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

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

Revision 01

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September 4, 1997

Prepared for:

**U. S. Department of Energy
Yucca Mountain Site Characterization Project Office
P.O. Box 30307
Las Vegas, Nevada 89036-0307**

Prepared by:

**Office of Civilian Radioactive Waste Management System
Management and Operating Contractor
1180 Town Center Drive
Las Vegas, Nevada 89134**

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Civilian Radioactive Waste Management System
Management & Operating Contractor

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Prepared by:



D. A. Thomas, Lead Coordinating Author
Waste Package Development

Date:

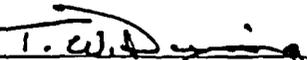
09/03/97

Authors:

R. A. Barnard, Performance Assessment
Peter Gottlieb, Waste Package Development
J. R. Massari, Waste Package Development
C. W. Mays, Waste Package Development,
Lead Technical Author

J. K. McCoy, Waste Package Materials
J. A. McNeish, Performance Assessment
M. L. Scott, Licensing
D. A. Thomas, Waste Package Development,
Lead Coordinating Author

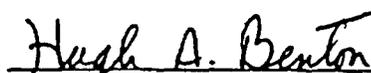
Checked by:


T. W. Doering, Manager
Waste Package Design

Date:

9.3.97

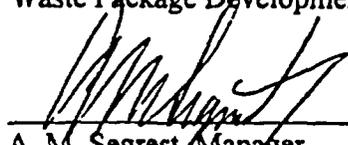
Approved by:


H. A. Benton, Manager
Waste Package Development

Date:

9/3/97

Approved by:


A. M. Segrest, Manager
Mined Geologic Disposal System

Date:

9/3/97

Civilian Radioactive Waste Management System
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Concurred by: K. L. Ashe Date: 9/2/97
K. L. Ashe, Manager
Licensing

Concurred by: R. W. Andrews Date: 09/03/97
R. W. Andrews, Manager
Performance Assessment

Concurred by: David Stahl Date: 9/3/97
David Stahl, Manager
Waste Package Materials

Reviewed by:

R. W. Andrews, Performance Assessment
K. L. Ashe, Licensing
H. A. Benton, Waste Package Development
B. M. Cole, Waste Management and Integration - Waste Acceptance
Mark Fortsch, Repository - Surface Design
C. R. Hasting, Project Engineering
F. H. Lentz, OCRWM Quality Assurance
R. D. Memory, Systems Engineering - MGDS Systems Analysis and Modeling
J. M. Skov, Systems Engineering - MGDS Safety Assurance
David Stahl, Waste Package Materials
Steve Su, Repository - Subsurface
N. D. Sudan, Systems Engineering - Requirements and Integration
W. E. Wallin, Product Checking Group
M. R. Wisenburg, Waste Management and Integration - Science & Engineering

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Minor revisions to Chapter 5

Chapter 6 moved to an Appendix (new Appendix B)

Minor revisions to Chapter 7, Chapter 7 moved (new Chapter 6)

Chapter 8 removed (dispersed to sections in other chapters)

Chapter 9 moved (new Chapter 7)

Minor additions to Appendices A.1 and A.2

Appendices B.1, B.2, C, and D removed (separate technical reports)

Appendix B major revisions (new sections, moved old Chapter 6)

Appendix C added on Aluminum-based DOE fuel example

PREFACE

The United States Department of Energy (DOE) is developing a postclosure methodology for criticality analysis to evaluate disposal of commercial spent nuclear fuel and other high-level waste in a geologic repository. A topical report on the postclosure disposal criticality analysis methodology is scheduled to be submitted to the United States Nuclear Regulatory Commission (NRC) for formal review in 1998 (to be verified). This technical report is being issued to describe the current status of the postclosure methodology development effort. Although it is structured similarly to the formal topical report, this technical report reflects work-in-progress, and contains inconsistencies in level-of-detail and completeness which will be remedied over the next year.

This report is intended primarily as a vehicle for obtaining feedback from reviewers regarding the methodology as it has evolved to this point in time. Preliminary sample applications of the methodology are provided in Appendices B and C as examples to facilitate more detailed review and comment. Where available, references are provided to sources of more detailed supporting data. Areas of this technical report that are incomplete or where additional supporting data is required for completion of the topical report are identified (i.e., marked "to be determined" (TBD) or "to be verified" (TBV)).

This technical report was prepared in accordance with the Civilian Radioactive Waste Management System (CRWMS) Management & Operating (M&O) Contractor Quality Administrative Procedures (QAPs). The responsible manager for Waste Package Development has evaluated the technical report development activity in accordance with QAP-2-0, Conduct of Activities. The *Prepare the Disposal Criticality Analysis Methodology Technical Report*^{P-1} evaluation concluded that the development of this report is subject to the DOE Office of Civilian Radioactive Waste Management (OCRWM) *Quality Assurance Requirements and Description* (QARD)^{P-2} controls. The methodology described in this report is related to the evaluation of the Mined Geologic Disposal System (MGDS) waste package and engineered barrier system; the waste package and engineered barrier system have been identified on the Yucca Mountain Site Characterization Project Q-List^{P-3} as items important to safety and waste isolation. The waste package is on the Q-List by direct inclusion by the DOE; an evaluation in accordance with procedure QAP-2-3, Classification of Permanent Items, has yet to be conducted. There are no determination of importance evaluations developed in accordance with Nevada Line Procedure NLP-2-0, since this report does not involve any field activity.

Much of the quality-affecting information in this report has not been verified under the OCRWM quality assurance program controls in accordance with the QARD. The quality-affecting information presented in this report has been developed using standard nuclear industry quality assurance practices (NQA-1). Therefore, the unverified information presented in this report will be treated as unqualified or unconfirmed and will be marked TBV or TBD, or otherwise clearly identified, and referenced to a source. In addition, Chapter 2 of this report addresses regulatory topics and issues that are considered as unqualified and unconfirmed by the M&O quality assurance program. The information presented in this report is not design information that can be used to support procurement, fabrication, or construction. The software used in this report's sample evaluations (Appendices B and C) has not all been validated in accordance with the M&O QAP computer software controls (QAP-SI series procedures). Sample results reported in the report are therefore designated as TBV in accordance with Attachment II of QAP-3-5/Revision 7.

This technical report has no interfaces outside the OCRWM program. This technical report does have some interfaces on common topics being developed in different areas of OCRWM, namely, burnup credit. The technical report references information also presented in the "Topical Report on Actinide-Only Burnup Credit for PWR Spent Nuclear Fuel Packages" (currently under review by the NRC). Some of the data and part of the methodology described in the "Actinide-Only" burnup credit topical report will be referenced as appropriate in describing the disposal criticality analyses methodology.

In reviewing this revision of the technical report, the reviewer should realize that this is not the final version of the topical report. It is intended to inform the reader of the current state of development of the methodology for disposal criticality analysis, to provide some of the supporting data for the methodology, and to identify the additional data and supporting analyses required.

References:

- P-1. *Activity Evaluation: Prepare the Disposal Criticality Analysis Methodology Technical Report*, CRWMS M&O, March 1997.
- P-2. *Quality Assurance Requirements and Description*, DOE/RW-0333P REV 7, U.S. DOE.
- P-3. *Q-List*, YMP/90-55Q REV 04, Yucca Mountain Site Characterization Project.

ABSTRACT

| This report describes the analysis methodology that is planned for use in demonstrating
| postclosure criticality control for the potential Yucca Mountain spent nuclear fuel and high-level
| waste repository. A risk-based methodology will be used to demonstrate disposal criticality
| control and to demonstrate that public health and safety is protected. The various models
| contained in the methodology are described and the validation process for these models
| presented. The criticality related criteria for determining the suitability of waste packages for
| emplacement in the repository are described along with the physical implementation and control
| procedures to be followed. Sample evaluations are provided in two appendices to illustrate the
| methodology presented in the report. Details of the experimental data used to validate the
| models, sources of information to establish the probabilities of events, and calculational data are
| provided in references, as indicated in the report. When complete, the methodology will provide
| a systematic approach for evaluating a waste form/waste package/engineered barrier/repository
| system combination for disposal criticality control through the entire postclosure period of
| regulatory concern.

When the development of the methodology described in this technical report is completed, it will
be documented in a topical report. The United States Nuclear Regulatory Commission staff will
be asked to review the topical report and accept the methodology. The United States Department
of Energy will then use the approved methodology in the license application for the potential
| Yucca Mountain repository to demonstrate the acceptability of proposed systems for control of
| criticality.

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TABLE OF CONTENTS

Chapter - Section	Page
PREFACE	v
ABSTRACT	vii
1.0 INTRODUCTION	1-1
1.1 Background	1-1
1.2 Objective	1-2
1.3 Scope	1-3
1.4 Methodology Implementation Strategy	1-5
1.5 Disposal Criticality Control Methods	1-6
1.5.1 Burnup Credit	1-7
1.5.2 Basket Design as a Criticality Control Method	1-8
1.5.3 Neutron Absorber Credit	1-9
1.5.4 Limiting the Amount of Moderator	1-9
1.6 Overview of the Report	1-10
1.7 References	1-12
2.0 REGULATORY PERSPECTIVE	2-1
2.1 NRC Guidance and Industry Standards	2-2
2.1.1 NUREGs	2-2
2.1.2 Industry Standards	2-2
2.1.3 Regulatory Guides	2-5
2.2 Risk-Based Analysis and the Current Regulatory Framework	2-6
2.3 Burnup Credit	2-8
2.4 References	2-8
3.0 METHODOLOGY	3-1
3.1 Approach	3-1
3.2 Features, Events, and Processes	3-3
3.2.1 FEPs Which May Lead to Internal Criticality	3-4
3.2.2 FEPs Which May Lead to Near-Field Criticality	3-9
3.2.3 FEPs Which May Lead to Far-Field Criticality	3-10
3.2.4 Evaluation of FEPs with Respect to Criticality Potential	3-14
3.3 Probabilistic Evaluations of Events and Processes	3-14
3.3.1 Probabilistic Evaluations Beyond the Capability of Traditional PRA ..	3-15
3.3.2 Introduction to Probabilistic Methodology	3-16
3.3.3 Scenario Identification, Generation, and Evaluation	3-19
3.3.4 Configuration Generator	3-21
3.4 Criticality Analysis	3-23
3.4.1 Computer Codes	3-23
3.4.2 Material Composition of SNF	3-23
3.4.3 SNF Principal Isotopes for Burnup Credit	3-25
3.4.4 Criticality Evaluations	3-26

TABLE OF CONTENTS

Chapter - Section	Page
3.5 Criticality Consequence Analysis	3-27
3.5.1 Type of Criticality Event	3-27
3.5.2 Evaluation of Direct Criticality Event Consequences	3-28
3.6 Criticality Impact on Risk Assessment and Performance Assessment	3-29
3.6.1 Risk Assessment Definitions	3-29
3.6.2 Methodology for Incorporation into TSPA	3-30
3.7 References	3-31
4.0 MODEL DESCRIPTION AND VALIDATION	4-1
4.1 Neutronics Models	4-1
4.1.1 Isotopic Model	4-1
4.1.2 Criticality Model	4-3
4.1.3 Neutronics Model Validation	4-5
4.2 Scenario Evaluation and Configuration Generation	4-12
4.2.1 Configuration Generation Code	4-13
4.2.2 Probability Combination Methodology	4-15
4.2.3 Abstraction of Models	4-15
4.2.4 Model Details	4-18
4.3 Criticality Consequence Model	4-32
4.4 Total System Performance Models	4-33
4.5 References	4-38
5.0 WASTE DISPOSAL CRITICALITY ACCEPTABILITY CRITERIA	5-1
5.1 Waste Package/EBS Criticality Acceptability Criteria	5-1
5.2 Physical Implementation and Controls	5-2
5.2.1 Fuel Assembly Records	5-2
5.2.2 Burnup/Fissile Content Verification	5-3
5.2.3 Waste Package Loading Procedure	5-4
5.3 References	5-4
6.0 SUMMARY AND CONCLUSIONS	6-1
7.0 LIST OF APPENDICES	7-1
ACRONYMS AND ABBREVIATIONS	Appendix A.1
GLOSSARY	Appendix A.2
SAMPLE OF THE DESIGN PROCESS AND METHODOLOGY APPLICATION	Appendix B
SAMPLE APPLICATION OF THE METHODOLOGY TO DOE SNF	Appendix C

LIST OF FIGURES

	Page
Figure 3-1. Overview of Disposal Criticality Analysis Methodology	3-2
Figure 3-2. Overview of Scenarios for the Three Locations of Potentially Criticality Configurations	3-5
Figure 3-3a. Internal Criticality Scenarios for General Waste Forms	3-7
Figure 3-3b. Internal Criticality Scenarios for General Waste Forms	3-8
Figure 3-4. Near-Field Criticality Scenarios for General Waste Forms	3-11
Figure 3-5. Far-Field Unsaturated Zone Criticality Scenarios for General Waste Forms .	3-12
Figure 3-6. Far-Field Saturated Zone Criticality Scenarios for General Waste Forms ...	3-13
Figure 3-7. Example Waste Package Configuration Logic Tree	3-18
Figure 3-8. Criticality Analysis Process	3-24
Figure 4-1. Components of the Repository Integration Program which are Used for Total System Performance Assessment	4-37

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LIST OF TABLES

	Page
Table 3-1. SNF Principal Isotopes for Burnup Credit	3-26
Table 4-1. Materials Proposed for Use in Disposal Containers	4-23
Table 4-2. Current Waste Package Materials Selection	4-24

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DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

1.0 INTRODUCTION

The United States Congress assigned the Department of Energy (DOE) the responsibility of managing the geologic disposal of commercial spent nuclear fuel (SNF) and high level waste (HLW) vitrified glass by enactment of the Nuclear Waste Policy Act¹⁻¹ of 1982 and the Amendments Act¹⁻² of 1987. Criticality control is an important aspect of geologic disposal and must be evaluated for license applications. This report describes a methodology that is being developed to provide a technical basis for postclosure disposal criticality evaluations. The completed methodology will be presented to the Nuclear Regulatory Commission (NRC) in a topical report and will, after acceptance by the NRC, be used in the license application for the potential Yucca Mountain repository to demonstrate acceptability of proposed systems for postclosure control of criticality.

1.1 Background

The planned DOE approach for demonstrating postclosure disposal criticality control is risk-based. The risk-based approach is expected to be able to demonstrate, in a licensing proceeding, that the health and safety of the public will be protected against the consequences of potential criticality events. Risk is defined in this document as the product of the probability of a given event or set of processes representable as an event occurring and its consequences. The risk-based approach may be thought of as a "bottom-line" approach that bases acceptability of the system design for criticality control on its projected effect on the health and safety of the public. When dealing with radioactivity, the measure of effect on health and safety is radioactive dose projected to be received by the public.

The Yucca Mountain Project planning assumption, to be validated during development of the disposal criticality analysis methodology, is that the risk-based approach to dealing with disposal criticality is not only the best approach, but also that it is the only feasible approach. The reasons for this assumption are discussed in Chapter 2 of this technical report.

Although a risk-based approach is being pursued, criticality events are considered undesirable even if the risks posed are determined to be small. Therefore, the approach also includes defense-in-depth to minimize the probability that potential postclosure criticalities will occur.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

The methodology presented in this technical report is not yet mature. It will be fully developed in fiscal year 1998 and will be submitted in the form of a topical report to the NRC for acceptance. If accepted by the NRC, it will be used and referenced in a future potential license application to demonstrate compliance with the disposal criticality requirements.

The methodology will be used to estimate the probability and nature of potential criticality events. These estimates will be used to predict increments to the repository radionuclide source term and the repository thermal effect. Chapter 3 of this technical report provides additional information on how these results will be used as input into total system performance assessments to predict the effects of potential disposal criticality on the ability of the repository to protect the health and safety of the public.

1.2 Objective

The objective of this report is to present the methodology being developed for performing criticality analyses for the postclosure period of geologic repository performance. This technical report is intended to describe the methodology at its present state of development. The completed methodology will be documented in a topical report. This technical report also provides a preliminary sample application of the methodology for commercial light water reactor (LWR) SNF (Appendix B) and for an aluminum-based DOE-owned SNF (Appendix C).

The topical report will specifically seek NRC acceptance of the following (references are to sections of this technical report that provide information on the associated topics):

1. The methodology for performing postclosure criticality analyses for disposal of commercial LWR SNF including the following models supporting this methodology:
 - a. The neutronics models (Section 4.1). These include:
 - i. The commercial SNF isotopic model (Section 4.1.1) for determining concentrations of the 14 actinides and 15 fission products (29 principal isotopes) analyzed.
 - ii. The criticality calculational model (Section 4.1.2) for determining the criticality potential (k_{eff} , effective neutron multiplication factor) of configurations. Upper subcritical limits are then determined from analysis of

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

experimental criticality data and represents an upper bound for the calculated k_{eff} of the type of system being analyzed.

- b. The configuration generation models (Section 4.2). These include:
 - i. The repository environment model (Section 4.2.4.1).
 - ii. The waste package/engineered barrier material degradation model (Section 4.2.4.2).
 - iii. The waste form degradation model (Section 4.2.4.3).
 - iv. The material transport model (Section 4.2.4.4).
 - v. The transport retardation/precipitation models (Section 4.2.4.5).
- c. The criticality consequence model (Section 4.3) for determining the potential impact of a criticality event on the radionuclide inventory and thermal effect, should such assessment be determined to be necessary based on the results of criticality analysis.

2. Validation of the following neutronics code systems for use in criticality analyses of commercial SNF for disposal in a repository, based on the neutronics models (item 1.a.) validation strategy presented in Section 4.1.3:

- a. SAS2H sequence of the SCALE-4.3¹⁻³ code system using the 44 energy group cross section library.
- b. MCNP 4A¹⁻⁴ code system with its associated continuous energy cross section libraries.

Addenda to the topical report (TBD) will seek NRC acceptance of the necessary extensions to the methodology to cover application to other waste forms (e.g., aluminum-based DOE-owned SNF).

1.3 Scope

This technical report is to be used for informational purposes only. This document presents a risk-based disposal criticality analysis methodology for the postclosure period. The scope of the

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

technical report and planned topical report (to be developed from this technical report) is limited as follows:

- Applies, in general, to any waste form but the details described in this report (with the exception of Appendix C) apply specifically to SNF from commercial LWRs. Specific models in the methodology will not apply to all waste forms (e.g., isotopics model for burnup credit). Addenda to the topical report will contain extensions to these models to accommodate other waste forms (e.g., HLW vitrified glass, DOE-owned SNF, MOX SNF, and immobilized Pu).
- Applies to analysis of potential criticality events both inside and outside the waste packages, for the postclosure period.
- Describes the criticality analysis methodology, validation of certain codes and models as part of that methodology, and uncertainties and conservatisms (TBD; to be determined) in the methodology. Does not describe the design basis or design strategy for providing disposal criticality control. The design basis will be provided or referenced in the license application.
- Describes the approach for establishing the probability and process of assembling spent nuclear fuel material into potentially critical configurations.
- Describes the range of applicability of the methodology for criticality analyses in the repository (TBD).
- Describes the approach for predicting radionuclide source terms and thermal effects used as input to total system performance assessment (TSPA) but does not discuss in detail the TSPA analyses.

[Note: As stated, the full proposed methodology in this report is specifically for commercial LWR SNF. Most of the models in the base methodology should cover any of the waste forms (TBD; to be verified). Future amendments or addenda will be made, as appropriate, covering any of the other waste forms selected for disposal and will address any special aspects or differences from the base methodology (e.g., different waste form corrosion model). An example application of the methodology for aluminum-based DOE-owned SNF is provided in Appendix C.]

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

1.4 Methodology Implementation Strategy

The disposal criticality methodology will be implemented within a well defined overall methodology that will assure timely input from all the affected technical disciplines. The objective of this overall strategy is to assure the timely identification of all possible scenarios that can lead to criticality and the criticality evaluation of the configurations that can result from these scenarios, over the range of parameters that can characterize such configurations. The overall methodology is summarized as follows:

1. The features, events, and processes (FEPs) which can lead to criticality are identified and combined into a preliminary set of scenarios by an interdisciplinary team. This team has already met in a three-day workshop¹⁻³ and produced the preliminary set of FEPs and scenarios. These are identified in Section 3.2, together with plans for future reviews as the methodology evolves. These future reviews will also cover the values to be used for environmental and material performance parameters (ranges or probability distributions).
2. The chemical and geochemical processes acting on the waste package, the waste form, and any additional criticality control material are analyzed theoretically to determine the solubilities and concentrations of neutronically significant species in altered forms and precipitates, using the computer codes and methodology described in Section 3.2.4. These results will be reviewed by representatives of the interdisciplinary team.
3. The configuration generation code is used to calculate the range of concentrations of neutronically significant species in the configurations identified in the previous two items. In this code the solubility sub-model will be modified to include the abstraction of the theoretical solubility results (representing the solubility as an empirical or analytic function of solution pH, etc.), and the transport submodel will be consistent with any detailed transport calculations performed as part of the TSPA process. The code and its calculations will be reviewed by representatives of the interdisciplinary team to verify the abstractions of the solubility and transport calculations and to assess the reasonableness of the results. A description of the configuration generation code is given in Section 3.3.3.
4. The values of k_{eff} are calculated for the configurations and representative values from the range of concentrations identified in the previous item (according to the methodology given

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

in Section 3.4). These values are used to establish regressions for k_{eff} as a function of the concentrations of the neutronically significant elements in the configurations considered.

5. The criticality configuration generation code is used to evaluate the criticality of the configurations using the regressions for k_{eff} from the previous item. The results are expressed in terms of probability distributions of the parameters representing criticality performance (e.g., earliest time to criticality, number of critical configurations before some time, and peak value of k_{eff}), based on probability distributions of the input values of environmental and material performance parameters. These results can also be represented by single parameters of the distribution, particularly mean and probability of exceeding a specific value (threshold). Changes in such summary parameters measure sensitivity of criticality performance to the material performance parameter distributions and to alternative design features (e.g., enhancement barrier * drip shield, denaturing with depleted uranium). Such sensitivities are used to evaluate design alternatives and demonstrate that the incorporation of the appropriate alternatives provides defense-in-depth.
6. The direct criticality consequences are estimated for representative configurations which indicate criticality in step 5, above. The principal direct consequence of a criticality is the expected increase in radionuclide inventory, which is computed according to the methodology given in Section 3.5.2.
7. The risk associated with potential criticalities is estimated from the product of the probability of occurrence multiplied by the dose at the boundary of the accessible environment and summed over all possible criticality events (or probability-consequence pairs). The performance assessment model is used to evaluate the dose attributable to the criticality alone and to compare it with the dose from the radionuclide inventory emplaced in the repository, according to the methodology described in Section 3.6.2.

1.5 Disposal Criticality Control Methods

Criticality control methods are required to ensure compliance with regulatory requirements. An overview of criticality control methods that may be used for disposal criticality is presented in this section. In addition to these methods, burnup credit (taking credit for fuel depletion and the generation of neutron absorbers in spent nuclear fuel assemblies) may be used to assist in

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

meeting regulatory requirements. Although burnup credit is not a design method that is implemented for criticality control, burnup is an intrinsic property of spent nuclear fuel that may be considered in designing criticality control systems. The disposal criticality analysis methodology must be able to evaluate the effectiveness of burnup credit and the design methods used for controlling criticality. Validation of the codes and models used to evaluate the criticality control potential of these methods and the range-of-applicability of this methodology are addressed in Section 4.1.

