter derailment, transporter runaway, closure of transporter door onto a waste package, and emplacement gantry causing a collision with another waste package)
- Missile and explosive overpressure (including a missile from a pressurized system, and an overpressure due to a fire or explosion)
- Fire or other thermal hazards (including the loading of a disposal container with a waste form that exceeds the thermal design basis [thermal mis-loading], fire in a disposal

container cell, transporter breakdown between the waste handling building and the north portal with the accompanying solar incidence, thermal mis-loading of waste packages within an emplacement drift, loss of underground ventilation, and rock fall burying emplaced waste package with debris)

- Fuel rod rupture and internal pressurization
- Criticality (including the loading of a disposal container with a waste form that exceeds the waste package criticality design basis, waste package flooding, and waste package internal geometry failure).

6.6.5 Waste Package Defects Considered

Eleven generic types of defects have been identified in the *Analysis of Mechanisms for Early Waste Package Failure* (CRWMS M&O 2000a) as having potential consequences for the early failure of the waste package. These defects are:

1. Weld flaws
2. Base metal flaws
3. Improper weld material
4. Improper heat treatment
5. Improper weld flux material
6. Poor weld joint design
7. Contaminants
8. Mislocated welds
9. Missing welds
10. Handling or installation damage
11. Administrative or operational error.

These defects could be introduced to the waste package during the fabrication, transport, storage, loading, closure, or emplacement processes. However, of these eleven defects identified, only the following seven were found to be applicable to the waste package:

1. Weld flaws
2. Base metal flaws
3. Improper weld material
4. Improper heat treatment
5. Contaminants
6. Handling or installation damage
7. Administrative or operational error.

7. SUMMARY

No developed data were created in this report. This report describes the methodology used by the Waste Package Design Section to design the various waste packages, emplacement pallet, and drip shield; however, it does not make any recommendations regarding the final design of either the waste packages or the repository. The accounting of uncertainties in the methodology falls into one of two categories. For most, parameters are selected that produce net conservative results. These require no additional treatment. For a few, comparison against benchmarks, either experimental or high-order computational methods, must be performed. Comparisons against such benchmarks are planned to be addressed in later revisions to this document. Since this is a design methodology, subsequent use is restricted only to the extent that such use would invalidate the theory undergirding the particular application.

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

8. INPUTS AND REFERENCES

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8.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

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10 CFR 51. Energy: Environmental Protection Regulations for Domestic Licensing and Related Regulatory Functions. Readily available.

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10 CFR 71. Energy: Packaging and Transportation of Radioactive Material. Readily available.

10 CFR 72. Energy: Licensing Requirements for the Independent Storage of Spent Nuclear Fuel and High-Level Radioactive Waste. Readily available.

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8.3 SOURCE DATA, LISTED BY DATA TRACKING NUMBER

MO0007RIB00077.000. In Situ Rock Conditions. Submittal date: 07/18/2000.

MO0009THERMODYN.001. Input Transmittal for Thermodynamic Data Input Files for Geochemical Calculations. Submittal date: 09/20/2000.

MO9808RIB00041.000. Reference Information Base Data Item: Rock Geomechanical Properties. Submittal date: 08/05/1998.