Criticality control requirements for waste-package disposal can be satisfied by using burnup credit and the following design control methods, separately or in combination:

1. Geometry restrictions.
2. Limiting the amount of fissionable material.
3. Adding neutron absorber material.
4. Limiting the amount of moderator.

Burnup credit and the other control methods used to satisfy requirements are addressed in the following subsections.

[Note: "Fissionable" is used in most places in this report instead of "fissile", although fissile may be applicable for most configurations from commercial SNF.]

1.5.1 Burnup Credit

Burnup credit is the process of accounting for the reduced reactivity of spent nuclear fuel (commercial LWR SNF) as compared to fresh fuel of the same initial enrichment. The approach recognizes that the fuel has been irradiated and accounts for the net depletion of fissionable material and for the creation of neutron-absorbing isotopes as a result of fission in an operating reactor. The criticality potential of SNF also varies with cooling time (the time since removal from the reactor core) as radionuclides are created and subsequently decay. Neutronics models used to estimate the criticality potential of SNF show that the reduced reactivity (criticality potential) due to burnup is a valuable contributor to long-term criticality control.

Evaluation, using the burnup credit approach, of an engineered barrier system design requires a reasonable and conservative prediction of the isotopic composition of the SNF and analysis of

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

the system reactivity based on these isotopes. The burnup credit methodology is validated using experimental data. This includes laboratory criticality experiments, commercial LWR criticality data, and chemical assay data for commercial SNF. Analysis of these data establishes the biases and uncertainties in the methodology and extends these biases and uncertainties to the range of applicability for long-term waste disposal in a repository. The burnup credit methodology presented in this report is applicable for configurations internal to waste packages. For external configurations, the material separation, transport, and deposition processes are such that credit cannot be taken for fission products which were formerly present in the ceramic form of the SNF. However, credit is still applicable for most actinides. More discussion on the applicability of burnup credit is provided in Sections 3.4 and 4.1.3.

The methodology described in this report references the data and parts of the methodology presented to the NRC in the "Topical Report on Actinide-Only Burnup Credit for PWR Spent Nuclear Fuel Packages"¹⁻⁶.

[Note: Current plans(TBV) are to only apply burnup credit with commercial LWR SNF.]

1.5.2 Basket Design as a Criticality Control Method

Geometry restrictions are implemented in the waste package through the use of a basket, which restricts the arrangement of fuel within the canister or container. The amount of fissionable material (number of fuel assemblies) in the waste package is also limited by the basket design. (Limiting the amount of fissionable material is the ultimate criticality control method.) The basket design controls the number of fuel assemblies and their arrangement within the waste package, and therefore affects the criticality potential of the system. The degradation of the basket over time (and the potential loss of geometry control) is an important consideration for the criticality analysis methodology.

The disposal criticality analysis methodology, as described, will account for the geometry of materials and amounts of fissionable material in systems being analyzed. Validation of neutronics models for analyzing various amounts and geometric arrangements of fissionable materials is described in Section 4.1.3. The material performance aspects of the basket are presented in Section 4.2.4.2.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

1.5.3 Neutron Absorber Credit

Neutron absorbers are materials that capture neutrons to prevent them from continuing to add to the fission chain reaction. The use of supplemental neutron absorber materials is an accepted method for criticality control. Neutron absorber credit is routinely used as a criticality control measure in reactors, spent fuel pools, and cask systems.

Maintaining criticality control with a neutron absorber depends upon retaining the absorber in the carrier material. Potential mechanisms for loss of the absorber material through physical removal (e.g., leaching or preferential corrosion) must be considered. Material performance and neutron depletion evaluations must be made for the neutron absorber material loaded into a control system (e.g., panel or rod). This will determine the amount of absorber available for criticality control at future times during disposal in the repository. More discussion on neutron absorber credit as it applies to disposal criticality analysis appears in Chapter 4. The neutronics aspects are presented in Section 4.1.3, while the material performance aspects are presented in Section 4.2.4.2.

1.5.4 Limiting the Amount of Moderator

The presence of moderator material in a waste package containing commercial LWR SNF increases the reactivity of the package. Since the engineered barrier system is designed to reduce the presence of moderating material, the only source of moderator of concern for criticality control internal to the waste package results from the condition in which water enters the waste package. The inclusion of additional (filler) material to limit the amount of water that can enter the waste package is referred to as moderator displacement. Moderator displacement is an effective criticality control mechanism. Use of a particular filler material for criticality control requires quantification of the amount of the filler material that can be loaded in the package, the reactivity effect of displacing an equivalent amount of moderator, the impact on waste package mass due to the addition of the filler material, and whether the filler material remains in a breached waste package. The waste package should also be evaluated against the thermal requirements after the addition of filler to the design. Evaluations and experiments are being performed (TBD) to ensure that the material performance characteristics of the possible filler will permit it to last over the time period of concern. More discussion of moderator displacement filler material as it applies to disposal criticality analysis appears in Chapter 4. The neutronics

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

aspects are presented in Section 4.1.3, while the material performance aspects are presented in Section 4.2.4.2 (TBV).

In addition to the specific criticality control features of a filler material, the following issues concerning degradation must also be considered when using a filler material:

- a. Chemical interactions between the filler and waste must not compromise the function of the waste package,
- b. Filler materials with explosive, pyrophoric or chemically reactive characteristics are precluded,
- c. Filler materials that are liquid under ambient repository conditions are precluded,
- d. Galvanic interactions between the filler material and other components must not compromise the function of the waste package, and
- e. Filler materials or their decomposed/reacted components must not accelerate the transport of radionuclides through any of the barriers.

[Note: Other methods exist for limiting moderator (i.e., moderator exclusion and rod consolidation), but are not preferred for disposal applications due to material performance issues and impacts on functions other than criticality. The analysis methodology will be able to evaluate the other methods, if they are used for disposal.]

1.6 Overview of the Report

This report presents a methodology for performing criticality analyses for long-term disposal of commercial spent nuclear fuel in a geologic repository. Chapter 1 presents the objectives and scope of this report, briefly summarizes the methodology and presents the strategy for implementation, and provides an overview of criticality control methods for an engineered barrier system in a repository. It was noted that the methodology presented in this report is a risk-based methodology.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

Chapter 2 discusses industry technical standards and regulatory guidance documents used or proposed to be used in whole or in part in development of the methodology. This chapter also addresses the need for a risk-based disposal criticality analysis, and it describes the current status of efforts to obtain credit for burnup.

Chapter 3 presents the methodology being developed for evaluating the criticality potential of commercial spent nuclear fuel emplaced in the potential Yucca Mountain repository. This methodology is based on specific models. These models and their validation are discussed in Chapter 4. The neutronics models for performing disposal criticality analyses, the models for identifying configurations for criticality analyses, and the criticality consequence model are described. The relevant total system performance models are also briefly described for informational purposes. The neutronics models are used in determining the isotopic composition of SNF and performing criticality analyses for various configurations of SNF. The computer code systems, cross section libraries, and measured data used in the model development and validation are described. Included in the configuration generator are models for the repository environment, material and waste form degradation, material transport, and transport retardation/precipitation. Some of these models are identical to the total system performance models, since similar processes and events are considered by both functions. The criticality consequence model evaluates the impact of a potential critical configuration. Both steady-state and transient models are discussed. Measured/experimental data used in model development and validation are included in the references.

Chapter 5 presents the waste disposal criticality acceptability criteria for waste shipments received at the repository, along with the physical implementation and administrative controls relating to the loading of waste packages. The required documentation accompanying the shipments is discussed, as well as the verification process.

Chapter 6 summarizes the methodology presented in this report and provides conclusions regarding the purpose, potential uses, and limitations on the uses of the methodology. A listing of the appendices is included in Chapter 7.

A listing of acronyms and abbreviations is presented in Appendix A, along with a glossary of terms. Appendix B provides a sample evaluation using the methodology described in this report for commercial SNF. An example of extending the methodology to aluminum-based DOE-owned SNF is provided in Appendix C. References are provided at the end of each chapter.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

1.7 References

- 1-1. *Nuclear Waste Policy Act of 1982, Public Law 97-425*. January 7, 1983.
- 1-2. *Nuclear Waste Policy Amendments Act of 1987, Public Law 100-23*. December, 1987.
- 1-3. *SCALE 4.3, RSIC Computer Code Collection, CCC-545*, Oak Ridge National Laboratory, October 1995.
- 1-4. *MCNP 4A - Monte Carlo N-Particle Transport Code System, Version 4A*, RSIC Computer Code Collection, CCC-200, Oak Ridge National Laboratory, February 1994.
- 1-5. *Criticality Abstraction/Testing Workshop Results*, DI Number: B00000000-01717-2200-00187 REV 00, CRWMS M&O.
- 1-6. *Topical Report on Actinide-Only Burnup Credit for PWR Spent Nuclear Fuel Packages*, DOE/RW-0472 Rev. 1, DOE OCRWM, Washington, D.C., May 1997.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

2.0 REGULATORY PERSPECTIVE

| This chapter addresses regulatory topics and issues and shall be considered as unqualified and unconfirmed information in accordance with the Civilian Radioactive Waste Management (CRWMS) System Management and Operating Contractor (M&O) Quality Assurance Program. This information was developed by the M&O Licensing Department using the Chapter 2 references identified in Section 2.4. It should be noted that this chapter does not contain design information.

| The purpose of the Disposal Criticality Analysis Methodology Technical Report is to present a risk-based methodology for criticality analysis that is appropriate for use in analysis of the postclosure period in a potential repository. As discussed in Chapter 1, this technical report describes the methodology at its present, incomplete state of development. Development and refinement of the methodology will continue to support development of the Disposal Criticality Analysis Methodology Topical Report. This topical report will provide a methodology for disposal criticality analysis that will be used to demonstrate compliance with applicable NRC regulations. The framework within which the DOE will ensure compliance with regulatory requirements is contained in the Office of Civilian Radioactive Waste Management (OCRWM) technical document hierarchy. Details of this hierarchy are provided in Section 1.2 of the CRWMS Requirement Document.²⁻¹

| In contrast to the topical report, this technical report is not a regulatory document and has no specific regulatory-related function. However, the methodology described in this technical report (revised and further developed as needed) is proposed for use in the topical report. Therefore, the information presented in this technical report may eventually be used to support a regulatory function.

| This chapter of the technical report provides information on certain regulatory-related aspects of criticality control and analysis. It describes NRC guidance and industry standards that have been used in development of the postclosure disposal criticality analysis methodology. It also discusses the need for a risk-based criticality analysis methodology. Finally, it discusses burnup credit, an important aspect of demonstrating compliance with disposal criticality regulations.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

2.1 NRC Guidance and Industry Standards

The DOE has used NRC guidance and various applicable industry standards in the development of this criticality analysis methodology. Additional guidance may be used in the further development and refinement of the methodology.

2.1.1 NUREGs

The DOE, in developing the disposal criticality analysis methodology, has reviewed the information and guidance contained in *NUREG/CR-2300²⁻², A Guide to the Performance of Probabilistic Risk Assessments for Nuclear Power Plants*. This guide provides methods and information for performing the three levels of analysis for a nuclear power plant risk assessment. In general, much of the information contained within NUREG/CR-2300 is specific to the analysis of nuclear power plants, and is not applicable to disposal criticality analysis. However, the flow of the disposal criticality risk analysis as described in this technical report is consistent with the three levels of Probabilistic Risk Assessments (PRA) discussed in NUREG/CR-2300.

The methodology entails the following steps: 1) identifying sequences of events and/or processes leading to criticality and determining the probability of each sequence; 2) estimating the power, duration, and radionuclide inventory increase resulting from each criticality sequence; and 3) estimating the consequences of each criticality sequence on the performance of the repository as part of the Total System Performance Assessment (TSPA).

The DOE has also used *NUREG/CR-6361²⁻³, Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages*, as a source of guidance in selecting benchmark cases to validate the criticality code system in the disposal criticality analysis methodology.

The DOE may use other NUREGs in refining the methodology for the topical report. The topical report will explicitly reference each such document that is used.

2.1.2 Industry Standards

The DOE, in developing this criticality analysis methodology, has assessed the following industry standards:

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

- *ANSI/ANS-8.1-1983, American National Standard for Nuclear Criticality Safety in Operations with Fissionable Materials Outside Reactors.*^{2,4} This standard provides guidance for the prevention of criticality accidents in the handling, storing, processing, and transporting of certain fissionable material, specifically U-233 and U-235 and Pu-239. It provides basic criteria and limits for certain simple geometries of fissionable materials. It also states requirements for establishing validity and ranges of applicability of any calculational method used in assessing criticality safety.

The methodology described in the technical report for criticality analyses external to a waste package (both near-field and far-field locations) uses and is consistent with this standard. The guidance in this standard is followed in establishing subcritical limits. Its guidance for establishing bias by correlating the results of criticality experiments with results obtained for these same systems by the method being validated has been used, as has its guidance for using trends in the bias to extend the range of applicability of the calculational method (TBD).

The standard describes use of the double contingency criterion, which states that criticality should not be allowed to occur unless at least two unlikely and independent events occur. The Yucca Mountain Project is currently considering the appropriate position to be taken on use of this criterion in the repository postclosure period. The risk-based postclosure criticality analysis methodology described in this technical report will comprehensively address features, events, and processes that pose the potential for criticality. Attempting to show that a single change in conditions will not lead to criticality appears to be incompatible with the uncertainties associated with the long postclosure period of regulatory concern and with the probabilistic approach necessary for postclosure criticality analysis. Some other "defense-in-depth" criterion of a similar nature but more compatible with the probabilistic nature of postclosure analyses may be proposed in the future.

- *ANSI/ANS-8.17-1984 (R1989), Criticality Safety Criteria for the Handling, Storage, and Transportation of LWR Fuel Outside Reactors.*^{2,5} This standard provides guidance for criticality safety for a specific waste form, light water reactor spent fuel, as opposed to the more general scope of ANSI/ANS-8.1-1983. ANSI/ANS-8.17-1984 (R1989), which is intended to provide supplemental guidance for ANSI/ANS-8.1-1983, allows reliance on neutron absorbers for criticality control. In addition, it allows credit to be taken for burnup through reactivity measurement or through analysis and verification of exposure history. It

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

provides criteria to establish criticality, though it does not require a specific margin to criticality be maintained.

The methodology described in this technical report for criticality analyses internal to a waste package is consistent with this standard. The standard allows neutron absorber credit, which will be sought as determined appropriate through use of material degradation and transport models. The Yucca Mountain Project planning assumption (TBV) is that the analysis and verification method will be used for burnup verification. Use of burnup/reactivity measurement is a subject currently under discussion between the DOE and the NRC. Finally, the standard's guidance is used in establishing the subcritical limit (referred to in the standard as "Criteria to Establish Subcriticality").

The standards discussed above are expected to be used in development of the methodology. Additional standards may be identified as applicable. These standards will be used as appropriate and referenced in the topical report. The following standards are already under consideration for use in the topical report:

- *ANSI/ANS-8.10-1983, Criteria for Nuclear Criticality Safety Controls in Operations with Shielding and Confinement.*²⁻⁶ This standard, though intended for application to fissionable material process facilities outside of reactors, could be interpreted to apply to the postclosure repository, in which adequate protection (including shielding provided by the rock surrounding the repository) for the public against radiation and release of radioactive materials can be demonstrated. The approach described in ANSI/ANS-8.10 requires designing for one unlikely event rather than for two unlikely events as required by ANSI/ANS-8.1-1983 and ANSI/ANS-8.17-1984 (R1989). The Yucca Mountain Project planning assumption is that the approach described in ANSI/ANS-8.10-1983 is consistent with the methodology for demonstrating disposal criticality control that is presented in this technical report, though the applicability of this standard to postclosure repository conditions must be verified.
- *ANSI/ANS-8.15-1981, American National Standard for Nuclear Criticality Control of Special Actinide Elements.*²⁻⁷ This standard provides guidance for prevention of criticality accidents in the handling, storage, processing, and transportation of special actinide elements. The document provides guidance for 14 nuclides ranging from Np-237 to Cf-251. This standard is the counterpart of ANSI/ANS-8.1-1983 for materials that, while generally much less abundant than those within the scope of ANSI/ANS-8.1-1983, are nevertheless a potential criticality

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

concern. The appropriate use of this standard for guidance on postclosure disposal criticality analysis has not yet been determined.

2.1.3 Regulatory Guides

Guidance from NRC Regulatory Guides was assessed in development of the methodology as follows:

- *Regulatory Guide 3.4, Nuclear Criticality Safety in Operations with Fissionable Materials at Fuels and Materials Facilities.*²⁻⁸ This Regulatory Guide endorses use of ANSI/ANS-8.1-1983 for general storage and transport of fissionable materials. As described in the previous subsection, the methodology presented in this technical report is consistent with ANSI/ANS-8.1-1983, and therefore with Regulatory Guide 3.4.
- *Regulatory Guide 3.58, Criticality Safety for Handling, Storing, and Transporting LWR Fuel at Fuels and Materials Facilities.*²⁻⁹ This Regulatory Guide endorses ANSI/ANS-8.17-1984 (R1989) for storage and transportation of light water reactor spent fuel, though it takes exception to verification of exposure history as an acceptable method to verify burnup in order to take burnup credit. This method is one of two that is presented in the standard. The Regulatory Guide states that credit for fuel burnup may be taken only when the amount of burnup is confirmed by reactivity measurements that are appropriate for each type of fuel assembly in the environment in which it is to be stored.

As noted in the previous subsection, the methodology presented in this technical report is consistent with ANSI/ANS-8.17-1984 (R1989). With regard to burnup verification, it should be noted that the DOE's *Topical Report on Actinide-Only Burnup Credit for PWR Spent Nuclear Fuel Packages*,²⁻¹⁰ which has been submitted to the NRC for acceptance, includes the verification of exposure history as a partial verification of burnup and also requires that burnup be verified by measurements. The extent to which measurements would be needed to verify exposure history is the subject of ongoing DOE and NRC discussion.

The Regulatory Guides discussed above are planned for use in development of the topical report. The DOE may use additional Regulatory Guides; such use will be explicitly described in the topical report.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

2.2 Risk-Based Analysis and the Current Regulatory Framework

The existing NRC repository criticality regulation (10 CFR 60.131(h)) is deterministic in nature. The disposal criticality analysis methodology presented in this technical report incorporates probabilistic analyses. The Yucca Mountain Project planning assumption to be validated (and the view of many knowledgeable persons in the scientific community) is that it is unlikely that a nuclear waste repository can be shown to limit the occurrence of a criticality to a probability that is zero, or vanishingly small. It is very difficult, for the extremely long period of regulatory concern likely to apply to a geologic repository, to define a credibility standard that is acceptable to all parties in a licensing proceeding. Accepted standards exist in reactor licensing, but the period of regulatory concern is many orders of magnitude smaller than that likely to be applicable to a geologic repository. For example, should the period of regulatory concern be substantially longer than 10,000 years, an event with a very low probability of occurring in one year could have a relatively high probability of occurring over the much longer period. There is no precedent for establishing a credibility threshold in this type of situation.

In keeping with the recent recommendations of the National Academy of Sciences²⁻¹¹, the repository's ability to meet risk-based performance objectives to protect the health and safety of the public is the focus of the methodology presented in this technical report. Risk is defined in this document as the product of probability and consequence of a process or event under consideration.

Using a risk-based criticality analysis, criticality would be evaluated as a potential threat to overall repository performance. The probabilities and consequences of potential criticality events would be used as input into the overall repository performance assessment, and evaluated along with other potential risks. Redesign would be required if the design, considering criticality and all other analyzed phenomena, were found to not meet the performance objectives, however augmented design features are evaluated based on the criticality analysis. Use of risk-based analysis in regulatory matters is encouraged by the NRC in its recent policy statement entitled *Final Policy Statement on Use of Probabilistic Risk Assessment Methods in Nuclear Regulatory Activities*²⁻¹².

Notwithstanding the emphasis on risk, the Yucca Mountain Project approach to dealing with potential postclosure criticalities also includes defense-in-depth against criticalities. Criticality events are considered undesirable even if the risks they pose are determined to be small. The

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

Yucca Mountain Project's approach to postclosure criticality is considered to be consistent with the NRC's regulatory philosophy that there should be diverse and redundant barriers against undesirable conditions and that appropriate margins should be used in design and analysis. The diverse and redundant barriers and protection modes are intended to minimize the probability of criticality because even if one barrier fails, another remains to provide protection.

The current Yucca Mountain Project approach to defense-in-depth against criticality includes the following aspects. The first aspect involves taking advantage of many natural and engineered features of the site and repository to make the probability of postclosure criticality as low as practical. Such features are expected to provide barriers to postclosure criticality that are both diverse (multiple barriers performing different functions that reduce the probability of criticality) and redundant (multiple barriers performing the same function that reduces the probability of criticality). Examples of diverse barriers that reduce the probability of criticality are: the inner barrier, borated stainless steel plates in the basket, and the iron in the basket materials. Similarly, use of two separate waste package shell materials to impede water entry into the waste package is an example of the use of redundant barriers. (Discussions of how these features perform as barriers to criticality is provided in Appendix B.) Numerous other features are either planned for use or under consideration. The end result is expected to be a site and repository with considerable resistance to postclosure criticality. Because specific site and design features are outside the scope of this technical report, design of the repository and use of the site to provide defense-in-depth is not further discussed in this technical report.

The second aspect of defense-in-depth will be implemented in conjunction with the postclosure criticality analysis methodology described in this technical report. In addition to assessing risks associated with potential criticality events, the probability of the events and the contributing factors to their potential for occurrence will be analyzed. This analysis will attempt to identify processes, conditions, and events most likely to lead to criticality. With this information, the design team will seek reasonable and practical approaches to reducing the probability of occurrence of potential criticality events as just described.

The third aspect of defense-in-depth is the use of appropriate conservatism in postclosure criticality analyses. The approach to conservatism in the analysis methodology is discussed in various places throughout this technical report.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

2.3 Burnup Credit

The time dependence of the isotopics of spent fuel is an issue that is an essential part of the methodology for demonstrating control of postclosure disposal criticality. The DOE plans to seek burnup credit for disposal criticality of commercial SNF as described in Section 1.5.1 of this technical report.

The NRC has approved burnup credit for use in PWR spent fuel pools. To date the NRC has not granted burnup credit for transportation. The DOE is working to obtain burnup credit, concentrating on transportation of fissionable material, and has submitted to the NRC a topical report on the subject, titled *Topical Report on Actinide-Only Burnup Credit for PWR Spent Fuel Packages*.²⁻¹⁰ The DOE has addressed NRC comments and has submitted a revised report for additional NRC review. The DOE is also planning to develop topical reports to obtain NRC acceptance of credit for selected fission products in reducing criticality potential during storage and transportation.

The Disposal Criticality Analysis Methodology Topical Report will include or reference information that is expected to be sufficient to allow the NRC to grant burnup credit for selected radionuclides to be used in disposal criticality analysis. Data and other information from the *Topical Report on Actinide-Only Burnup Credit for PWR Spent Nuclear Fuel Packages* and from future topical reports related to burnup credit for storage and transportation will be used in this effort to the extent appropriate.

2.4 References

- 2-1. *Civilian Radioactive Waste Management System Managing and Operation Contractor Requirement Document (CRD)*, DI Number: A00000000-00811-1708-00003 REV 03, CRWMS M&O.
- 2-2. *A Guide to the Performance of Probabilistic Risk Assessments for Nuclear Power Plants*, NUREG/CR-2300, J.W. Hickman, American Nuclear Society/Institute of Electrical & Electronic Engineers, January 1983.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

- 2-3. *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages*, NUREG/CR-6361, NRC, March 1997.
- 2-4. American Nuclear Society, October 1983. *American National Standard for Nuclear Criticality Safety in Operations with Fissionable Materials Outside Reactors*, ANSI/ANS-8.1-1983, La Grange Park, IL.
- 2-5. American Nuclear Society, January 1984 (Revised 1989). *Criticality Safety Criteria for the Handling, Storage, and Transportation of LWR Fuel Outside Reactors*, ANSI/ANS-8.17-1984 (R1989), La Grange Park, IL.
- 2-6. American Nuclear Society, 1983. *Criteria for Nuclear Criticality Safety Controls in Operations with Shielding and Confinement*, ANSI/ANS-8.10-1983, La Grange Park, IL.
- 2-7. American Nuclear Society, November 1981. *American National Standard for Nuclear Criticality Control of Special Actinide Elements*, ANSI/ANS-8.15-1981, La Grange Park, IL.
- 2-8. *Nuclear Criticality Safety in Operations with Fissionable Materials at Fuels and Materials Facilities*, Regulatory Guide 3.4, Revision 2, NRC (U.S. Nuclear Regulatory Commission), March 1986.
- 2-9. *Criticality Safety for Handling, Storing, and Transporting LWR Fuel at Fuels and Materials Facilities*, Regulatory Guide 3.58, NRC (U.S. Nuclear Regulatory Commission), October 1986.
- 2-10. *Topical Report on Actinide-Only Burnup Credit for PWR Spent Nuclear Fuel Packages*, DOE/RW-0472 Rev. 1, DOE OCRWM, Washington, D.C., May 1997.
- 2-11. *Technical Bases for Yucca Mountain Standards*, National Academy of Sciences, Washington, D.C., August 1995.
- 2-12. *Use of Probabilistic Risk Assessment Methods in Nuclear Regulatory Activities; Final Policy Statement*, 60 FR 42622, NRC (U.S. Nuclear Regulatory Commission), August 1995.

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DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

3.0 METHODOLOGY

The methodology for performing criticality analyses of commercial spent nuclear fuel for long-term disposal in a repository is presented in this chapter. This methodology is applicable for disposal criticality control analysis following permanent closure of the potential repository. Although the methodology will apply to the entire postclosure period of regulatory concern, there will be variations in the application of the individual models as conditions, events of interest, and levels of uncertainties change.

An overview of the methodology is presented in Figure 3-1. The intent of this figure is to show the flow process of the various analyses performed and the models used for these analyses. Descriptions of the analyses performed are provided in the following sections of this chapter. The specific models and their validation will be described in Chapter 4. The repository environmental model and the radionuclide transport/precipitation models are discussed briefly in Chapter 4, but they are developed primarily as part of the TSPA process, as indicated in Figure 3-1. The scenario/configuration generator and criticality configuration generator are two aspects of the same code. As indicated in Figure 3-1, they are applied at several places in the overall methodology.

3.1 Approach

Waste packages will be designed to preclude nuclear criticality occurring in the sealed, undamaged state. Waste package failure, followed by some degradation of the basket and/or waste form must occur before nuclear criticality is possible. This fact will be demonstrated by criticality calculations for the intact basket and waste form (TBV). The design objective of criticality analysis is to estimate the effectiveness of criticality control methods implemented for long-term disposal. The effectiveness of these methods will vary as a function of time after emplacement and as a function of waste package degradation which can occur as a result of changes in repository environment. These changes are dependent on features, events, and processes (FEPs). A natural sequence of FEPs and the resulting degradation of the waste package are collectively referred to as a scenario. The final configurations (material composition and geometry) resulting from the range of possible scenarios will be evaluated for criticality. The probability of criticality for each configuration and consequence of criticality are combined

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

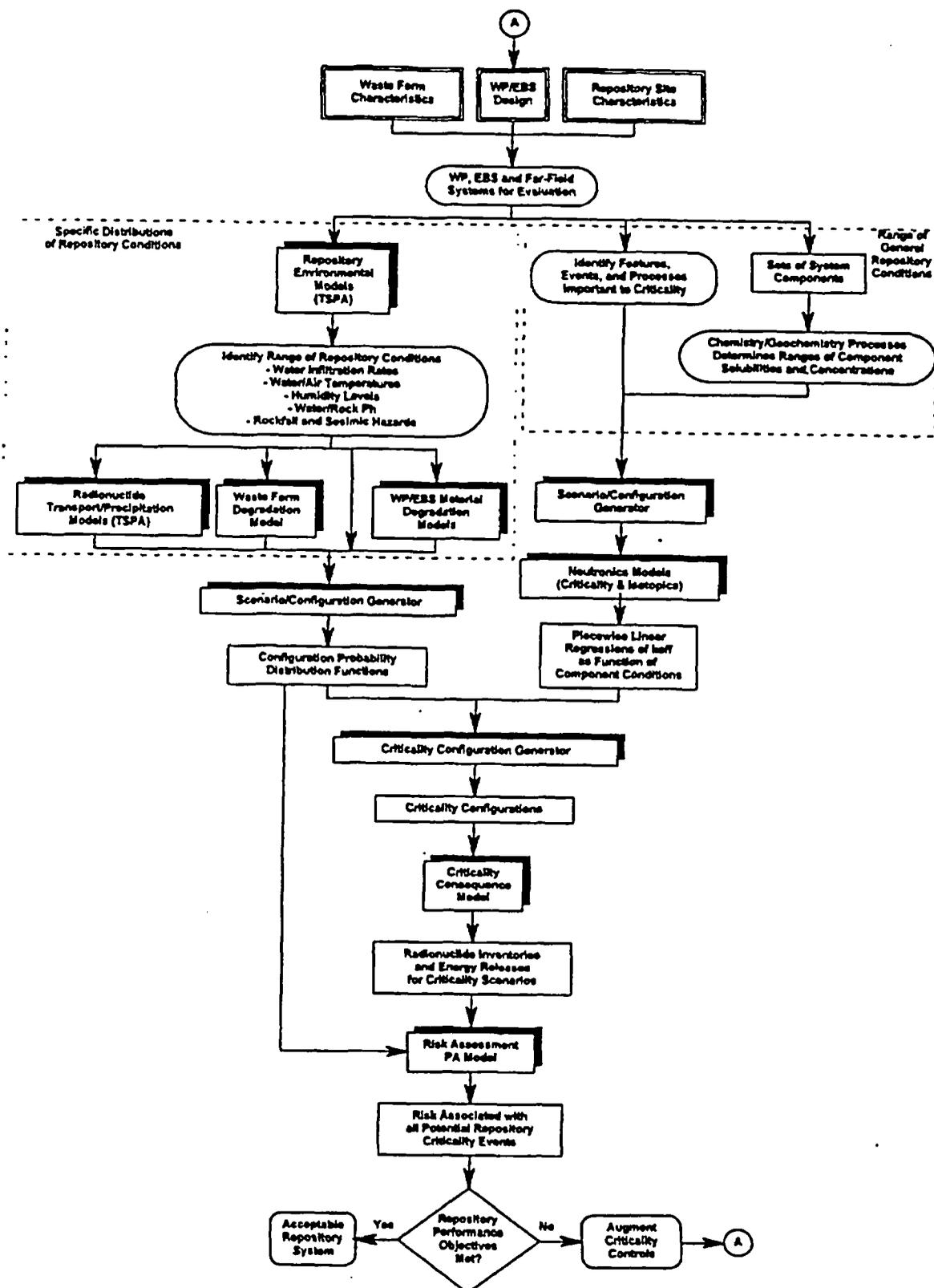


Figure 3-1. Overview of Disposal Criticality Analysis Methodology

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

to estimate risk. The effectiveness of the criticality control is ultimately measured by the risk of increased radiation dose due to the increase in radionuclide inventory and energy release that can result from potential criticalities. The increased radiation dose is determined as part of the TSPA process.

The use of FEPs in building scenarios which may lead to potential critical configurations is described in Section 3.2. A description of the probabilistic methodology used to prioritize configurations for criticality evaluations and for the risk analysis process is provided in Section 3.3. The approach for evaluating nuclear criticality of fissionable material configurations in the repository is summarized in Section 3.4. This includes establishing an upper bound for k_{eff} (subcritical limit) for potential fissionable material configurations. A criticality consequence analysis (described in Section 3.5) is performed for configurations not satisfying the subcritical limit criteria. Section 3.6 describes the process followed in evaluating the potential impact of criticality events on repository performance. The acceptability of the risk associated with the configuration is determined by whether it meets the performance objectives.

3.2 Features, Events, and Processes

The purpose of this section is to illustrate the features, events, and processes which make up the scenarios which can lead to potentially critical configurations. These FEPs are a central part of the demonstration of completeness of inclusion of all significant mechanisms of degradation of the waste package and its contents, and subsequent removal of the contents from the waste package and reconcentration.

Features are defined as topographic, stratigraphic, physical, or chemical characteristics of the site that may influence the criticality problem; examples of features are faults that may focus or block groundwater flow, or topographic lows in geologic strata that may provide locations where fissionable solutes can collect. Processes are the physical or chemical interactions that can take place between the emplaced material and the surroundings; examples include groundwater flow, corrosion, precipitation, etc. Events are a subset of processes that have a definable starting time, an observable duration, and possibly a more extreme intensity or effect on the emplaced material; examples include rockfall in a drift onto a waste package.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

The FEPs important to scenarios which can lead to potentially critical configurations in the three general locations – internal, near-field, and far-field – all include water reaching the waste package and the subsequent container degradation as the initiator. Such degradation can occur from the combination of water reaching the waste packages and elevated temperatures. The rate at which waste package corrosion occurs, and the mode of failure are dependent on the amount of water present, its chemical constituents, and the waste package temperature. Figure 3-2 is a logic diagram which identifies, at the highest level, the scenarios that could potentially lead to critical configurations in the three locations. The principal FEPs for criticality are represented by boxes in Figure 3-2. For in-package criticalities, various FEPs can occur that could separate the fissionable material from the neutron absorbers. If the waste form degrades faster than the criticality-control structures, then the fissionable material can be removed from the waste package and separated from the criticality-control elements. Reconcentration mechanisms in the near-field or far-field could then potentially result in critical configurations at those locations.

The FEP descriptions given in the following sections are those having the greatest impact on commercial SNF, however, the FEP trees outlined in Figures 3-3 through 3-6 are sufficiently general to be applied to all waste forms for which there may be a criticality issue (e.g. DOE SNF, immobilized plutonium).

The FEP trees discussed in the following sections have been developed as an outcome of a workshop on postclosure criticality for the TSPA-VA abstraction/testing effort. The workshop participants and other experts will review them to identify those scenarios that are relatively likely, or have indications of high consequence. The scenarios so identified will be evaluated using detailed codes which simulate the behavior of the FEPs and the results will be abstracted to determine the range of essential parameters for final configurations (concentrations of neutronically significant elements, using the configuration generator code). Additionally, the FEP trees will be screened to eliminate from further consideration those scenarios that appear to have little possibility of leading to a critical configuration. What is presented here has not been screened; it is intended to represent a catalog of possible scenarios.

3.2.1 FEPs Which May Lead to Internal Criticality

There are four general modes of the waste form and criticality control structure degradation inside a breached waste package: 1) both the waste form (e.g., SNF) and the basket are intact; 2) the basket has degraded more quickly than the SNF (the expected mode for commercial SNF);

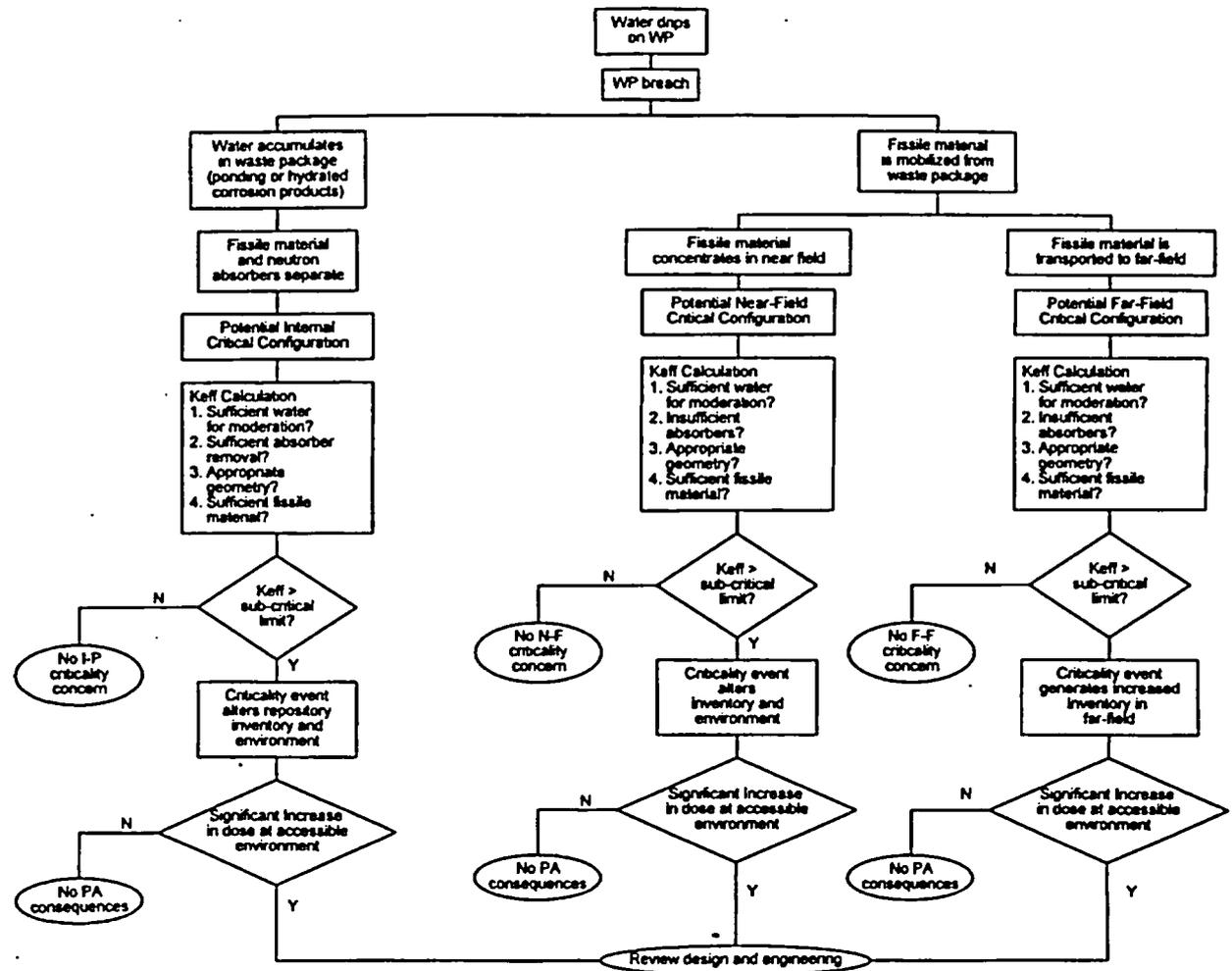


Figure 3-2. Simplified Illustration of Scenarios for the Three Locations of Potentially Critical Configurations

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September 4, 1997

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

3) the SNF has degraded more quickly than the basket (the expected mode for aluminum matrix SNF); and 4) both are comparably degraded. Degradation can include both corrosion and alteration mechanisms that can release the neutron absorbers from the basket and the fissionable material from the waste form. The four modes listed above may have different mechanisms to separate absorbers from fissionable material, but all could result in potentially critical configurations if the other physical requirements are met – presence of a moderator, sufficient fissile fuel, and favorable geometry.

Figure 3-3 shows the branches of the FEP tree illustrating the above degradation modes. The primary criticality scenarios are illustrated by the left-hand branch of the tree, Figure 3-3b. Any mode leading to criticality must eventually have standing water in the package providing moderator for some minimum number of assemblies. Some standing water will accumulate in the waste package if the rate of infiltration in (through holes in the upper portion of the waste package) is greater than the rate of leakage out (through slow leaking cracks in the bottom of the waste package). As long as such a condition of accumulation exists, the water level in the package is limited by the lowest location of any significant size hole in the package wall. Once the package is filled to this level, the standing water will overflow through these hole(s), and the total outflow will equal the inflow. Within the standing water in the waste package, there will be some circulation driven by the heat from assemblies covered with water, so that the soluble corrosion products are flushed out. The initial filling to this level may take between 2 and 100 years (Reference 3-2), during which time there will be no flushing; as a consequence there could be a temporary buildup of soluble corrosion products in solution, which could, in turn, accelerate the corrosion of the waste package contents. The right-hand branch of Figure 3-3b illustrates release of neutron absorbers and degradation of the basket structure before there is extensive waste form degradation. Depending on the design of the basket, the mechanical structure (especially the spacing) may remain unchanged from the as-emplaced configuration while the absorbers degrade, or the basket may collapse before significant degradation of the absorbers occurs. In either case, the timing of such a condition is dependent on the amount and chemical constituents of the water and the temperature. Once the material containing the neutron absorbers degrades, the mobilized absorbers may either precipitate in the waste package or remain in solution. If they precipitate, sufficient separation may occur to result in a critical configuration; if they remain in solution, additional water flushing (by circulation and overflowing) of the waste package may dilute the absorbers sufficiently to permit the occurrence of a critical configuration. Because the waste form structure has not changed, the degraded basket might be more favorable for criticality.

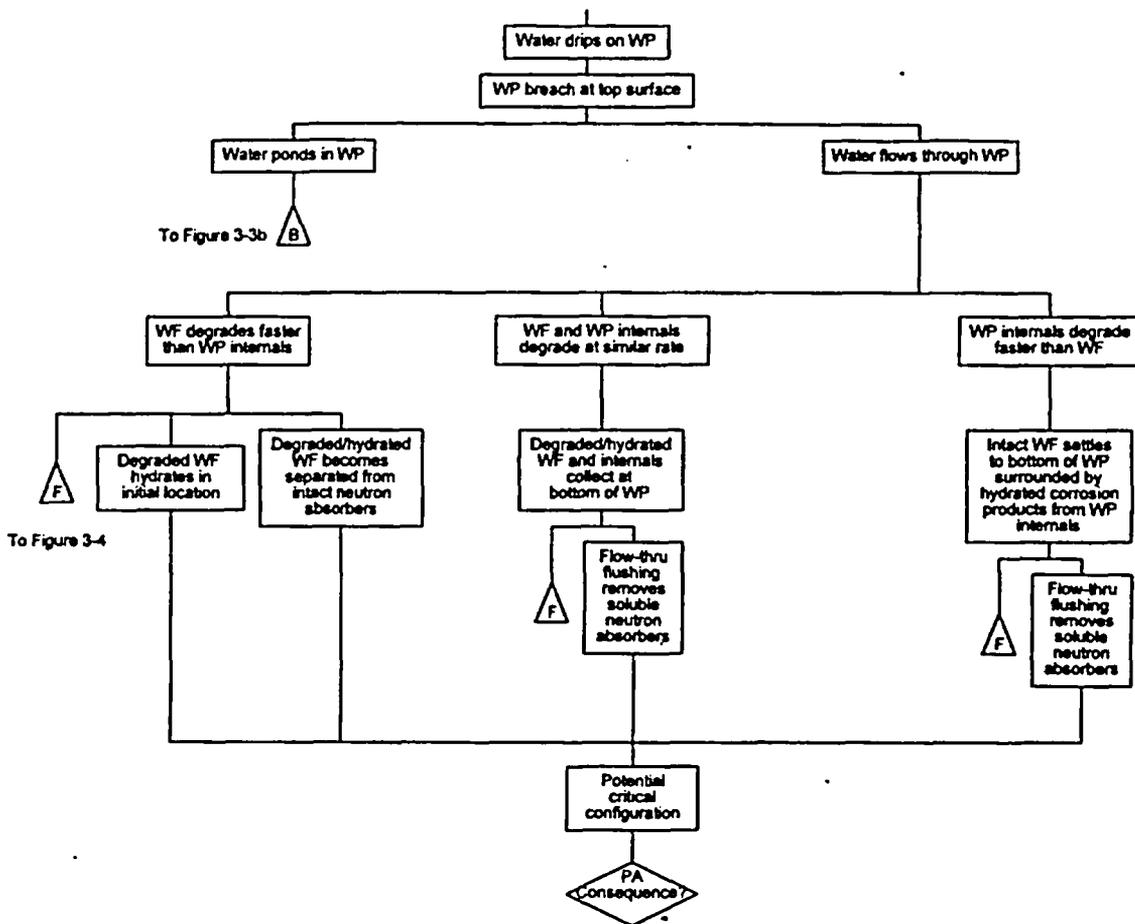


Figure 3-3a. Internal Criticality Scenarios for General Waste Forms*

* - All branches do not apply to all waste forms

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3-8

September 4, 1997

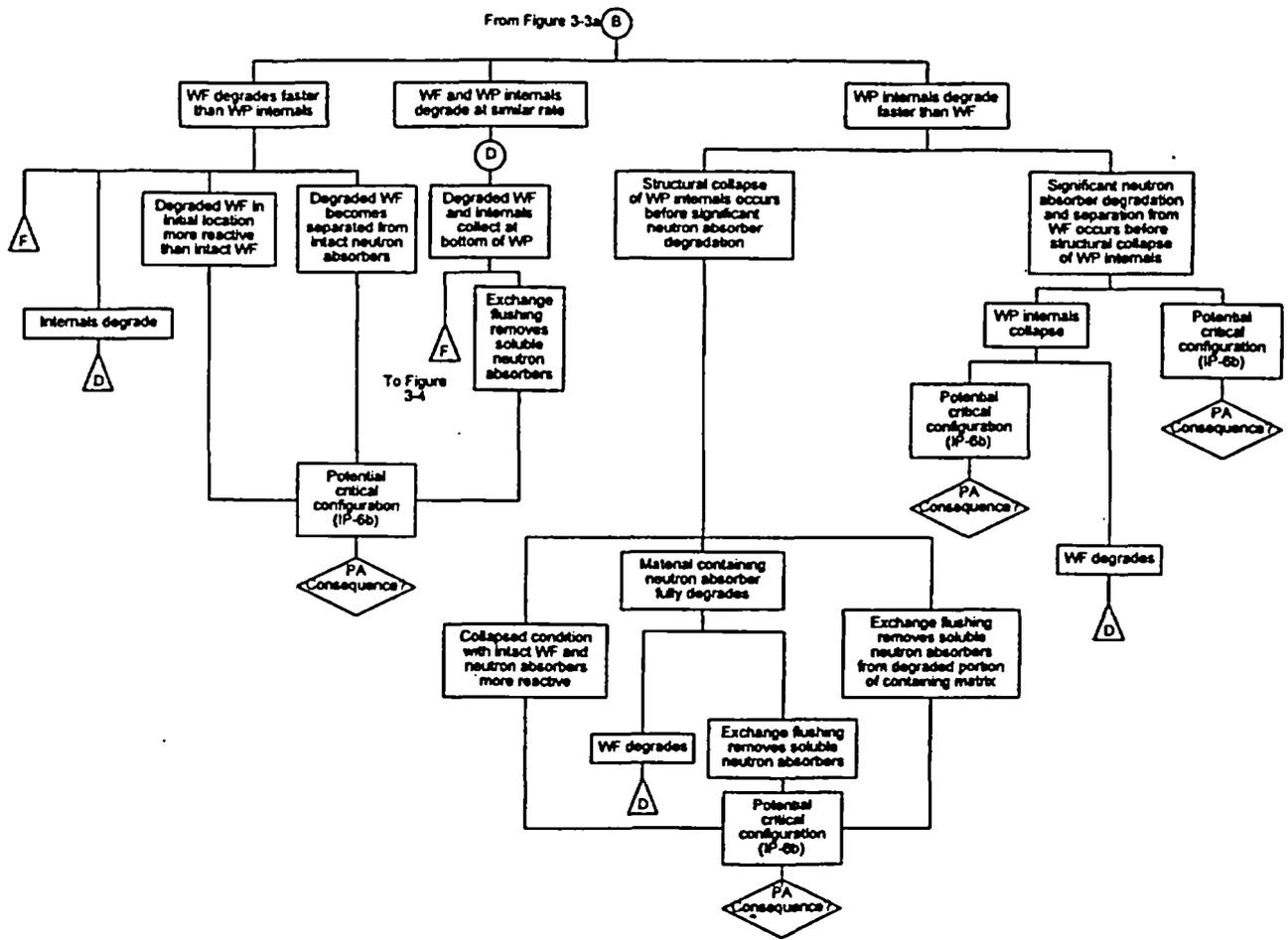


Figure 3-3b. Internal Criticality Scenarios for General Waste Forms

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

The center branch illustrates FEPs associated with degradation of both the basket structure and the waste form at approximately the same rate, ultimately resulting in a mixture of degradation products from both sources at the bottom of the waste package. This path is also the final internal configuration for the both the right and left hand branches of Figure 3-3b.

The left-hand branch of Figure 3-3b covers degradation of the waste form before basket degradation. This applies only to easily degradable waste forms, such as aluminum clad/aluminum matrix DOE owned SNF (illustrated in Appendix C). After such degradation, the fissile material can collect in the bottom of the waste package. If sufficient fissile material and moderator are accumulated, a critical configuration could form in the bottom of the waste package. It may also be more reactive in the initial location if degradation products become more hydrated and homogenized than the intact waste form.

Figure 3-3a describes the case in which the waste package bottom is penetrated to a significant degree so that generally there is insufficient standing water to provide moderator for internal criticality. The only exception is for the co-disposal (with HLW glass canisters) of waste forms other than commercial SNF. The silica in the HLW glass canisters may be degraded to clay which is sufficiently hygroscopic that it can retain sufficient water to provide moderation for fissionable material also trapped in the clay.³⁻⁸

3.2.2 FEPs Which May Lead to Near-Field Criticality

Fissionable material released from the waste package (either as solutes, colloids or other fine particulates) can be transported into the concrete/crushed tuff invert beneath the waste packages. Physical or chemical processes which may act to collect the fissionable material in the near-field or the far-field will be evaluated. Because of differences in geochemical interactions between the contaminants in the water flowing out of the waste package and the surrounding materials (usually represented by differences in retardation factors), the neutron absorbers and the fissionable material might be separated as the plume moves through the invert. (This mechanism is usually referred to as chromatographic separation, because of the analogy with the chromatograph used for chemical analysis of liquids or gasses.) Thus, the processes exist to possibly concentrate fissionable material in the near field in the presence of water or other moderators, without significant concentration of neutron absorbers.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

The left-hand branch of Figure 3-4 illustrates separation and concentration of fissionable-material solutes by sorption and precipitation in the invert. Since both water and SiO₂ are present, the possibility of critical configurations with both thermal and more energetic neutrons (epithermal) are indicated. The right-hand branch of the figure illustrates largely the same FEPs for fissionable material transported as colloidal suspensions. Physical processes acting on particulates, such as filtration by concrete or waste-package degradation products, are indicated in this branch. The center branch of the figure illustrates the transport of fissile material which is already concentrated, to some extent, in the medium doing the transport.

3.2.3 FEPs Which May Lead to Far-Field Criticality

The contaminant plume can move through the near-field materials into the host rock surrounding the drift. Groundwater transport in the host rock will pass through the interfaces between geologic strata with different hydrologic or sorptive properties. Such discontinuities can provide a mechanism for concentration near the interface. However, this mechanism is not as species specific as the chromatographic described above. This mechanism is analogous to the one responsible for the perched groundwater reservoirs usually encountered.

In the unsaturated zone, alteration of strata by thermo-chemical processes from repository heat can also result in concentration. Figure 3-5 illustrates some of the FEPs for the unsaturated zone beneath the repository. The right-hand branch of the FEP tree identifies some of the interactions with the altered Topopah Spring basal vitrophyre. Hydrothermal processes can convert some of the materials in this stratum to clays, reducing the permeability and providing sorption sites for the fissionable material.

If, and when, the contaminants reach the water table, they might interact in other ways with the materials there. Figure 3-6 is a segment of the FEP tree illustrating a number of possible processes for concentration of fissionable material. Waters from deep beneath Yucca Mountain might have sufficiently different chemical or redox characteristics that fissionable material from the contaminant plume concentrates by precipitation at the interface. Alternatively, the presence of organics provides a reducing zone, potentially creating conditions appropriate for a fissionable-material "ore body" to form. One possible location for such organic materials to be found is at the Franklin Lake Playa, several tens of km down-gradient from the Yucca mountain site.

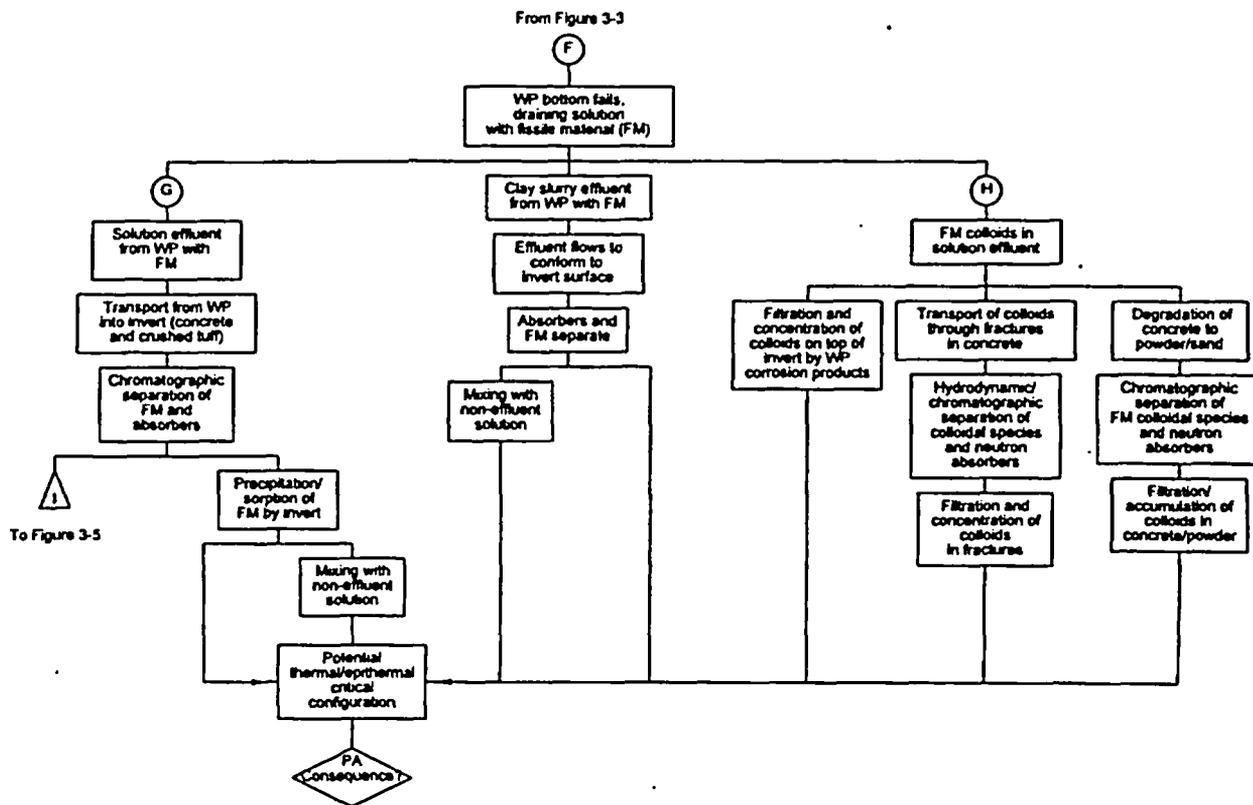


Figure 3-4. Near-Field Criticality Scenarios for General Waste Forms

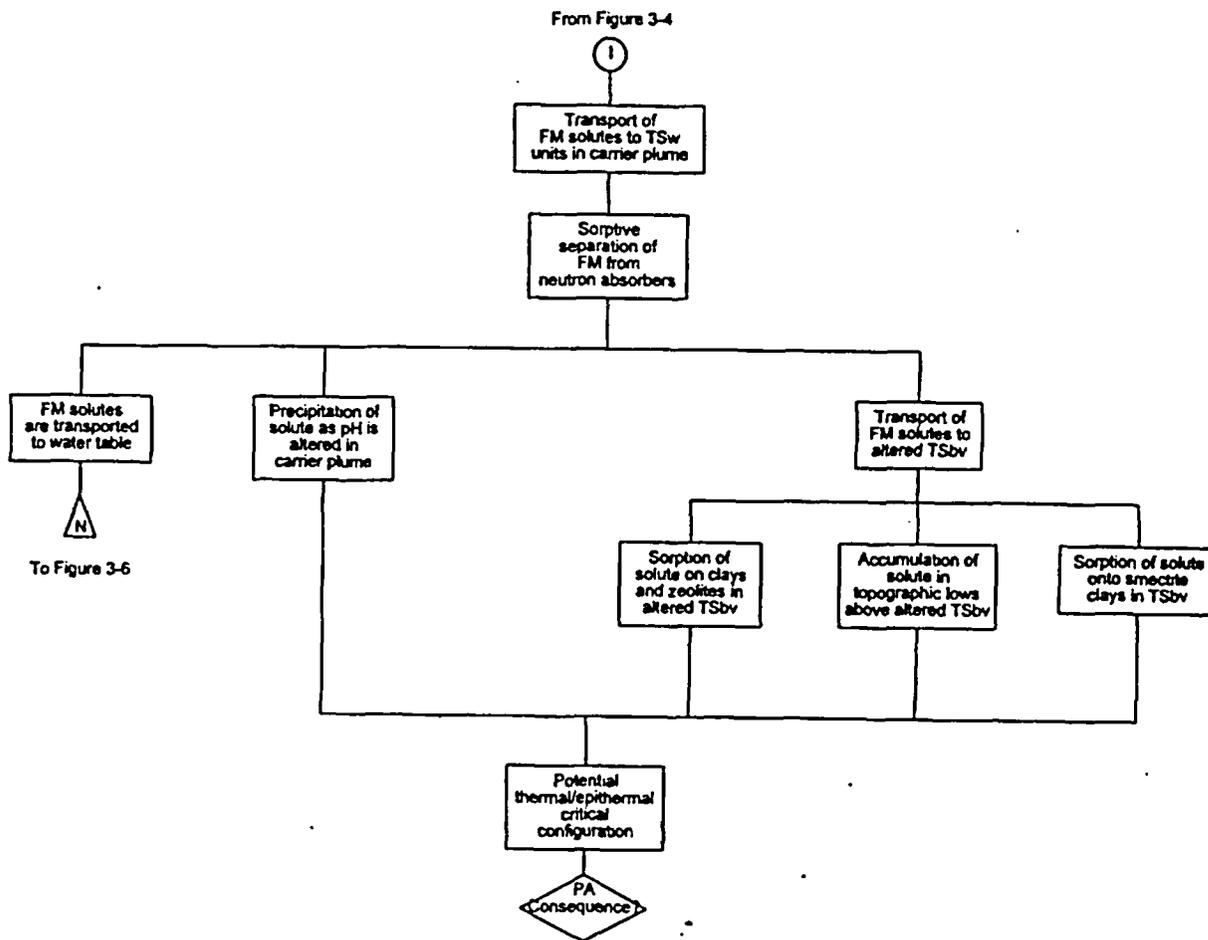


Figure 3-5. Far-Field Criticality Scenarios for General Waste Forms - Unsaturated Zone

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3-13

September 4, 1997

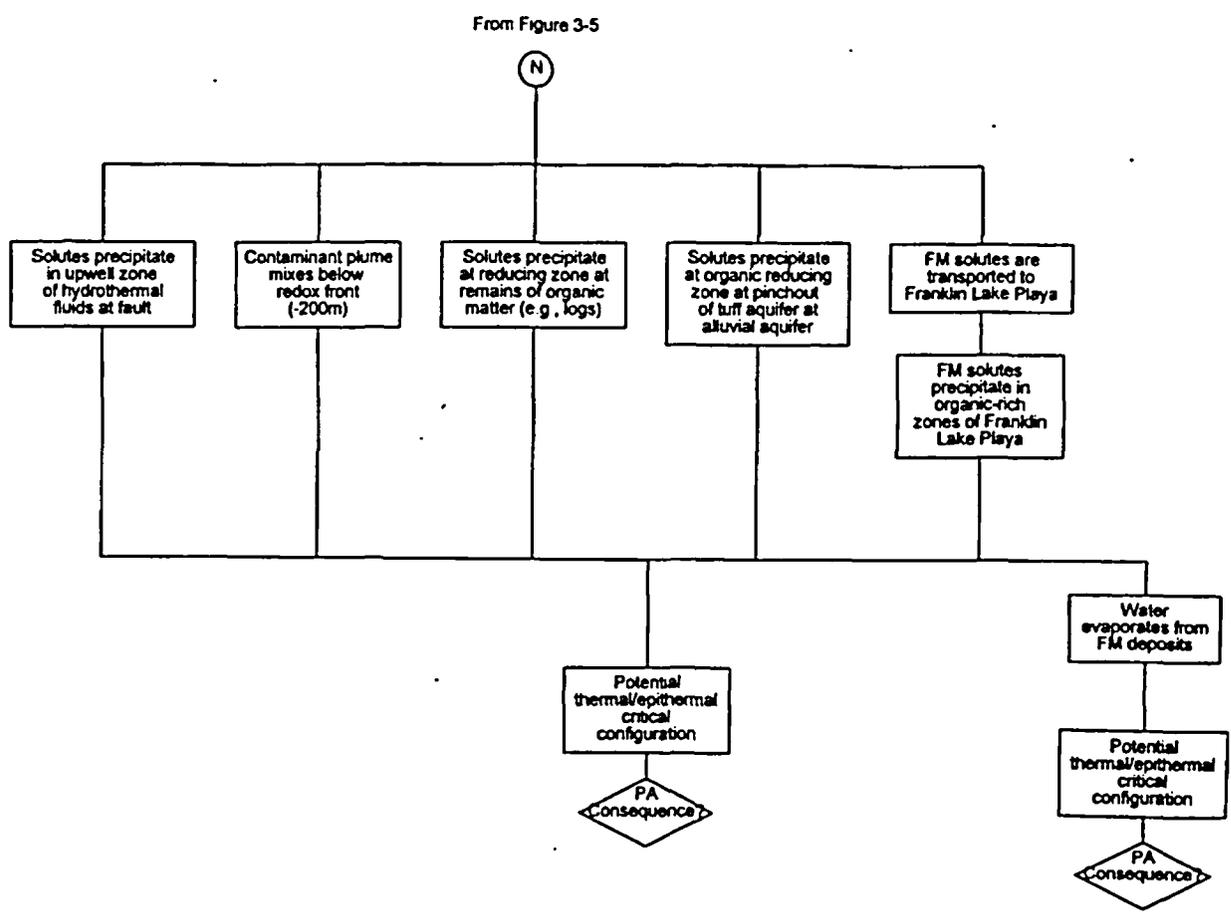


Figure 3-6. Far-Field Criticality Scenarios for General Waste Forms - Saturated Zone

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

3.2.4 Evaluation of FEPs with Respect to Criticality Potential

Theoretical chemical analysis is applied to those processes involving chemistry or geochemistry, and leading to concentration of fissionable material or removal of neutron absorber material. In particular, the geochemical codes EQ3/6^{3-10,3-11} are used to determine the composition and amounts of precipitates containing neutronically active species, and the concentration of such species in solution. This type of theoretical analysis is applied in the three general locations of interest: inside the waste package, external to the waste package in the drift (particularly the invert immediately beneath the waste package), and external to the waste package in host rock.

- Concentrations of neutronically significant species in precipitates and adsorbates are used to estimate criticality of such configurations.
- Concentrations of neutronically significant species in solution are used to determine the transfer of such species between locations (e.g., removal from the waste package).

For locations external to the waste package, these theoretical analyses will also include the use of groundwater transport codes and combined transport-chemistry codes such as AREST-CT³⁻¹².

The use of these codes is described further in Section 4.2.4.1.2, as part of the detailed description of the modeling process. As with all the waste package environmentally related analyses, this work will be coordinated with the analyses conducted for overall repository performance assessment to assure consistency and avoid duplication.

3.3 Probabilistic Evaluations of Events and Processes

Probabilistic evaluation of waste package criticality is the analysis of waste package performance across the spectrum of possible: 1) environmental conditions, 2) waste form performance parameters, and 3) waste package material performance parameters. A preliminary screening of scenarios for minimal credibility (probability) can be illustrated with a Failure Modes and Effects Analysis (FMEA) type analysis. In the overall scheme of criticality analysis, probabilistic evaluations have two purposes: 1) the probabilistic results are used to prioritize the configurations for the calculation of k_{eff} ; and 2) they also constitute the first step of the risk analysis process which expresses the hazards from the repository in terms of the expected dose

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

(or some other risk measure) impacting some population (e.g., humans at the accessible environment). The prioritization of configurations for criticality analysis according to probability may be revised if the overall risk analysis identifies such large consequences with a configuration having a very low probability, that the expected dose to a population turns out to be significant.

3.3.1 Probabilistic Evaluations Beyond the Capability of Traditional PRA

A well known example of probabilistic evaluation in the nuclear industry is the PRA. PRA is widely used by the nuclear power industry for judging the importance of plant systems and components to radiological safety. Nuclear power plant PRAs are used for identifying potential vulnerabilities and guiding design change and maintenance decisions towards optimizing plant safety; they are also used to show that risk has been reduced to an acceptable level. While the goal of the probabilistic evaluations discussed in this technical report remains the same as that for nuclear power plants, differences in conditions require methods which differ from those utilized in traditional PRA. Principal examples of these different conditions are as follows:

1. Analyses must cover longer periods of time. Assumptions of constant failure rates, or even constantly increasing or decreasing failure rates, may not be correct due to potentially fluctuating environmental conditions.
2. Partial component failures must be accounted for (e.g., partial degradation of basket, partial degradation of waste form), since they may have a significant effect on the associated scenario and resulting configuration.
3. In many cases, component failures cannot be assumed to be independent. Failures are often dependent on previous component failures or environmental changes (FEPs).
4. Due to changing isotopics, the time in which a failure or event occurs may also affect the consequences of the event.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

3.3.2 Introduction to Probabilistic Methodology

A good introduction to the probabilistic methodology is provided by the application of the traditional failure mode effects analysis (FMEA) to the waste package. The waste package/EBS/repository long-term probabilistic evaluation differs from the traditional nuclear power plant PRA in that there is no discrete failure event associated with the waste package. Nevertheless, the continuous degradation processes can be understood by discrete summary representations such as a logic tree or a fault tree. One such representation is the FMEA, which, for application to the waste package, will be called "pseudo-FMEA" since it has no discrete failure modes. For internal criticality, the goal of this pseudo-FMEA is to identify how waste package component (e.g., barriers, welds, fuel assemblies, basket plates or tubes, fuel rods) degradation events and processes will produce changes in the configuration/geometry of the waste package (barriers and contents). The pseudo-FMEA also considers any prior failures or degradations which are required antecedents for the downstream (in time) degradation of some component. For example, the waste package barriers must be breached, and water must enter the waste package, before the neutron absorbing material can be removed from the waste package basket.

If necessary, component failure events may be grouped into general configuration change categories. These categories are discrete representations of a continuum of parametric values.

This grouping is used to reduce the number of configurations to a manageable level. This discretization also provides a better analog of the traditional FMEA concepts of discrete configuration changes (or discrete failure modes).

In the next step, the categories of discrete configuration changes or component failures defined in the FMEA are used to build a waste package configuration logic tree. An example waste package configuration logic tree is shown in Figure 3-7. This logic tree is visually and conceptually similar to the event trees used in nuclear power plant PRAs. There are two principal differences for the present application: 1) For many of the steps, the probabilities are conditioned upon the occurrence of prior events so many events must occur in sequence; and 2) for most of the steps the events represent a continuum of processes, which are represented by probability density functions instead of discrete probabilities. The configuration change categories (or events) are listed across the top of the tree (E_1 thru E_n), and all possible configurations (regardless of likelihood) are listed down the right side.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

In Figure 3-7, the prime notation has been used to indicate complement. For example E_2' indicates a configuration where the inner barrier has not been breached. These changes may or may not be dependent on a previous configuration change. For example, the category E_2 indicates a configuration where the inner barrier has been breached. Corrosion breach of the inner barrier cannot occur until breach of the outer barrier exposes it to the external environment.

The probabilities are best expressed by the continuous probability density function (PDF) and the cumulative distribution function (CDF). The PDF, $f(t)$, is defined by:

$$\Pr \{t \leq T \leq t+dt\} = f(t)dt$$

where dt is an arbitrarily small time interval; since $t \geq 0$, the CDF, $F(t)$, is defined by either:

$$F(t) = \int_0^t f(\tau) d\tau$$

or

$$F(t) = \Pr\{T \leq t\},$$

which are equivalent.

If $f_1(t)$ represents the PDF for corrosion breach of the outer barrier, and $f_2(t)$ represents the unconditional PDF for corrosion breach of the inner barrier, then the PDF for category E_2 is defined as the convolution of the two PDFs, $f_{12}(t)$, which is given by:

$$f_{12}(t) = \int_0^t f_1(\tau) f_2(t-\tau) d\tau$$

Of course, the dependence of inner barrier corrosion on outer barrier breach is more complex than is represented by this convolution. The inner barrier corrosion or degradation will be proportional to the amount of inner barrier exposed to corroding water, which will, in turn, be proportional to the outer barrier surface area which has been penetrated (for designs with no gap between barriers). The more complex dependence is reflected, to some degree, in the barrier

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

corrosion model of TSPA-95³¹, and will be even more refined for TSPA-VA and for the topical report.

The probability that the logic tree category E_2 has occurred by a given time is then represented by the CDF, $F_{12}(t)$, which is obtained by integrating the convolved PDF, $f_{12}(t)$. This particular illustration of the causal relationship is supported as long as the breach is due to corrosion from the outside. The probability that a given configuration (shown to the right of the tree) has occurred by time t would generally be determined by taking a multiple convolution over the times of occurrence of each event. Since many of these events (or processes) are independent, the convolution may degenerate into the product of the probabilities that each of the categories has or has not occurred by time t (as indicated), which is obtained from the CDF for each category at time t .

This logic tree is described here to illustrate the process of considering all relevant configurations. The logic tree cannot actually describe the very many degrees of partial process completion (e.g., partial barrier corrosion) which are significant in the overall waste package degradation. In addition, the logic tree is unable to conveniently handle certain combinations and non-corrosion modes of degradation, such as rockfall on a partially corroded package, and would be unable to support external criticality analyses. For these and other reasons, the comprehensive methodology described below will be used.

3.3.3 Scenario Identification, Generation, and Evaluation

Three typical scenarios leading to the three types of criticality (internal, near-field external, and far-field external) are shown in the three branches of Figure 3-2. These scenarios can be said to be probabilistic in their initiation, because their initiation depends on environmental parameters which are best described by a probability distribution. For the preliminary evaluations, the scenarios are said to be initiated probabilistically and to evolve deterministically. In other words, once the environmental parameters are selected randomly at the beginning of the scenario, they are assumed to be constant throughout the time of evolution of the scenario, so the scenario evolution becomes deterministic. Both the probabilistically determined initial environmental parameters and the subsequent process evolution will be consistent with, and/or derived from, the methodology and results of TSPA-VA.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

The implementation of the scenario generation process is provided by a computer code, called the scenario generation tool, which tracks the parameters which characterize configurations with the greatest criticality potential. The algorithms of the scenario generation tool computer code will generally be abstractions of the physical processes of the physics and chemistry codes used in TSPA.

Construction of the scenario generation tool will consist of the following activities, in approximately the indicated sequence:

- Determination of the species of importance (particularly fissionable nuclides and neutron absorbers).
- Definition of the sample space consisting of bins formed from the discretization of the range of parameters representing phases and locations of the species of importance. Examples of such compartments are the amount of iron in the basket steel, iron in solution, boron in solution, etc.
- Abstraction of transfer rates between the sample space compartments based on physical and chemical process models as provided by TSPA, either through the parameterization of the results of physics and chemistry codes like FEHM and EQ3/6, or through the results of summary model codes like RIP.
- Development of mass balance equations (first-order, time-dependent differential equations) using the transfer rates determined in the previous step. These mass balance equations will be implemented in a computer code incorporating the following models:
 - Repository environment model (abstracted from results of TSPA). Some of the components will be concerned with the immediate waste package environment, such as temperature, humidity, or infiltration rate. Other components will be concerned with the far-field rock, such as the probability of a reducing zone existing in the saturated zone.
 - Material degradation models for:
 - (1) waste package barriers, and
 - (2) waste package basket.
 - Waste form degradation model.
 - Material transport model (abstracted from results of TSPA).

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

- Material precipitation and retardation models (abstracted from results of TSPA). In addition to straightforward physical adsorption or precipitation processes, chemical changes analogous to mineral deposition will also be evaluated on the basis of recommendations of experts who will also review the resulting analysis.
- Estimation of probabilities and uncertainties associated with the five models of the previous item.

A preliminary implementation of part of the scenario generation tool has been developed to determine concentration of neutron absorbers in the waste package as a function of time and used in the *Second Waste Package Probabilistic Criticality Analysis: Generation and Evaluation of Internal Criticality Configurations*³⁻², which was completed in March 1996.

The scenario generation tool will be applied using the following steps:

- The mass balance equations are solved (using the computer program) to yield the average expected values of concentrations in the various compartments of the sample space, and as a function of time. Emphasis will be on those compartments which participate in configurations having the greatest chance of criticality. This step defines the configurations for evaluation in the subsequent steps.
- Probabilities are estimated for the mean value configurations, using the parameter distributions and uncertainties in the parameters in the models.
- Those external criticality configurations that rely on some specific capability of fissionable material precipitation or adsorption (e.g., reducing zone) will incorporate the probability of the fissionable material laden repository effluent encountering such a reducing zone.

3.3.4 Configuration Generator

The configuration generator code tracks the concentration of neutronically significant isotopes at the various locations at which a critical configuration could occur. For this purpose, the waste package/repository system is divided into two sets of locations: 1) ponds (potential) in which there is sufficient water for moderation and the fundamental processes of interest are dissolution (only in the waste package, which is always the first pond), precipitation, and adsorption;

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

2) paths, in which the principal processes are movement of the fissionable material bearing solution through the host rock, transporting the fissionable material from one pond to the next in the sequence defined by the scenario.

The configuration generator implements a set of first-order, time-dependent differential equations which are integrated numerically, typically with a time step of greater than one year. Since the chemical properties of an element are determined by its atomic number, the isotopic concentrations must be combined for purposes of calculating solubility, adsorption, and precipitation. However, for neutronic calculations the isotopic concentrations must be tracked individually. Therefore, the following updates are performed at each time step for each element which has more than one neutronicly significant isotope:

- The increments to isotopic concentrations in solution are calculated from the dissolution of the waste form and criticality control material.
- The relative isotopic concentrations are recorded (stored).
- The isotopic concentrations are combined to update the amounts in solution according to the maximum concentration permitted (solubility limit) for the isotopically combined concentration; the combined increment (or decrement) to the amount in solution is recorded.
- The amounts of the individual isotopes in solution and precipitate are recalculated according to the previously recorded isotopic percentages and the combined decrement (or increment) to the amount in solution.
- The amounts of individual isotopes removed from the pond are calculated according to the recorded isotopic ratios and the amount of solution flushed from the pond at that time step.

In the current version of the code, the only element tracked by isotope is uranium (235, 238).

The revised version will also track isotopes of plutonium, which will be important for times less than 20,000 years. The configuration generator can also describe the concentrations probabilistically by simply combining the probabilities associated with the set of input parameters (e.g., infiltration rate, dissolution rate) and assigning that combined probability to the resulting configuration.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

3.4 Criticality Analysis

The part of the methodology for evaluating nuclear criticality of fissionable material configurations in the Yucca Mountain repository is summarized in this section. The potential for nuclear criticality is determined by material composition and geometry of the material composition. The initial material composition of a commercial SNF assembly is governed primarily by the operating history of the assembly in a nuclear reactor. One component of the methodology addresses the effects of reactor operating history on the initial material composition of SNF. For the long disposal time period the material composition and geometry will change from their initial state based on isotopic decay and material degradation processes. Thus the potential for nuclear criticality will change during the disposal time period. The disposal criticality analysis methodology must be applicable for evaluating nuclear criticality of fissionable material configurations from the time of repository closure through the period of regulatory concern. The flow of the criticality analysis process is presented in Figure 3-8.

3.4.1 Computer Codes

Criticality analyses for disposal are performed using a combination of computer codes to calculate the material (isotopic) composition of SNF and the reactivity of geometric configurations of SNF. The isotopic compositions are obtained from computer codes contained in the SAS2H sequence of SCALE 4.3³⁻³. Reactivities (criticality potential) are calculated with the MCNP 4A³⁻⁴ code which uses the isotopic compositions of the materials and a system of nuclear data libraries (generally termed ENDF - the Evaluated Nuclear Data File system), plus a detailed model of the geometry, to calculate the k_{eff} of the system. A description of the code systems and their associated nuclear data libraries used in criticality analyses for disposal is provided in Section 4.1.

3.4.2 Material Composition of SNF

The criticality analysis methodology starts with the determination of the isotopic concentrations of fissionable and absorbing isotopes to be used for criticality evaluations (Figure 3-8). The calculations performed in determining the isotopic concentrations are based on conservative model input parameters (discussed in Chapter 4), fuel assembly burnup data, disposal time period of interest, and fuel assembly design data.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

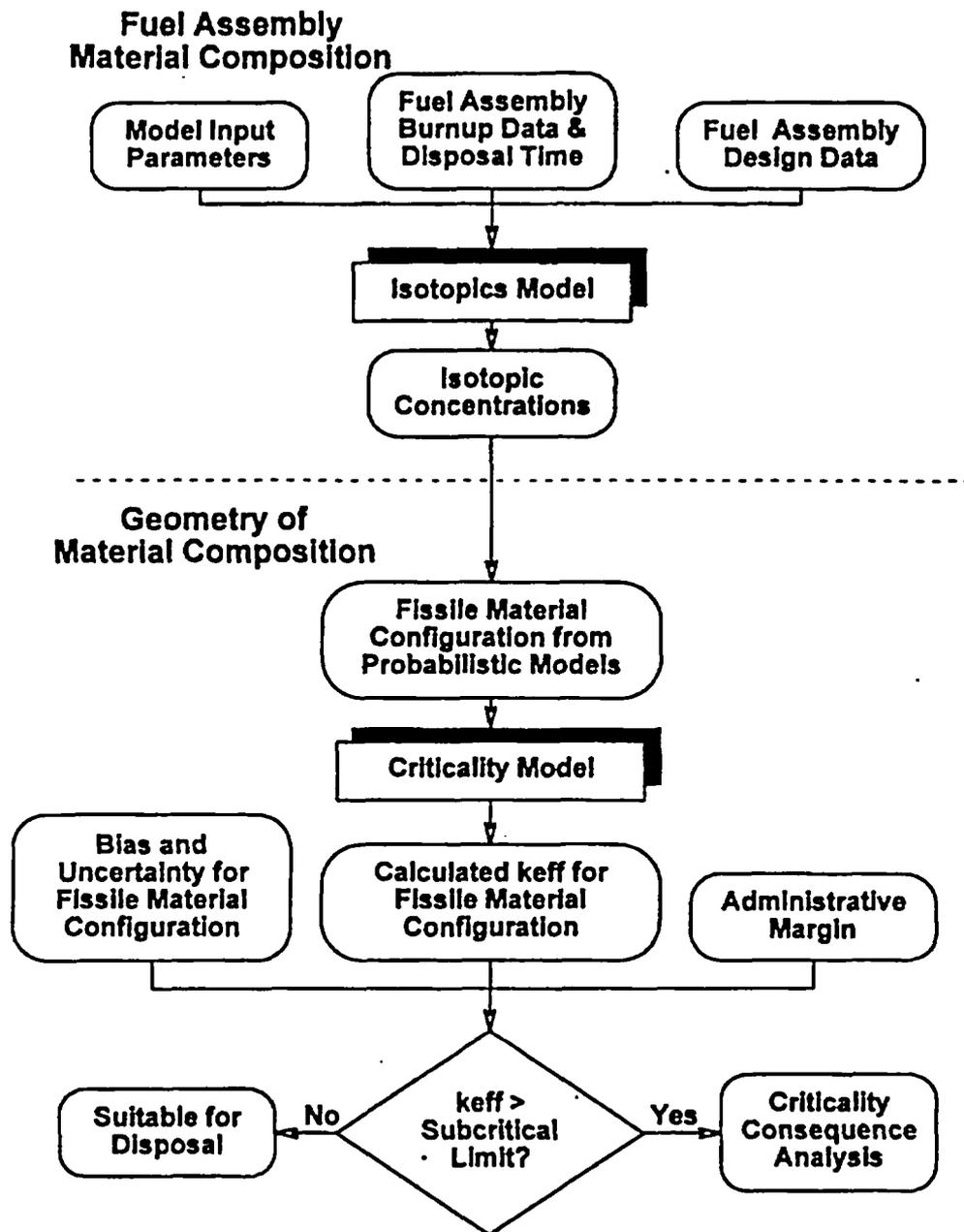


Figure 3-8. Criticality Analysis Process

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

Taking credit for the reduced reactivity associated with the net depletion of fissionable isotopes and the creation of neutron absorbing isotopes during the period since nuclear fuel was first inserted into a reactor is referred to as burnup credit. Both the time that the fuel was in a reactor and exposed to a high neutron flux (in a power production mode) and the "cooling time" since it was removed from the reactor should be considered. Burnup is the amount of exposure (irradiation) of a nuclear fuel assembly, in a power production mode, expressed in units of gigawatt days per metric ton of uranium (GWd/MTU) initially loaded into the assembly. Burnup credit accounts for the reduced reactivity potential of a fuel assembly associated with this power production mode and varies with the fuel burnup, cooling time, and the initial enrichment of U-235 in the fuel.

Local conditions in the reactor core during burnup that affect the neutron spectrum, and therefore the isotopic composition of the fuel at discharge from the reactor, must be quantified if burnup credit is to be appropriately applied. These conditions include reactor power density variations (and associated moderator and fuel temperature variations), addition of neutron absorbing materials (e.g., soluble boron, control rods, and burnable poison rods), and alteration of the amount of moderator material (e.g., moderator displacement by non-fuel rods). Investigations of some of these conditions are discussed in Reference 3-5. The disposal criticality analysis methodology examines local variations in these conditions in reactor cores when commercial SNF is being produced. The treatment of these local variations by the methodology is discussed as part of the model validation process in Chapter 4. The model input parameters in Figure 3-8 represent conservative values for these conditions that are determined as part of the model validation process.

3.4.3 SNF Principal Isotopes for Burnup Credit

For the criticality analysis methodology, a subset of the isotopes present in SNF will be used in criticality evaluations of waste packages in a repository. The selection process to determine the isotopes to be included in these evaluations was based on the physical, nuclear, and chemical properties of SNF isotopes. The nuclear properties considered were cross sections and half-lives of the isotopes. The physical properties were concentration (amount present in the SNF) and state (solid, liquid, or gas). The chemical properties included the volatility and solubility of the isotopes. In selecting the isotopes to be included, time effects (during disposal) and relative importance of isotopes for criticality (combination of cross sections and concentrations) were considered. During the selection process no isotopes with significant positive reactivity effects

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

(fissionable isotopes) were removed from consideration. The only isotopes removed from consideration were non-fissile absorbers. Thus, the selection process was conservative.

The actinide isotopes selected for the Actinide-Only burnup credit criticality analysis methodology³⁻⁶ are also selected for the disposal criticality analysis methodology. Four additional isotopes have been added to this list. For long disposal times U-233 buildup becomes significant and is added to the list. Np-237 (which decays through Pa-233 to U-233) also increases during the containment phase due to the decay of Am-241 and is added to the list. The isotopes Am-242m (which has a significant fission cross section) and Am-243 (which decays through Np-239 to Pu-239) are also included.

Using this selection process, 14 actinides and 15 fission products (referred to as "Principal Isotopes") were chosen as the SNF isotopes to be used for disposal burnup credit evaluations. A list of these isotopes is presented in Table 3-1. Analyses supporting the selection of these isotopes are presented in *Disposal Needs for Isotopic Data*.³⁻⁷ The conservatism in the use of the

principal isotopes for criticality analyses with spent nuclear fuel is addressed as part of the validation process in Chapter 4.

Table 3-1. SNF Principal Isotopes for Burnup Credit

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

3.4.4 Criticality Evaluations

Configurations of fissionable material are identified for criticality evaluations for each of the three repository regions previously described: 1) inside the waste package, 2) outside the waste package in the near-field, and 3) outside the EBS near-field in the far-field. For these analyses,

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

an upper bound is identified to represent the maximum calculated value of k_{eff} that will ensure subcriticality of the configurations analyzed. This upper bound, called the subcritical limit (Figure 3-8), contains the criticality analysis method bias, the bias uncertainty, and an additional arbitrary margin (consistent with applicable regulatory requirements) to ensure subcriticality. Although the same criticality analysis method is used for each of the three regions, the method bias and uncertainty, and thus, the subcritical limit values can be expected to be different for each region. The subcritical limit values are determined during the validation process for the criticality analysis methodology. Since material composition and geometry (i.e., configurations of fissionable material) are different for each of the three repository regions, different sets of experimental data are used in the validation process for each region. The determination of bias and uncertainty, the subcritical limit values, and the applicability of the subcritical limit values for criticality evaluations for each of the three repository regions will be described in Section 4.1.

3.5 Criticality Consequence Analysis

Criticality analyses are performed for configurations identified within the waste package, outside the waste package in the near-field, and outside the EBS in the far-field. When the k_{eff} of the configuration analyzed exceeds the subcritical limit (upper bound established by the methodology), a criticality consequence analysis is performed. This analysis determines the impact of a potential criticality event on the radionuclide inventory and on the thermal effect (based on the energy yield) within the repository. Probabilities of criticality events and the results of the criticality consequence analyses provide input for a performance assessment to demonstrate that the repository performance objectives are met.

3.5.1 Type of Criticality Event

The consequence of a criticality event is dependent upon the type of event, and the configuration in which the criticality occurs. The following criticality classification scheme is illustrative:

- Thermal versus fast criticality: For a given fissionable material and geometry, the lowest critical mass will generally occur (absent a relatively large amount of thermal neutron absorber) with a neutron spectrum dominated by thermal energies (less than 0.1 eV). A thermal spectrum is produced by sufficient moderator material. A criticality that occurs with no moderator at all is called a fast criticality because all the participating neutrons are either

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

absorbed or lost from the system before they can slow down. For commercial SNF there is no possibility of fast criticality; the effective enrichment is less than 6% which is too low to support fast criticality.³⁻⁹ For waste forms with a high effective enrichment (HEU) or with Pu, there is a possibility of fast criticality, but preliminary analysis has shown that the probability of assembling a sufficiently high mass/concentration of fissionable material with insignificant amount of neutron absorber is so small as to be incredible.

- Degree of moderation (amount of neutron slowing down): For thermally critical configurations there is an optimum moderator concentration which balances the slowing down properties of the moderator against the neutron absorbing properties. A configuration is said to be under-moderated if it has less than this optimum, and over-moderated if it has more. An over-moderated configuration has more than enough moderator for slowing down the neutrons, but removal of water will increase the k_{eff} , because of the decrease in neutron absorption while there is still enough moderating capability to support thermal criticality. If such a configuration becomes critical it will initially be autocatalytic (having positive feedback with respect to the removal of water).
- Reactivity insertion rate: Typical potential reactor criticality accidents could involve reactivity insertion times of less than 1 second. Most geologic processes will provide only very slow reactivity insertion (1 week or more), but certain configurations have the potential for more rapid insertion (10 to 100 seconds) if initiated by a sudden mechanical disturbance such as an earthquake or a rockfall.
- Steady-state versus transient: For transient criticality the energy produced is divided between thermal (molecular motion within a mass) and kinetic (macroscopic motion of a mass of material). Kinetic energy may be analogized to an explosion if it is sufficiently large. However, significant kinetic energy can only occur with the following conditions: 1) some limitation of the negative feedback processes, 2) confinement of the entire critical mass during the time of reactivity insertion (positive feedback), 3) increase in reactivity large enough to compensate for the deficiency of delayed neutrons (prompt critical).

3.5.2 Evaluation of Direct Criticality Event Consequences

Direct criticality consequences are of two types: increase in radionuclide inventory, and release of kinetic and thermal energy. The ultimate criticality consequences are measured by dose at the

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

accessible environment, which are discussed in Section 3.6, Criticality Impact on Risk Assessment and Performance Assessment.

The increase in radionuclide inventory can be calculated by two types of analysis: steady-state and transient. Both types are illustrated by example for commercial SNF in Appendix B. It is shown that the steady-state analysis provides a more conservative (larger) estimate of total radionuclide increase for the same initial conditions.

3.6 Criticality Impact on Risk Assessment and Performance Assessment

The importance of increased radionuclide inventory resulting from a criticality event is the potential for increased dose at the accessible environment. The following subsections indicate the methodology for estimating the increased dose at the accessible environment due to a criticality (if any) and the methodology for incorporating the result into TSPA-VA and for using the result for design guidance.

3.6.1 Risk Assessment Definitions

The risk associated with repository criticality is the product of the probability of occurrence multiplied by the consequence and summed over all possible criticality events (or probability-consequence pairs). If the probability distribution is continuous, then the summation becomes an integration. In practice the consequence will be measured by important impact parameters, such as the following:

- Radiation dose to the average nearby population, as a function of time.
- Radiation dose to the most affected individual in the nearby population.

Radiation doses will be estimated as part of TSPA, and will use, as input, the increased radionuclide inventory and thermal effects estimated by the criticality consequence model (described in Section 3.5).

Appendix B provides an illustration of the process for estimating total dose to the affected population as a function of time.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

3.6.2 Methodology for Incorporation into TSPA

The dose increments will be calculated using the TSPA methodology, for the worst case (largest) radionuclide inventory increases. Consistency with the TSPA then current will always be assured by using the same calculations in both the TSPA and the criticality evaluation wherever there is a corresponding configuration. If these dose increments are determined to be insignificant (compared with the doses expected from the commercial SNF without criticality), no additional TSPA will be conducted. If the dose increments are determined to be potentially significant, the consequence of significant criticality events will be evaluated as necessary: 1) within the failed waste package, 2) outside the waste package in the near-field, and 3) outside the EBS in the far-field. The approach to the evaluation of the potentially significant consequences for each of these regions is summarized as follows:

- Start with the already identified potential criticality events (Sections 3.2 and 3.3) and associated increments to the inventory of radionuclides and thermal effect (temperature at the source as a function of time) (Section 3.5);
- Use the thermal effect to determine timing of return of ambient ground-water flow conditions (if the event causes the removal of ambient ground-water) in the vicinity of the criticality and refine the inventory as necessary;
- Use geochemical models to estimate the release rate of radionuclides from the vicinity of the criticality caused by leaching of the inventory by the ground-water flow (i.e., develop the source term for the inventory produced by the criticality); and
- Use source term and the inventory in a TSPA model to evaluate the dose history at the accessible environment or at other locations as required by regulations.

The TSPA model tracks radionuclides as they are leached from the inventory, and transported through the unsaturated and the saturated zones, and provides the concentration of radionuclides in ground water at the accessible environment. For criticalities that occur within a failed waste package, or in the near-field, the source term is located in the unsaturated zone, but for those that occur in the far-field the source term is likely to be located in the saturated zone (TBV). Over the transport pathway from the source to the accessible environment processes such as retardation, dispersion, and dilution reduce the concentration of radionuclides. Radioactive

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

decay may either reduce or increase the concentration of a particular radionuclide over the transport path (the increase being produced by ingrowth of daughter products). It is assumed that at the accessible environment a person uses the ground water for drinking, or for both drinking and food production. The radionuclide concentration at the accessible environment is converted to dose using a conversion factor that is derived using a dose model and the water use scenario.

The performance assessment model used to evaluate the dose at the accessible environment has the capability of tracking several inventories simultaneously (e.g., defense high-level waste, commercial spent fuel, and release from a criticality). Because of this capability, the dose attributed to the criticality alone can be evaluated and compared to that from the entire repository. This comparison allows the investigator to determine the significance of the criticality in terms of total dose at the accessible environment. The performance assessment model also has the capability of including a distribution of criticalities in time and space to evaluate the long-term effects of multiple cyclic events on the total dose at the accessible environment.

3.7 References

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DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

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- 3-7. *Disposal Needs for Isotopic Data*, DI Number: BBA000000-01717-4200-00013 REV 00, CRWMS M&O.
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- 3-9. *Critical Dimensions of Systems Containing ^{235}U , ^{239}Pu , ^{233}U , 1986 Revision*, LA-10860-MS, LANL, Los Alamos, NM, p. 42.
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DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

4.0 MODEL DESCRIPTION AND VALIDATION

| An overview of the methodology for performing disposal criticality analyses for the proposed
| Yucca Mountain repository is provided in Chapter 3. This methodology is based on models for
| performing neutronics calculations, models for generating potential configurations of fissionable
| materials, models for assessing the consequence of potential criticality events, and repository
| performance assessment models. This chapter provides a description of these models along with
| possible information and data to be used in their validation. The model development and
| validation is an ongoing process.

4.1 Neutronics Models

| Two types of neutronics models are used in assessing the criticality potential of spent nuclear
| fuel. The first model uses the SAS2H⁴⁻¹ computer code system to determine the material
| isotopic composition of spent nuclear fuel from commercial light water reactors, and the second
| model uses the MCNP 4A⁴⁻² code for performing criticality analyses for various configurations
| of fissionable materials. These models are described in this section, followed by a discussion of
| the model validation strategy. The experimental data and supporting analyses for the validation
| process are discussed in References 4-3 through 4-5.

[Note: Additional validation analyses will be performed prior to release of the topical report.
The method biases and uncertainties, determined from all validation analyses performed, will
then be used in establishing the subcritical limit values for each of the three regions or locations
in the repository where criticality analyses are performed.]

4.1.1 Isotopic Model

| The isotopic model determines isotopic concentrations of the fissionable and absorbing isotopes
| to be used for criticality evaluations. The computer code system used by the isotopic model is
| described in this section. This model will be used for determining isotopic concentrations of
| commercial SNF for disposal and is validated using commercial SNF data. The isotopic
| concentrations determined with this model, for the 29 principal isotopes defined in Section 3.4.3,
| will be used for burnup credit for configurations internal to waste packages. There is currently no
| justification for including isotopic concentrations of the fission products (15 of the principal

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

isotopes) for configurations external to waste packages due to the different material separation, transport, and deposition processes for fission products versus the actinides.

[Note: This Isotopic Model section of the technical report is written for commercial SNF from light water reactors. Other waste forms (with potential for criticality), when selected for geologic disposal, will be addressed in Isotopic Model sections of addenda to the topical report.]

For the methodology developed in this report, the neutronics model for determining isotopic concentrations of SNF uses the SAS2H sequence of the SCALE-4.3 computer code system with the 44-energy group cross section library. SAS2H is the control module for the analytical sequence. The functional modules (or codes) within the sequence are BONAMI-S, NITAWL-S, XSDRNPM-S, COUPLE, and ORIGEN-S. SAS2H converts user input data into the forms required by the functional modules. BONAMI-S and NITAWL-S perform problem-dependent resonance processing of neutron cross sections. XSDRNPM-S is a one-dimensional discrete-ordinates code that produces a weighted cross section library and spectra data. This data is used by COUPLE to update an ORIGEN-S data library. ORIGEN-S is a point-depletion/decay code that computes the time-dependent isotopic concentrations using the matrix exponential expansion technique. For short-lived nuclides a form of the Bateman equation is used to ensure better accuracy. ORIGEN-S computes the isotopic concentrations (actinides and fission products) for all required conditions. This includes both power operation and shutdown intervals while the fuel is in the reactor. ORIGEN-S is also used in calculating radioactive decay and daughter isotope buildup after the fuel is withdrawn from the reactor core. Since ORIGEN-S is a point model, spatial and spectral effects are not explicitly modeled. However, spatial and spectral effects are incorporated in the model through the one-dimensional spatial and the 44 energy group spectral weighting of data by XSDRNPM-S.

A fuel assembly is modeled with SAS2H in one-dimensional cylindrical geometry. This modeling is a two step process. First, the fuel is represented as an infinite lattice of fuel rods with XSDRNPM-S, where resonance data is obtained from BONAMI-S and NITAWL-S. Second, cell-spectrum-weighted cross sections from XSDRNPM-S are then applied to the fuel zone in a larger cell model representing part or all of a fuel assembly within an infinite lattice. Material and volume ratios for the zones must be appropriate for the physical system being represented. Weighted cross section and spectra data from this model are used by COUPLE to update the ORIGEN-S data library. ORIGEN-S performs point depletion calculations to provide updated isotopic concentrations that are fed back to the one-dimensional model. The first step is

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

then repeated and new weighted cross section and spectra data are determined for the next depletion calculation. Updating of the ORIGEN-S library for depletion time steps is performed to appropriately represent changes (with depletion) in the neutron energy spectrum within the fuel assembly. A more detailed discussion of the SAS2H modeling for PWR fuel is presented in Reference 4-3. For BWR fuel, additional weighting of cross section data is necessary to accommodate the additional heterogeneities present within the fuel assemblies. A BWR SAS2H model is currently under development to accommodate these heterogeneities and will be described in the topical report.

4.1.2 Criticality Model

The criticality model is used to calculate the criticality potential (k_{eff}) of a wide range of potential fissionable material configurations during the disposal time period. An upper bound is identified to represent the maximum value of k_{eff} that will ensure subcriticality for the configurations analyzed. This upper bound, called the upper subcritical limit, is determined during the criticality model validation process. The computer code system used by the criticality model is described in this section. This includes a brief description of the Monte Carlo method and the material cross section data used for criticality evaluations.

4.1.2.1 Criticality Model Description

For the methodology developed in this report, the neutronics model for disposal criticality analysis uses the MCNP 4A computer code system to calculate nuclear reactivity (or chain reaction potential) of systems with fissionable material. MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport, including the capability to calculate eigenvalues for critical systems. The composition of the SNF materials, obtained from SAS2H (or ORIGEN-S), are input to the MCNP code. Nuclear cross section data are obtained by MCNP from the ENDF libraries in a compressed ENDF (ACE) format provided by Los Alamos National Laboratory (LANL). The neutron cross sections in the ACE libraries are not collapsed into energy groups (as is done for the KENO code variants); but instead, cross sections are provided at energies ranging from very low energies through 20 MeV in sufficient detail that the original ENDF data can be accurately reproduced by linear interpolation.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

MCNP uses pointwise cross section data, which tabulate the cross section for each different type of nuclear interaction as a function of energy. For neutrons, all interactions given in a particular cross section evaluation (such as ENDF/B-V) are considered for. Neutron interactions in the thermal energy range may be described by the free gas or $S(\alpha,\beta)$ models.

MCNP allows explicit geometrical modeling of systems through the use of geometric cells defined as the intersections, unions, and complements of first-degree and second-degree surfaces and fourth-degree elliptical tori.

4.1.2.1.1 The Monte Carlo Method

The Monte Carlo method is a method of simulating and recording the behavior of individual particles within a system. The behavior of the simulated particles is extrapolated to describe the average behavior of all of the particles within the system. The Monte Carlo method as applied to neutrons in an MCNP criticality calculation is based upon following a number of individual neutrons through their various transport experiences such as scattering, fission, absorption, or leakage. The fission process is regarded as the birth event that separates generations of neutrons. A generation is the lifetime of a neutron from birth by fission to death by either escape, parasitic capture, or absorption leading to fission. The average behavior of the sample set of neutrons is used to describe the average behavior of the system with regard to the number of neutrons in successive generations (i.e., effective neutron multiplication factor, k_{eff}).

4.1.2.1.2 Cross Section Data

Using the appropriate material cross section data in an MCNP criticality calculation is essential to obtaining credible results. The cross sections for the various neutron interactions are used to determine the flow of the criticality calculation at each interaction site. The MCNP neutron interaction tables are processed from evaluated data sets.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

The MCNP neutron interaction tables provide the following data:

1. all available cross section data,
2. angular distribution data for scattered neutrons,
3. energy distribution data for inelastically scattered neutrons,
4. data about secondary photon production,
5. Q-value data for each reaction, and
6. the average number of neutrons per fission data for fissionable isotopes.

A description of the MCNP cross section data used for the validation analyses presented in this report is given in References 4-3 and 4-4.

4.1.3 Neutronics Model Validation

This section outlines the overall strategy for validating the isotopic and criticality models, along with the associated SAS2H and MCNP codes and cross section libraries. The overall validation strategy considers potential critical configurations of fissionable material for three regions or locations within the repository. The first region is inside the waste package, the second region is outside of the waste package but inside the EBS (near-field), and the third region is outside the waste package in the host rock (far-field). For model validation the range of potential degradation conditions of the SNF is divided into three categories: 1) intact SNF that is still in a ceramic form (e.g., UO_2) and still maintains its regular lattice geometry, 2) fragmented SNF that still retains its as-emplaced chemical composition (modified by radioactive decay), but its geometry is no longer in a regular lattice, and 3) SNF dissolution products with individual elements distributed in solution or precipitated according to their individual solubilities. For degradation conditions 1) and 2) both actinides and fission products, from the 29 principal isotope set, will be accounted for in burnup credit calculations. For degradation condition 3) individual neutronically significant species from the SNF, as established by the configuration generator code (described in Section 4.2), will be considered. Internal to the waste package (region 1) all three degradation conditions can occur. For near-field locations (region 2) degradation conditions 2) and 3) are considered to occur. For far-field locations only degradation condition 3) is considered to occur.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

4.1.3.1 Region 1 - Inside Waste Packages

The initial (intact) lattice configuration (geometry) of SNF inside waste packages is known. All other configurations both inside and outside of waste packages are hypothetical. The initial geometry is dependent upon the fuel assembly design and the waste package design. The composition of the SNF inside the fuel assembly is dependent upon the fuel assembly design, the initial enrichment of U-235, and the operating history of the fuel assembly in a commercial light water reactor. The fuel assembly design parameters and initial enrichment of U-235 are known. The operating history of the fuel assembly in a reactor may be obtainable, but is generally not known. The isotopic model validation process must accommodate both the known and the unknown characteristics of the SNF.

The isotopic model validation is performed for region 1. For configurations of SNF external to waste packages, concentrations of those isotopes that can be shown to be neutronically significant are obtained from the same isotopic model, which is validated for region 1 (inside waste packages). The decay constants of non-stable isotopes are used in extending the range of applicability beyond the time period where model validation is performed. Uncertainties in these decay constants are used to account for uncertainties in the isotopic concentrations as a function of time.

The material composition within SNF assemblies from commercial reactors is complex. Various quantities of many individual isotopes are present. The spatial distribution of individual isotopic concentrations within a given fuel assembly varies significantly. Both the quantities and the distributions of the isotopes are governed primarily by the operating history of the nuclear reactor (and the accompanying local neutron spectra effects) that created the SNF. Since the material composition within SNF assemblies is complex, with significant variations in both the quantities and distributions of individual isotopes, the validation process for the isotopic model is also complex. For example, chemical assays will provide data for validating the concentrations of selected isotopes for either a very small segment of fuel within a fuel assembly (data from a single pellet within a fuel rod) or will provide assembly averaged data that doesn't represent axial distributions. It must be ascertained if the integrated neutron spectra that produced this assay data is representative of SNF assemblies for disposal.

Another class of experimental data is commercial reactor criticality (CRC) data for zero-power (ZP) conditions. Although this data provides excellent criticality benchmarks for SNF in a

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

reactor, it does not provide measured isotopic concentration data for individual isotopes. Thus, CRC data is addressing both isotopic model validation and criticality model validation with a single class of experiments. The CRC experiments contain fuel assemblies with a range of fuel enrichments, burnup values, and burnup distributions. This is similar to waste packages where fuel assemblies with various enrichments and burnup values will be loaded into a single waste package. The PWR CRC experiments contain soluble boron for reactivity control, whereas waste packages do not contain soluble boron. The CRC experiments may contain burnable absorber rod assemblies (BPRAs), rod cluster control assemblies (RCCAs), and axial power shaping rods (APSRs). The presence of soluble boron, BPRAs, RCCAs, and APSRs during reactor operation will affect SNF isotopic concentrations and their distribution within fuel assemblies. The waste packages will also contain neutron absorbing materials for reactivity control and will contain SNF whose isotopic concentrations are affected by various reactor control materials. Although waste packages will contain about one-tenth the number of fuel assemblies as a typical commercial reactor core, the neutron spectra for CRCs should be representative of intact configurations of SNF in waste packages. The validation process will evaluate the degree of similarity in the neutron spectra between the CRCs and SNF in waste packages

CRC data is being used as one component of both the isotopics model validation and the criticality model validation process. This approach is unique for obtaining burnup credit for use in criticality evaluations. However, this approach is the one used for reactor design (i.e., the reactivity effect of burnup is validated using CRC data). The model requirements for reactor design are more stringent since the capability to predict both small reactivity differences (reactivity coefficients and various differential and integral reactivity worths) and local power peaking within small limits is necessary in order to meet the requirements in the Final Safety Analysis Report (FSAR). The predictive capability of the neutronics models used for reactor design is demonstrated through reactivity measurements and through power distribution measurements with an incore detector system. A large CRC database containing some of the same measurements and measurement systems is used in the validation process for the neutronics models for disposal criticality with burnup credit. For reactor design the measurements demonstrate that the predictive capability of the neutronics models is sufficient to bound the FSAR requirements. For waste package design it must be demonstrated that the predictive capability of the neutronics models is sufficient to bound the 10 CFR 60⁴⁻⁶ requirements.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

For intact SNF inside the waste package, three types of experimental data are being used for the neutronics model validation. These include CRCs, LCEs, and chemical assays. The CRCs and LCEs are used in determining method bias and uncertainty for the criticality model. The CRCs represent SNF in known critical configurations, where the material composition of the SNF for each criticality statepoint analyzed is obtained from the isotopic model. The change in material composition with burnup is modeled with 16 to 24 axial nodes for each fuel assembly (will vary between plants) based on fuel assembly design and core operations data. Local thermal-hydraulic feedback effects during core operations are modeled based on core follow calculations (e.g., with the CASMO⁴⁻⁷ / NEMO⁴⁻⁸ code system).

Data for 90 CRC statepoints are being collected and analyzed. This includes PWR data from both Babcock & Wilcox and Westinghouse designed plants, and BWR data from General Electric (GE) designed plants with both GE and Siemens fuel designs. Additional PWR data is being sought for Combustion Engineering designed plants. The CRC database covers annual, 18-month, and 2-year fuel cycles; initial U-235 enrichments ranging from 1.6 to 4.96 wt%; soluble boron concentrations ranging from 0 to over 2200 ppmB; axial and radial zone loaded fuel; axial blanket fuel; and a variety of burnable poison designs. The CRC database also covers statepoints for beginning-of-life (BOL) with all fresh fuel, beginning-of-cycle (BOC) with a mixture of fresh and burned fuel, and middle-of-cycle (MOC) to end-of-cycle (EOC) with all burned fuel. The statepoint cases will be grouped according to parameters affecting k_{eff} (e.g., fuel enrichment, burnup, soluble boron concentration). The contribution of each parameter to variations in the calculated k_{eff} will be investigated and the results used to identify potential biases in the calculational model.

Approximately 80 LCEs with lattice configurations are also being analyzed to supplement the CRC database in identifying potential biases in the model. Each experiment is designed to vary a single parameter. The LCEs contain a wide range of water to fissionable material ratios (e.g., atom, mass, or volume) and contain neutron absorber materials that are similar to those in waste packages. Thus, a wide range of neutron energy spectra is represented by the LCEs, which will be shown to bound the neutron energy spectra of waste packages.

Sensitivity analyses will be performed to investigate potential non-conservatisms in the material compositions from the isotopics model that may be masked in the CRC benchmark analyses. Chemical assay data⁴⁻⁵ are being analyzed to define ranges of variation in the isotopic concentrations. These variations will be studied for the CRC statepoints to establish the potential

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

impact on the calculated k_{eff} and any uncertainty associated with the integral method used for SNF material composition.

Additional sensitivity analyses will be performed to establish input parameters for the isotopic model for waste package application. These analyses will address axial effects such as power density, burnup, moderator density, and fuel temperature distribution; effects due to the presence of absorber materials such as soluble boron, RCCAs, BPRAs, APSRs, and other absorber materials (e.g., Gd fuel rods) used in assembly design; and effects due to other design features such as axial blanket fuel and various types of zone loading of fuel and absorber materials. The result of these sensitivity analyses will be a set of input requirements to be followed in developing loading curves for waste packages. These input requirements were previously referred to in Figure 3-8 as "model input parameters." The degree of conservatism imposed on the neutronics models based on the input requirements and measured against the as-built/as-operated CRC data will be documented. The conservatism from these sensitivity analyses will be addressed in conjunction with the results from the sensitivity studies for the chemical assay data in establishing any uncertainty in the neutronics model associated with the integral approach used for validating SNF material composition.

The validation process for fragmented SNF inside the waste package that remains in a ceramic form but is no longer in a regular lattice uses additional LCE data. The SNF material composition is obtained from the same isotopic model previously described. The geometry of the material composition has changed, thus criticality experiments for non-lattice configurations of fissile oxide fuel will be used. Results from these experiments will be combined statistically with the CRC results in establishing model bias and uncertainty for degraded SNF inside the waste package.

Both metal and solution LCEs (over 200) for slab, cylindrical, spherical, and other geometries are being analyzed for model validation for degraded conditions inside the waste package with SNF dissolution products. The isotopic concentrations of those isotopes that remain is obtained from the same isotopic model previously described. The model validation process for these degraded conditions inside the waste package is similar to the model validation process for near-field locations. However, the condition of a mixture of fragmented SNF and SNF dissolution products must also be addressed.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

4.1.3.2 Region 2 - Near-Field Locations

For near-field locations (inside the EBS but outside the waste package) dissolution products from the SNF will be considered for criticality evaluations. (While the SNF in the near-field may be in a ceramic form and therefore contain fission products, this is not assumed at this time.) The SNF material composition of neutronically significant isotopes identified for this region by the configuration generator code is obtained from the same isotopic model previously described. Uncertainties in the decay constants of the isotopes that remain will be used to establish uncertainties in the isotopic data beyond the time period where model validation was previously performed. Both metal and solution LCEs for slab, cylindrical, spherical, and other geometries (that bound the range of configurations established by the configuration generation code) are being analyzed for model validation. These experiments are used in determining method biases and uncertainties for the criticality model for near-field locations. These biases and uncertainties will be used in developing subcritical limit values for criticality evaluations for this region.

4.1.3.3 Region 3 - Far-Field Locations

Configurations of fissionable material in far-field locations (outside the EBS) requiring criticality evaluations (including isotopic constituents) will be identified by the probabilistic models. The LCEs used for model validation will be similar to those used for region 2 (near-field). The application of these the LCEs in determining bias and uncertainty for potential configurations in the far-field may be different (i.e., may require extending range of applicability of experiments by extrapolating trends established for the bias). Neutronics model development and validation for this region will proceed in conjunction with the models for generating potential configurations of fissionable materials.

4.1.3.4 Applicability of Critical Experiments to Disposal

The recommendations presented in NUREG/CR-6361⁴⁻⁹ are followed (as applicable) in the selection of experiments for validating the neutronics model for disposal criticality evaluations. The recommendations for the determination of calculational bias and uncertainty will also be followed. Because of the complexities associated with the long time periods involved for disposal of SNF, additional considerations beyond those discussed in this NUREG are necessary and are discussed below.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

The NUREG identifies three fundamental parameters to be considered in selecting suitable experiments. These include materials of construction (including fissionable material), geometry of construction, and inherent neutron energy spectrum affecting the fissionable material(s). As noted in Section 3.4, the material composition (which is initially equivalent to materials of construction discussed in the NUREG) and geometry will change from their initial state based on isotopic decay and material degradation processes during the long disposal time period. The selection of suitable experiments for validating the neutronics model for disposal criticality evaluations accommodates this change.

Guidelines are provided in the NUREG for addressing the three fundamental parameters. These guidelines note that for the materials of construction, the fissionable and nonfissionable species used in the benchmark experiments should be as similar as possible as those materials in the package design under normal and hypothetical accident conditions. For waste packages, the materials of construction for the SNF assemblies are identical to the SNF assemblies in the CRC benchmark experiments. However, as previously noted, the initial composition of materials (material of construction) in the SNF assemblies are strongly dependent on the operating history of the assemblies in a commercial reactor. The effect of reactor operating history on material composition of SNF assemblies is being quantified as part of the validation process. This addresses the isotopics model and any (local or global) path dependent burnup effects on reactivity. Thus, additional considerations are being addressed for waste packages regarding materials of construction.

Other materials (e.g., stainless steel, carbon steel, neutron absorbers) may either be different or have different relative masses between the waste packages and the CRC benchmark experiments. The effect of these materials on criticality are addressed in the disposal criticality model validation process through LCEs.

Guidelines to address the similarity between experiments and package design for reflector and moderator materials, physical form and temperature of materials, and ratio of nonfissionable materials to fissionable material are also given in the NUREG. This is being addressed for the CRC benchmark experiments and the LCEs to ensure that the range of these parameters are applicable for waste package design for the long disposal time period of concern. The range of potential critical configurations that will be evaluated for waste packages is large, thus additional considerations beyond those presented in the NUREG are required. The NUREG lists items to consider regarding geometry of construction. These items are applicable for configurations

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

inside the waste package. However, the original waste package design does not resemble potential configurations of fissionable materials in far-field locations. Thus, LCEs are being chosen to bound potential configurations (identified by the probabilistic methodology) for degraded states for near-field and far-field locations.

Finally, guidelines are provided for comparing the neutron energy spectrum from the benchmark experiments and the waste package design. The neutron spectra for the CRC benchmark experiments will be compared with the neutron spectra for waste package designs containing SNF assemblies from various statepoints. Additional neutron spectra comparisons for benchmark LCEs and waste package designs (including degraded configurations) will also be made. These comparisons will include neutron leakage, absorption, production, and flux, as discussed in the guidelines.

NUREG/CR-6361 also provides guidance for the determination of bias and subcritical limits. Two methods are presented for the determination of an upper subcritical limit from the bias and uncertainty associated with the calculation of criticality. Guidance for applying each of the methods is provided. This methodology will be applied in determining upper subcritical limit values for the three regions previously discussed. This includes dividing the benchmark experiments (CRCs and LCEs) into subsets according to parameters studied (e.g., burnup, neutron spectrum characterization parameter) and applicability to a given region. The contribution of each parameter to variations in calculated k_{eff} is then established and the results used in establishing upper subcritical limit values for the three regions of concern.

[The various benchmark data (LCEs, CRCs, and chemical assays) for the topical report have been selected and are currently being documented (to meet QA requirements) and analyzed, and documentation of the analyses is being prepared. Statistical analyses will be performed and documented upon completion of the benchmark analyses. The sensitivity analyses mentioned in Section 4.1.3 are in the beginning stages, but will be completed for the topical report. Code-to-code is also being considered to support the validation process (TBD).]

4.2 Scenario Evaluation and Configuration Generation

Scenarios will be evaluated and configurations will be generated by a computer code called the configuration generator. The algorithms of this code will be abstracted from detailed

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

performance assessment models. These models are generally grouped into five categories. The first category (repository environment) provides input parameters to the other four. The other four model categories provide the parameters which go into the mass balance equations which determine the expected values of species concentrations in the various locations where criticality can occur. Alternative scenarios will be generated as a function of the input parameters which are determined from appropriate probability distributions. The evolution of the scenarios is described in terms of the environmental parameters and the location and concentrations of isotopic species which are major determinants of criticality (neutron absorbers and fissionable material).

4.2.1 Configuration Generation Code

The configuration generation code is being developed for this methodology to track the concentrations (or amounts) of neutronically significant isotopes (either fissile or neutron absorbing) and chemical species which can effect the solubility of the neutronically significant elements. As was mentioned in Section 3.3.4, the concentrations, or amounts, are tracked by time-dependent first-order differential equations, which are solved by numerical integration. The update process at each time step consists of the following:

- For the waste package:
 - Increment water in the package according to the difference between inflow and outflow from package.
 - Compute the increment to the solution from each solid being dissolved at this time step, according to the intrinsic dissolution rate and the solid surface remaining.
 - Compute the decrement to each element/isotope from the amount of solution removed at the previous time step.
 - Compute pH and solubilities as a function of the concentration of species which can effect pH and solubility (e.g., chromate, carbonate), including the effect of pH on solubility.
 - Compute precipitation and/or dissolution of the various species being tracked, according to the above determined solubilities for this time step; for elements with more than one neutronically significant isotope (only U-238 and U-235 in the current model implementation) the following refinement is implemented:

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

- The relative isotopic concentrations going into solution from the dissolution of the several possible source terms at this step and those isotopic concentrations already in solution are recorded (stored).
 - The isotopic concentrations are combined to update the amounts of each element or each chemical species in solution according to the maximum concentration permitted (solubility limit) for the combined isotopes; the increment of the combined isotopes (or decrement) to the amount in solution is recorded.
 - The amounts of the individual isotopes in solution and precipitate are recalculated according to the previously recorded isotopic percentages and the combined decrement (or increment) to the amount in solution.
- For the invert (first external potential pond):
 - Accept outflow from the package, augmented by any inflow from the drift (including dissolution from depleted uranium backfill, if any).
 - Decrement by outflow and compute new concentrations.
 - Compute pH and solubilities as a function of pH.
 - Compute precipitation and/or re-dissolution of the various solids in contact with solution, according to the above determined solubility for this time step. If there is an inflow from the drift containing depleted uranium, the isotopic composition can change with time, so the special bookkeeping of individual isotopic species used for the waste package solution will have to be repeated for the invert.
 - Compute the concentrations in the outflow for this time step.
 - For a designated path through the rock beneath the invert to the next pond location:
 - Accept the outflow from the invert and store in array element for this time.
 - Compute fracture travel time (assumed to be the same for all species).
 - Compute matrix travel time for each species (primarily Pu and U), using species specific retardation coefficients.
 - Compute outflow for this time from inflows at this time minus appropriate travel times.

The next pond location is handled the same as the invert and the pond-path cycle can be repeated.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

4.2.2 Probability Combination Methodology

The probabilities associated with the generated configurations (concentrations and amounts calculated from the configuration generator code) will be determined by combining the probabilities associated with the distribution of possible input parameter values. The following are typical sources of parameter uncertainty:

- Material properties (over the range of pH and ionic strengths): dissolution rates, solubilities, adsorption/partition coefficients; these uncertainties can be reflected in pdf's.
- Geologic conditions or environmental parameters: infiltration rate, fracture networks above the repository which can concentrate infiltration, matrix-fracture split for fissionable material bearing transport, focusing SZ flow to the accessible environment (like springs), existence of reducing zones; many reflected by pdf's, but the last two must be stated alternatives.
- Process models: passivating layers for dissolution protection, galvanic protection, colloid formation and persistence; nominally stated alternatives.

The full probability distributions of such uncertain parameters will be represented by discrete distributions having at least three parameter levels (high, average, low). In such a discrete distribution the associated point probabilities will sum to 1. It is expected that there will be between 6 and 10 uncertain parameters for each problem type, which implies at least between 3^6 and 3^{10} possible combinations (between 729 and 59049).

4.2.3 Abstraction of Models

The YMP total-system performance assessment for Viability Assessment (TSPA-VA) is developing abstractions of detailed process models to permit their use in stochastic TSPA-VA analyses. Abstraction is the process of capturing the essential features of a detailed model such that it can be used in a computationally efficient way in performance analyses generally. Several of the process models are directly applicable to analyses that will be done to quantify the scenarios which lead to configurations with the potential for criticality. The applicable models include:

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

- waste package degradation
- waste form degradation and mobilization
- geochemistry of near-field materials
- unsaturated-zone (UZ) thermohydrology
- UZ flow and transport
- saturated-zone (SZ) flow and transport

Subject-matter experts have identified potentially important parameters and processes for these detailed models, and they and PA analysts are performing sensitivity studies to determine which processes and parameters must be included in the abstracted TSPA-VA models. The result of the abstraction/testing activities for the above models will be an efficient means of investigating all the components of the scenarios developed (as described in Chapter 3).

For waste package degradation, the important issues being investigated toward abstraction include the corrosion processes (corrosion of waste package carbon steel outer barrier, corrosion of inner barrier, and including consideration of microbiologically-induced corrosion for both barriers), and effects on waste package degradation of variability in near-field environment conditions, in manufacturing, and in materials. In addition, other processes that can affect waste package degradation, such as galvanic protection are also considered. Responsibilities for models involving waste package degradation are shared among the Performance Assessment, Waste Package Development, and Waste Package Materials departments. Examples of the detailed modeling issues being addressed are:

1. Issues related to outer barrier corrosion:
 - refluxing and concentration of electrolytes
 - temperature dependence on corrosion
 - model of salt build-up
 - critical relative humidity (dry-humid
 - critical relative humidity (humid-aqueous
 - aqueous corrosion (localized/pitting
 - flow rate and episodicity of water
2. Issues related to inner barrier corrosion:
 - aqueous corrosion (localized/pitting

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

- crevice
- cathodic protection
- choice of waste package materials
- barrier interface environment

3. Issues related to microbially induced corrosion:

- maximum corrosion as a function of limiting factors, such as availability of water and nutrients, and available energy
- performance of specific materials (such as those that may be toxic to bacteria), and material processes and characteristics (such as weld materials and treatment history, impurities, and crystal/grain structure)

4. Issues related to galvanic protection against inner barrier corrosion by sacrifice of outer barrier:

- crevice corrosion (including at welds)
- limiting factors
 - ionic conductivity at
 - electrode area
 - contact
- water-contact mode inside and outside
- negative effects of ferric ions on the inner barrier

For waste form degradation and mobilization, important issues being investigated for abstraction include:

1. Issues related to spent fuel and other waste forms:

- dissolution rate, including dependence on pH, Cl⁻,
- formation of passivating and alteration layers

2. Issues related to mobilization and transport:

- physical processes - water contact
- colloids
- chemical processes - mobilization - fluid dependence
- physical processes - transport paths

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

The general issues of geochemistry and environmental conditions in the near-field can influence the rates and modes of waste package and waste form degradation. Areas identified for further analyses that will support the degradation studies include:

1. Issues related to the dissolution of solid phases:

- volume and flux of water in drift
- compositions, abundances, and distribution of natural and introduced materials (cement, alloys, organics, microbes, ceramics)
- aqueous and gas reactions on
- in-drift system open or closed

2. Issues related to gas phase:

- gas flux
- reactions with solids and microbes (excluding waste package)
- thermal effects (water reactions)
- temporal heterogeneity

3. Issues related to the aqueous phase:

- aqueous phase reactions with major introduced materials (excluding waste package)
- temporal evolution of aqueous phase composition

4. Issues related to colloids:

- reversibility of radionuclide sorption onto colloids
- water-composition
- waste form

4.2.4 Model Details

The following sub-sections provide further details of the performance assessment models, the results of which will be abstracted into the configuration generation code to address the issues identified in Section 4.2.3 above.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

4.2.4.1 Repository Environment Model

The repository environment sub-model provides the distribution of parameters to be used as input to the other four sub-models. All the algorithms and parameter values of this sub-model are derived directly from, are abstracted from the results of, or are in agreement with, corresponding sub-models of the TSPA model. Furthermore, the use of these sub-models will be consistent with their use in TSPA-95⁴⁻¹⁰ and TSPA-VA.

4.2.4.1.1 Fundamental Environmental Parameters

The hydraulic properties of the repository rock are determined by measurements taken primarily from surface drilling and from sampling in the Exploratory Studies Facility (ESF). These parameters will be updated as part of the Scientific Investigations and TSPA processes. Examples of the parameters are porosity, matrix permeability, and fracture permeability. In general, a higher permeability will increase the probability of internal criticality by increasing the rate of flushing the waste package, thereby increasing the rate at which the neutron absorber can be removed from the waste package. For external criticality, the spatial variations of fracture permeability will significantly affect the transport of nuclear significant species and the concentration of water available for moderation.

Other parameters will change under the influence of the heat from emplaced waste packages. Some typical parameters of this type are infiltration rate, initial water pH, and dissolved oxygen. The algorithms which model the changes in these parameters are indicated in Section 4.2.1.

4.2.4.1.2 Environmental Parameters Derived from Modeling Waste Package - Environment Interactions

Many environmental parameters will be changed significantly by the presence of the repository, particularly from the thermal load from the emplaced waste packages. The change in these parameters (with respect to their measured initial values) is estimated, as part of the TSPA process, from recognized computer codes which model the fundamental heat and mass transfer processes.

Starting with typical initial measurements as inputs, temperature, humidity, and infiltration rate are determined as a function of time using a hydrothermal code with the following principal

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

inputs: heat generation (by the waste packages), heat transfer (by mass transport, diffusion, radiation, and convection), and hydrologic permeability.

Water chemistry parameters (pH and principal ion concentration) are determined as a function of time by using a chemical thermodynamics code, such as EQ3/6, with input parameter values from rock sample measurements. Certain basic reaction rates are in the code database, and others are developed from the degradation models of waste package materials and the waste forms, described below.

These fundamental physical process codes will generally be run only a limited number of times as part of the TSPA process, and this will only be for the purpose of establishing a parameterization which will then be incorporated into the simple mass-balance equations of the scenario generation code. In fact, maximum use will be made of cases already run by performance assessment, for representative repository parameter values.

4.2.4.1.3 Environmental Parameters Derived from Modeling of Prior Geologic Processes

Certain environmental parameters cannot be measured directly, and their values must be estimated from models of geologic processes which could have taken place at some time in the past and would have left the geologic environment unchanged since then. An illustration of such a modeling process is given in Reference 4-38; this model estimates the probability of occurrence of a reducing zone at the lower boundary of the tuff at Yucca Mountain. In particular, the estimate is based on the probability of the occurrence of organic deposits of sufficient size and density to accumulate a critical mass of low enriched uranium from a groundwater stream flowing through the deposit. Further description of the model is given in Reference 4-38. This appendix also shows how the probability of occurrence is incorporated in a stand-alone analysis of this type of criticality. The probability will be incorporated into the configuration generator code when it becomes available.

The model illustrated in Reference 4-38 was developed in consultation with, and the product is being reviewed by, geologists expert in the uranium and other mineral deposits. Refinements of this model, and other models of this type, will also be developed in consultation with and reviewed by geologists and geochemists with appropriate expertise.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

4.2.4.1.4 Validation of Environment Model

The repository environmental models used in the scenario generation tool are mostly derived from performance assessment models, as indicated in Section 4.2.1. Therefore, the validation of these parts of the scenario generation tool is accomplished indirectly by the validation of the TSPA models from which the scenario generation sub-models are derived. The validation of the TSPA models is part of the TSPA process and is described in the appropriate planning documents.

Validation of Thermal Conditions and Groundwater Hydrology Model

These scenario generation tool models will be developed from the abstraction of corresponding hydrothermal performance assessment code results, particularly those used for TSPA. These codes have been extensively verified and validated. For this project, the final validation is expected to be against data from the ESF heater tests.

Validation of Groundwater Chemistry

These scenario generation tool models will be developed from the abstraction of corresponding chemical/thermodynamics performance assessment code results, particularly those used for TSPA. These codes have been extensively verified and validated. For this project, the final validation is expected to be against the results of various tests being conducted on dissolution rates of waste package materials and waste forms.

Validation of Models of Prior Geologic Processes

| These models, illustrated by the reducing zone formation model described in Reference 4-38,
| deal with phenomena which are not directly measurable. At present, there are no corresponding
| or antecedent models in the TSPA process. It is expected that these validations will be
| accomplished by peer review.

4.2.4.2 Material Degradation Model

This section discusses materials for disposal container components, mechanisms for degradation of these materials, models for such degradation, and methods of validating such models.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

4.2.4.2.1 Materials for Disposal Container Components

Waste packages for high-level radioactive waste will include several components. *Waste forms* and *canistered waste forms* are placed into *disposal containers*. Together, these components form a *waste container*. The waste container differs from a *waste package*, as defined in 10 CFR 60, in that materials surrounding the individual waste containers are excluded. The disposal container may include a *basket*, which supports the waste and may perform other functions such as stiffening and strengthening the containment barriers, absorbing neutrons, and conducting heat to the containment barriers. For some PWR fuel, *control rods* will be inserted into SNF assemblies to absorb neutrons. Although it is not used in current designs, filler material has been considered for inclusion in the waste package. A *filler material* would be placed in void spaces to absorb neutrons and/or to displace moderator; filler material would possibly be added in granular form. Outside the waste package, a *waste package support* may be placed under the containment barriers to hold the waste package in place during seismic events, aid heat removal from the bottom of the waste package, and separate the containment barriers from potentially corrosive materials in the invert. Degradation of the basket material could lead to removal of the neutron absorber from the waste package, which would increase the probability of internal criticality. Scenarios of greatest interest include breaching of the containment barriers, which could allow water to fill the waste package and act as a moderator, and dissolution of neutron-absorbing isotopes from control rods or neutron-absorbing panels in the basket.

Materials that have been proposed for use in disposal containers are listed in Table 4-1. Table 4-2 lists the current materials selection for major components of the waste package⁴⁻¹¹. These are the materials that, in light of current knowledge, are expected to provide the best overall cost and performance. Research on other materials is continuing, however, because of the possibility that current understanding of the near-field environment and waste package degradation may be incorrect. ASTM A 516 is a low-carbon steel. ASTM B 443 is a nickel-base alloy (Alloy 625). Neutronit A978 is a proprietary grade of stainless steel with boron; its composition is based on that of Type 316. For PWR fuel, the fuel basket includes not only stainless steel-boron alloy plates but also carbon steel tubes that provide structural support and promote conduction of heat from the fuel to the containment barriers.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

Table 4-1. Materials Proposed for Use in Disposal Containers ^{4-11, 4-12, 4-13, 4-14}

Material	Proposed Uses
Carbon steel Low alloy steel	Corrosion-allowance containment barrier Filler material Heat-conducting material for basket Structural support tubes for SNF assemblies Basket guides Canister guide
Austenitic stainless steel	Moderately corrosion-resistant containment barrier Internal structural material, structural material for basket
High-nickel alloys Nickel-base alloys	Corrosion-resistant containment barrier
Copper-base alloys Copper-nickel alloys	Moderately corrosion-resistant containment barrier
Titanium alloys	Corrosion-resistant containment barrier
Ceramic coatings	Corrosion-resistant containment barrier
Aluminum-boron alloys and composites	Neutron-absorbing material for basket
Aluminum alloys without boron	Heat-conducting material for basket
Austenitic stainless steel with boron	Structural and neutron-absorbing material for basket Neutron-absorbing material for control rods
Zirconium-hafnium alloys	Neutron-absorbing material for control rods

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

Table 4-2. Current Waste Package Materials Selection

Component	Material
Corrosion allowance barrier for SNF waste forms	ASTM A 516
Corrosion resistant barrier for SNF waste forms	ASTM B 443
Fuel basket tubes for SNF waste forms (PWR only)	ASTM A 516
Fuel basket plates for SNF waste forms	Neutronit A978 or equivalent
Waste container fill gas for SNF waste forms	Helium
Basket guides for SNF waste forms	ASTM A 516

4.2.4.2.2 Degradation Mechanisms for Disposal Container Components

Because of the wide variety of materials under consideration and uncertainty about the repository environment, many forms of degradation are possible. For the metallic components, corrosion is the major degradation mode of concern. Possible forms of corrosion include atmospheric and aqueous general corrosion, dry oxidation, pitting, crevice corrosion, galvanic corrosion, stress corrosion cracking, and microbiologically influenced corrosion. For some of the proposed containment barrier materials, some of these corrosion forms occur in liquid water or in humid air; others require liquid water.

The ceramic materials that have been considered, notably spinel, mullite, and alumina, are not subject to the electrochemical forms of corrosion but are subject to dissolution if they are contacted by liquid water. The rate of dissolution will depend on the water chemistry, with pH being particularly important. Ceramic materials may also be susceptible to mechanical loading from rockfall.

Environmental attack on the waste package supports and the outermost containment barrier may begin immediately upon emplacement. Inner barriers and any internal structure will be protected by the outer barrier until the outer barrier is breached; it is expected that an inert environment will be provided inside the waste package^{4-15,4-16,4-17}.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

4.2.4.2.3 Models for Material Degradation

Because of the importance of corrosion control to industry, there is a substantial body of information on corrosion rates and mechanisms under various conditions. Unfortunately, 1) industrial conditions are normally different from (and often much more aggressive than) expected repository conditions, 2) repository time scales are much longer than industrial time scales, and 3) many corrosion measurements are not sufficiently sensitive to detect corrosion rates that would be significant to repository performance. As a result, most corrosion predictions must be extrapolated from tests under conditions that are more severe than those expected in the repository.

Dry oxidation of metallic materials is not expected to be significant under postulated repository conditions. Calculations for expected repository temperatures and humidities indicate that the penetration depths for dry oxidation will be much smaller than those for corrosion in humid air^{4-18, 4-19}.

The current level of understanding varies for different mechanisms of corrosion. At present, models for dry oxidation and atmospheric and aqueous general corrosion have been developed. These models are discussed briefly below. Other models are under development and will be discussed when they become available.

For corrosion-allowance materials, the most important degradation mechanism is expected to be general corrosion. Stahl⁴⁻¹⁸ has presented a model, with coefficients, for corrosion depth as a function of time and temperature for exposure to water under constant conditions. Two extensions of this model have been proposed^{4-10, 4-19}; both of these give corrosion rate for atmospheric corrosion in humid air as a function of temperature and humidity. In the limiting case of 100% relative humidity and constant temperature, they reduce to Stahl's model.

The rate of galvanic corrosion depends on (among other things) the galvanic potential difference between the two coupled materials, the surface areas of the materials, and water chemistry. Quantitative prediction normally requires measurement. Galvanic corrosion can be mitigated by proper waste package design. For example, the current design uses two barriers and puts the more active material on the outside, so that after breaching any remaining metal from the outer barrier would provide cathodic protection to the inner barrier. Similarly, the basket guides and

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

| basket tubes are more active than the basket criticality control material (plates and/or rods) and
| will corrode sacrificially to protect the material, which must provide long term criticality control.

For corrosion-resistant materials, the most important degradation mechanisms are expected to be various forms of localized corrosion. Localized corrosion (pitting, stress corrosion cracking, and crevice corrosion) is strongly dependent on water chemistry, and microbiologically influenced corrosion is strongly dependent on humidity or the presence of liquid water and on the presence of suitable nutrients. Microbiologically influenced corrosion is poorly understood. Since it is
| difficult to control postclosure repository conditions, these forms of corrosion can only be controlled by material selection. It is possible that for many waste packages the near-field environment will be so benign that none of the forms of localized corrosion will be significant. Under such conditions, the containment barrier will remain intact for an extremely long time.

More information on and better models for materials degradation will be produced by the ongoing materials research effort. These will be used when available and as applicable.

4.2.4.2.4 Validation of Models

For times up to a few years, integrated corrosion tests in a laboratory are expected to provide the best tests of the applicability of these models. Long-term (at least five-year) corrosion tests
| under expected and postulated repository conditions began during the 1996 fiscal year⁴⁻²⁰.
| Because of the extremely long times over which repository materials must perform, complete validation of models by laboratory experiments is not practical. Laboratory results may be supplemented by data for natural or historical analogs, but analogs are not expected to be available for all materials. It appears that the best approach to validation of performance under repository conditions is to predict performance by using conservative bounding models backed
| by adequate experimental data (such as those provided by the long-term corrosion tests), then conduct a performance confirmation program in an operating repository. Such a program could have a duration that is an order of magnitude longer than what is practical for laboratory experiments. Predictions of long-term performance must ultimately rely on models that will allow extrapolation from shorter-term data.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

4.2.4.3 Waste Form Degradation Model

This section discusses materials for waste form components, mechanisms for degradation of these components, models for such degradation, and methods of validating such models.

4.2.4.3.1 Waste Form Components

| The bulk of the waste will be commercial spent nuclear fuel and defense high level waste glass.
| Other types of waste forms include highly enriched Navy fuel, DOE fuel from production
| reactors, fuel from research reactors, and waste forms for surplus fissile materials. The scope of
| this report is limited to commercial spent nuclear fuel (although an example of DOE-owned
| aluminum-based fuels is discussed in Appendix C). Other waste forms will be treated in
| addenda.

Components of commercial spent nuclear fuel that significantly affect criticality include the cladding, the spacer grids and end plates, and the oxide (fuel pellet fragments). Since commercial PWR fuel is slightly undermoderated, collapse of a fuel assembly will tend to reduce reactivity. However, commercial BWR fuel is overmoderated and the opposite reactivity effect is observed with partial collapse of a fuel assembly. Spacer grids and end plates are made of corrosion-resistant materials, typically nickel-base alloys or austenitic stainless steel. Fuel cladding is normally made of a zirconium-base alloy, though some older fuels have a stainless steel cladding, and some newer fuels will have zirconium alloyed with niobium rather than tin⁴⁻²¹. The fuel pellets, which are typically fragmented when discharged from the reactor, are uranium dioxide (UO₂) with a mixture of activation and fission products.

4.2.4.3.2 Degradation Mechanisms for Waste Form Components

| Metallic components of commercial spent nuclear fuel are made of corrosion-resistant and heat-resistant materials. Because of the limited amounts of available reactive species, no significant degradation due to oxidation or corrosion can occur in an intact disposal container containing commercial spent nuclear fuel⁴⁻¹⁵.

Since the spacer grids and end plates are made of corrosion-resistant material, their degradation is expected to be slow even if the waste package is flooded. Localized corrosion is the most likely form of degradation since these materials resist general corrosion.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

The zirconium-base alloys used for fuel cladding are also quite corrosion resistant. However, some degradation of these materials can occur even in an intact disposal container. Substantial research efforts have been made in this area^{4-22,4-23,4-24}. Degradation mechanisms that have received significant attention include creep rupture, iodine stress corrosion cracking, various forms of hydrogen degradation, and oxidation.

The fuel pellet fragments are also subject to degradation. At sufficiently high temperatures in an oxidizing environment, the fragments will oxidize, from UO_2 to U_4O_9 and from U_4O_9 to U_3O_8 ⁴⁻²⁵. The first step results in a slight reduction in volume and opening of grain boundaries. The second step results in a large increase in volume and reduction of the fragments to powder. The increase in volume could result in splitting of the cladding. The oxides are also subject to dissolution. Oxidation (particularly oxidation to U_3O_8) and dissolution are coupled effects. By splitting the cladding, the formation of U_3O_8 will increase exposure of the fuel to water, and by breaking the fuel fragments into powder, it will greatly increase the surface area and dissolution rate. Oxidation can be controlled until the disposal container is breached by providing an inert environment for the fuel while the temperature is high.

Since fuel cladding is in the form of slender, thin-walled tubes, it might also be damaged by mechanical loading. Probably the most severe mechanical damage would occur if the containment barriers corrode away and a rock falls on exposed fuel assemblies. The importance of mechanical damage is being evaluated.

4.2.4.3.3 Models for Material Degradation

Models for corrosion of corrosion-resistant metals, such as those that are used in spacer grids, end plates, and cladding, are described in Section 4.2.2.3 above.

Iodine stress corrosion cracking of zirconium-base alloys has been considered and rejected as a significant cause of cladding failure⁴⁻²² because in typical spent nuclear fuel neither the concentration of free iodine in spent nuclear fuel nor the stress intensity factor is high enough to cause stress corrosion cracking.

Failure of cladding by creep rupture has been considered by several authors^{4-24,4-26,4-27}. A significant result of this work is that cladding failures by creep rupture will tend to produce small perforations in the cladding rather than gross ruptures⁴⁻²³. Upon such a failure, the fuel rod

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

pressurization gas (helium) will escape, and the driving force for further damage by creep rupture will be eliminated. It is possible that even cladding that has been perforated by creep rupture will act as a significant barrier to release of radionuclides from the waste form.

Various forms of hydrogen damage to cladding have been discussed and generally dismissed as a concern for dry storage⁴⁻²². Since conditions in an intact disposal container are similar to those for dry storage, significant hydrogen damage is not expected under these conditions⁴⁻¹⁵. Even after failure of the disposal container, significant hydrogen damage is not expected because of the modest temperatures and low water pressures.

Fuel oxidation has been investigated by Einziger⁴⁻²⁵ and the results have been applied to model degradation under expected repository conditions⁴⁻¹⁹. It was concluded that failure by fuel oxidation will not be significant because the requirements for protection by the disposal container are modest. The time for which protection is required will depend on repository design but is typically a few tens to a few hundreds of years. It has also been found that the fuel becomes cool enough that oxidation is negligible before the surface of the disposal container cools to the boiling point of water. While the disposal container is hot, aqueous corrosion is not possible, so there is great confidence that the container will provide sufficient protection against fuel oxidation.

Although its dissolution rate is slow, oxide fuel is subject to dissolution. Experiments⁴⁻²⁸ indicate that dissolution involves the formation of a complicated series of mineral phases. The overall process, however, might be approximated by congruent dissolution. Because of the relatively low solubility of uranium oxides, significant fuel dissolution requires that material be removed from the waste package. Accordingly, dissolution does not increase criticality potential inside the waste package, but it may need to be considered as contributing to critical configurations outside the waste package.

4.2.4.3.4 Validation of Waste Form Degradation Models

For spent nuclear fuel, the processes that could result in significant changes in reactivity are corrosion of the metal components of the fuel assemblies, oxidation of the UO₂ fuel pellet fragments, and dissolution of the UO₂ fuel. Experimental work is planned or under way on all of these processes⁴⁻²⁹. Particular attention is being paid to choosing conditions that are relevant to

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

disposal. The data from these experiments will be used as the basis for validating the models of waste form material degradation.

A systems study has been completed to determine what measures should be taken in an operating repository to monitor the degradation of emplaced waste packages⁴⁻³⁰. Such efforts will provide data on degradation under actual repository conditions, and they will allow measurements over time scales that are impractically long for laboratory experiments, but such results will not be available until long after license application.

4.2.4.4 Material Transport Model

The material transport (aqueous) sub-model will follow the TSPA methodology. For the unsaturated zone models ranging from the simplified methodology of RIP (Repository Integration Program) which is one dimensional with bulk permeability properties only, to the very comprehensive TOUGH2 (including explicit representation of fracture flow) have been applied.

The sophisticated techniques are also available for the saturated zone, but a simple plume dispersion model is often adequate. An illustration of the plume dispersion model applied to the possible combination of fissile bearing streams from several waste packages is given in Reference 4-38.

The material transport model will be validated with respect to the underlying TSPA models (TBV).

4.2.4.5 Transport Retardation/Precipitation Models

The retardation sub-model will follow the TSPA methodology, which presently models the simple equilibrium sorption reaction using the standard differential material-balance equations, incorporating a sorption (or distribution) coefficient, K_d , which is defined as the moles of radionuclide per gram of solid phase divided by the moles of radionuclide per milliliter of aqueous phase. The result of the mass-balance analysis can usually be expressed as a reduction of the nominal groundwater velocity (Darcy velocity) by a factor known as the retardation coefficient:

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

$$R_d = 1 + \rho_{bd}K_d/(\phi S_w),$$

where ρ_{bd} is the dry bulk density, ϕ is the porosity of the rock, and S_w is water saturation in the porespace.

- | The most likely mechanism for precipitation of uranium is a chemically reducing zone, the strongest potential examples of which are organic material and hydrothermal fluids containing hydrogen sulfide or methane. The likelihood of occurrence and the likely extent of such geochemistry in Yucca Mountain depends on many unknown factors, but the little known evidence gives no indication of such accumulating capability. The proposed criticality control methodology will evaluate these possibilities using some conservative models.
- | Retardation/precipitation of fissionable material is important in the determination of time at which a critical mass can be accumulated and the size of the rock region over which the material is distributed. The region over which the precipitated fissionable material is distributed is inversely related to the maximum concentration.
- | Sorption will be strongest in minerals known as zeolites, which account for over 50% of the rock in the Calico Hills (CH), which lies below the planned emplacement horizon. Reference 4-38 provides an illustration of the calculation of the maximum possible sorption of UO_2 in zeolite which shows that for commercial SNF the maximum possible density will be far less than is necessary for criticality. Since the calculation in Reference 4-38 was concerned only with the maximum sorptive capacity of the zeolite, there was no use of the transport model to determine whether, and when, the fissionable material could be available in the water flowing through the zeolite.
- | The transport retardation and precipitation models will be validated with respect to the underlying TSPA models (TBV). It should be noted that the prior geologic processes models mentioned in Section 4.2.4.1.3 and illustrated in Reference 4-38, also have some effect on the material retardation and precipitation parameters.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

4.3 Criticality Consequence Model

There may be up to six distinct criticality consequence models: either steady state or transient, and for three different types of location (internal, external near-field, and external far-field). The steady state model is concerned only with the increased radionuclide content remaining after the duration of the criticality. The transient model is concerned with the characterization of the energy release in the possibly very high power pulse over the short duration of the peak, as well as the cumulative buildup of radionuclide increments over a periodic pulsing.

It is expected that the transient models will be used to demonstrate the impossibility of a large kinetic energy yield for any criticality. It is also expected that the radionuclide increments from a pulsed criticality will be less than from the equivalent steady state reactor. Therefore, the steady state reactor is expected to be the more conservative method for estimating the increased radionuclide inventory, so the more elaborate transient model will not be used for this purpose.

Some of the six consequence models have been developed, and some are still in the design and development process. The models for internal criticality are summarized in the following subsections.

4.3.1 Internal Steady-State Criticality

As the criticality power level increases, the temperature will increase and the evaporative water loss will increase. Therefore, the steady state temperature is that at which the evaporative water loss is just equal to the total (net) water infiltrating into the waste package. If the temperature were to increase beyond this point, the net decrease in moderator would shut down the criticality. Once the temperature is determined, the power level can be computed as the total of the power lost through conduction, convection, radiation, and evaporation. The duration of the criticality is conservatively bounded by the length of the high moisture part of a climatological cycle, which might be as long as 10,000 years. It should be noted that this concept can be applied to criticality in which there is no standing water, but only water loosely bound to clay. Such water can be removed by evaporative heating, although the evaporation rate as a function of temperature and clay composition has not been sufficiently measured to support quantitative analysis at this time.

The principal direct consequence of a steady state criticality is an increase in radionuclide inventory, which is computed from a point-depletion code, such as ORIGEN, for a given initial

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

set of isotopes with a criticality of a specified power level and duration. In using the point-depletion code, the isotope concentrations are taken as those which lead to the criticality. Since criticality was assumed at a threshold value of k_{eff} which was significantly less than 1, the isotopic concentrations are not consistent with a steady state criticality at $k_{eff}=1$. The inconsistency is acceptable because it errs on the side of conservatism.

4.3.2 Internal Transient (or Quasi-static) Criticality

The reactor transient code, RELAP5, will be used to model the time dependent increase in k_{eff} with the following negative feedback mechanisms: Doppler broadening, void coefficient, thermal expansion, evaporation and/or boiling at the free water surface. There will be an evaluation of possible positive feedback mechanisms, particularly the autocatalytic effect which can arise in an over moderated system (which is not expected to be possible with the low enrichments of commercial SNF, but which will be a possibility for the higher enriched waste forms). Particular attention will be given to relatively rapid reactivity insertion mechanisms such as one or more assemblies shifting (or falling) from above the waste package water level to below the waste package water level due to some mechanical disturbance. Such a reactivity insertion mechanism might typically have a period of approximately 0.3 seconds (the time it might take to fall such a short distance).

4.4 Total System Performance Models

If the initial performance assessment evaluation indicates the need to conduct detailed TSPA calculations using the incremented radionuclide inventory, several models are required. Prior to using a total system performance assessment model, the source term for the criticality (i.e., the rate of release of radionuclides over time from the vicinity of the criticality) will be determined. This will be conducted to evaluate the solubility and alteration of the inventory produced by the criticality. The EQ3/6 code package is used to evaluate geochemical models of the criticality produced inventories. The result will be an estimate of the dissolved concentrations of radionuclides. The release rate over time as a function of groundwater flow and temperature, and the total inventory of radionuclides are then used in the total system performance assessment model.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

Because of the variability and uncertainty in models and model parameters, TSPA analyses will calculate numerous realizations of the processes comprising the scenarios important to repository performance. These calculations will provide a statistical representation of the effects of the variability and uncertainty. TSPA-VA calculations may be done using a variety of computer codes, and example of which is RIP. This code was used for the TSPA-95 analyses and may be used again for TSPA-VA.

The current approach to TSPA of a potential radioactive waste repository makes use of the computer program RIP in conjunction with detailed process-level models. The proposed methodology for this report is to use the same codes unless preferable alternatives are developed for TSPA prior to the time at which analyses are required. The RIP code, and the detailed process models are described in TSPA 1995⁴⁻¹⁰. The RIP code was specifically developed by Golder Associates Inc. in order to evaluate the performance of a potential radioactive waste disposal facility at Yucca Mountain^{4-31,4-37} and has subsequently been applied to a wide variety of proposed radioactive waste disposal facilities both in the U.S. and abroad. Most recently, the RIP code has been applied to the WIPP site in New Mexico^{4-32,4-34} and has been used to evaluate alternative disposal options for low-level waste for the State of New York⁴⁻³⁵. The RIP code is fully documented in a Theory Manual and User's Guide⁴⁻³³ and has a context-sensitive help package. The program has recently been formally verified consistent with ASME NQA-1 and ISO-9000 standards⁴⁻³⁶. It is expected to be qualified in accordance with OCRWM-QA in the near future.

The major features of the four component models of RIP (see Figure 4-1) that comprise the performance assessment model are: 1) waste package behavior and radionuclide release component model; 2) radionuclide transport pathways component model; 3) disruptive events model; and 4) biosphere dose/risk model. These models are summarized briefly below. For evaluation of the consequences of a criticality, the waste package component model could be modified or replaced by the source term for the criticality that is supplied to the TSPA.

The *waste package behavior and radionuclide release component model* input requirements are descriptions of the radionuclide inventories in the waste packages, a description of near-field environmental conditions (which may be defined as temporally and spatially variable), and subjective estimates of high-level parameters describing container failure, matrix alteration and dissolution, and radionuclide mass transfer. The waste package component model can simulate two layers of containment (e.g., outer package and zircaloy cladding). Waste package failure

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

rates, along with matrix alteration and dissolution rates, are used to compute the rate at which radionuclides are *exposed*. Once the radionuclides are exposed, RIP computes the rate of *mass transfer* out of, and away from, the waste package (or the vicinity of the criticality). Parameters describing waste package failure and radionuclide exposure and mass transfer can be functions of near-field environmental conditions. The output from this component (for each system realization) consists of time histories of release for each radionuclide from the waste packages (or from the vicinity of a criticality), and acts as the input for the transport pathways component.

The *radionuclide transport pathways component* model simulates radionuclide transport through the near and far field in a probabilistic mode. The RIP model uses a phenomenological approach that attempts to describe rather than explain the transport system. The resulting transport algorithm is based on a network of user defined *pathways*. The geosphere and biocell pathways reflect the major features of the hydrologic system and the biosphere, and are conduits through which transport occurs. The pathways may be used for both flow balance and radionuclide transport purposes, and may account for either gas or liquid transport. The purpose of a pathway is to represent large-scale heterogeneity of the hydrologic system, such as geologic structures and formation-scale hydro stratigraphy.

Geosphere pathways may be subdivided into *flow modes*, which address heterogeneity at the local scale (e.g., flow in rock matrix, flow in fractures). The flow modes are primarily distinguished from one another based on flow velocity, although retardation parameters may also differ between flow modes.

The transport of radionuclides along a geosphere pathway is based on a *breakthrough curve*, which is calculated as a cumulative probability distribution for radionuclide travel times along the pathway. The breakthrough curve combines the effects of all flow modes and retardation on the radionuclide travel time, and determines the expected proportion of mass that has traversed the pathway by any specified time. The breakthrough curve is computed based on a Markov process algorithm for exchange between different flow modes.

The third performance assessment component model represents *disruptive events*. Disruptive events are defined as discrete occurrences that have some quantifiable effect on the processes described by the other two component models. Examples of disruptive events include volcanism, faulting, and human intrusion. The user first identifies all significant events (i.e., events that are both credible and consequential). Having done so, each event is assigned a rate of

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

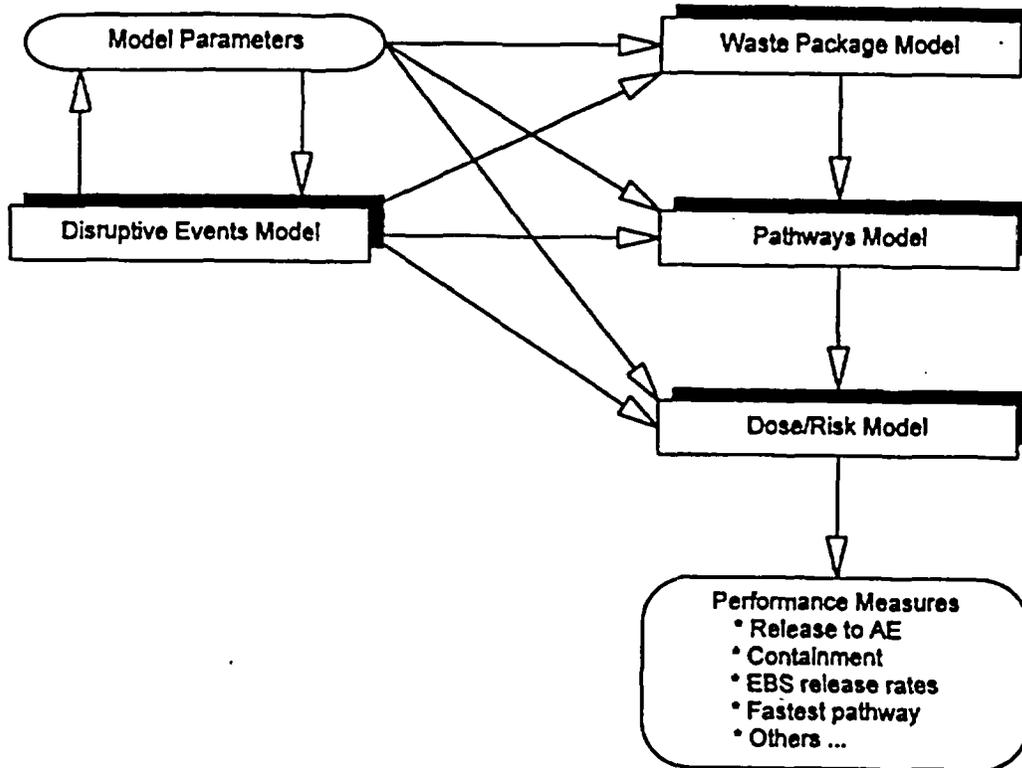
occurrence and, if desired, one or more descriptor parameters, which define the characteristics and magnitude of the event (e.g., length of a volcanic dike). Descriptor parameters may be represented stochastically. Event occurrences are simulated as Poisson processes.

The user defines probability distributions for the event consequences (which may be functions of event descriptors). A consequence may take the form of a number of discrete responses (e.g., disrupting a number of waste packages, moving radionuclides from some waste packages directly to the accessible environment). It is also possible for an event to directly modify parameters defined in the other two component models. This capability can be used to specify long-term consequences (e.g., raising the water table or opening a new pathway).

The fourth performance assessment component model describes the fate and effect of radionuclides in the biosphere. The *biosphere dose/risk model* allows the user to define *dose receptors* in the system. Receptors receive radiation doses from specified geosphere (e.g., a water supply aquifer) or biosphere (e.g., a pond, or flora and fauna) pathways. Concentrations in these pathways are converted to radiation doses (or cancer risks) based on user-defined conversion factors.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

| Figure 4-1. Components of the Repository Integration Program which are Used for Total System Performance Assessment.



DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

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DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

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DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

5.0 WASTE DISPOSAL CRITICALITY ACCEPTABILITY CRITERIA

[Note: This chapter of the technical report provides only a general description of the disposal criticality acceptability criteria. The chapter will be expanded in the topical report to address the establishment of the detailed disposal criticality acceptability criteria and the physical implementation and administrative controls for loading waste packages.]

| Prior to emplacement of nuclear waste containing fissionable material in a deep geologic repository, it must be demonstrated with reasonable assurance that criticality control of the waste will be maintained in accordance with the governing regulations. This chapter presents the approach to determining the criticality acceptability criteria for emplacement of waste within the repository and to determining the physical implementation and control requirements which will ensure that the criteria are met. The waste disposal criticality acceptability criteria are related to the Waste Receipt Criteria for acceptance of waste at the repository, which are not the same as the waste acceptance criteria applied to waste received by the DOE OCRWM from waste owners/generators. Waste disposal criticality acceptability criteria are the criteria for ensuring that the waste as emplaced in a repository is in a configuration suitable for disposal, from a standpoint of criticality.

The basic criterion for geologic disposal of SNF waste packages as part of the repository EBS is that the established limits on the release of radionuclides to the accessible environment (or other limits established in future regulations) shall not be exceeded through the period of regulatory concern. The waste package/EBS criticality acceptability criteria must support this basic criterion for geologic disposal plus any additional criteria established for control of criticality events. The overall basis and details for the criteria are discussed in Chapter 2. This chapter will discuss more of the details of addressing the criteria, with limits on the waste form characteristics and waste package/EBS designs.

5.1 Waste Package/EBS Criticality Acceptability Criteria

| The criticality acceptability criteria are based on the results of the evaluations performed using the methodology from Chapter 3. Loading criteria are determined for the waste form characteristics that a given design can accept and still meet the criticality acceptability criteria.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

Loading criteria are established for a category of waste (PWR SNF or BWR SNF) to be sealed in a given waste package design for emplacement in a given underground repository EBS design. The combination of waste form, waste package design, EBS design, and repository site must meet the criticality acceptance criteria for the waste to be acceptable for disposal. If the criticality acceptance criteria are not met, the designs must be modified or the amount of waste must be reduced until the criteria are met.

Evaluations must be performed to establish the loading criteria for each category of waste to be loaded into the specific waste package/EBS design. Once the loading criteria are established for each design, confirmation is then required that the waste packages are loaded according to the loading criteria determined by the evaluations.

5.2 Physical Implementation and Controls

The physical implementation and administrative controls relating to the loading of a disposal waste package are to be addressed in this section. Procedures are developed (TBD) to ensure that the SNF intended to be loaded into a specific waste package is loaded in that waste package, and that any requirements imposed relative to criticality control of the waste package (e.g., enrichment, burnup, fissile content, etc.) are met. The implementation of the procedures for controlling the loading of waste packages depends upon documentation of the waste form characteristics, identification of the waste forms, and verification of the information.

5.2.1 Fuel Assembly Records

Part of the requirements for determining suitability for emplacement of SNF shipments received at a repository is the receipt of supporting documentation. The supporting documentation will include all the records determined to be necessary to document criticality related information. It is assumed (TBD) that the *Spent Nuclear Fuel Verification Plan*⁵⁻¹ will require the specific records needed for determining compliance with the criticality acceptability criteria (TBD). The plan will also specify the mechanism by which such records will be obtained.

Records are maintained for every commercial nuclear fuel assembly. The reactor records track each assembly from the time it is received at the reactor site until it is shipped off site. The record for each assembly includes its initial properties, its operating history in the reactor core,

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

and any modifications made to it. The initial fuel assembly properties in the reactor record include the assembly design type (components, dimensions, and masses) and the initial enrichments. The operating history records include individual assembly burnup information. The records will also contain documentation of any modifications performed on a fuel assembly for Special Nuclear Material Control and Accounting purposes.

For tracking purposes, a unique identification number is stamped on each fuel assembly. Part of the Waste Disposal Receipt Criteria for bare SNF shipments includes checking the fuel assembly identification numbers against the numbers listed in the accompanying documentation.

[Note: Similar records and identification numbers will accompany shipments of HLW vitrified glass pour canisters. A similar verification will be performed by checking the identification number on the canister against the accompanying records. (TBD)]

5.2.2 Burnup/Fissile Content Verification

The records accompanying the commercial SNF assemblies shipped to a repository will include a record of each fuel assembly's initial enrichment and burnup. These pieces of information are key to criticality evaluations. No special verification beyond checking the fuel assembly records is expected to be required for fuel enrichment information. It is expected that additional verification will be required for fuel assembly burnup information.

Burnup measurement systems are expected to provide the required additional verification of the records. Fuel assemblies shipped in burnup credit transportation casks or as canistered fuel (CF) are expected to have the burnup verification measurement performed prior to shipment to the repository. Fuel assemblies shipped in non-burnup credit casks or dual-purpose canisters may need to be measured at the repository surface facility prior to loading into a waste package. The final details regarding the necessity of the burnup measurement system are still being determined.

[Note: The HLW vitrified glass pour canister shipments will be accompanied by records documenting the fissionable isotope contents of each canister. The fissionable isotope content is controlled during the manufacturing process within limits. The verified records of this controlled process will accompany the shipment.]

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

5.2.3 Waste Package Loading Procedure

| The waste package loading procedure (TBD) will ensure that the fuel assemblies to be loaded in
| a waste package are properly identified prior to emplacement in the repository. The waste
| package loading procedure will use the limits established in the loading criteria as a basis for
| what fuel assemblies are acceptable for loading into in which waste package design and which
| assemblies may be combined with which other assemblies in a specific waste package design.
| [The methodology for establishing loading criteria will be presented in the topical report.]

| Independent double verification of the identification numbers of the fuel assemblies received and
| the loading of these fuel assemblies into the specified waste package will be performed.
| Independent double verification will also be performed for the incorporation of any additional
| criticality control material (i.e., loaded according to specifications). Similarly for CF,
| independent double verification of the CF identification numbers received and the loading of
| commercial SNF canisters into the specified waste package for disposal will be performed.

| [Note: For HLW vitrified glass canisters, each unit will be identified according to identification
| number and fissile content. These canisters will then be loaded into a waste package as specified
| and the entire process from identification to emplacement in the repository shall be
| independently double verified.]

5.3 References

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DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

6.0 SUMMARY AND CONCLUSIONS

A methodology for performing nuclear criticality analyses for disposal of commercial light-water reactor spent nuclear fuel in the potential repository at Yucca Mountain is presented in this report. The starting point for this methodology is the establishment of the range of waste forms, WP/EBS design, and repository site characteristics. This determines the range of system characteristics to be evaluated. A broad range of system characteristics of neutronically significant species, along with the features, events, and processes important to criticality, are used to generate preliminary scenarios. Configurations from the preliminary scenarios are evaluated with the neutronics models. The resulting k_{eff} values are used to establish a regression expression for k_{eff} as a function of the concentrations of the neutronically significant species in the configurations considered. The detailed distribution of system characteristics is used to generate the specific scenarios for further evaluation. The specific configurations and their probability distributions from these scenarios, along with the regression expression for k_{eff} , are used to determine the range of potential critical configurations. Direct criticality consequences (increase in radionuclide inventory and energy release) are estimated for the representative configurations that indicate potential for criticality. The risk associated with repository criticality is the product of the probability of occurrence and the consequence, summed over all possible criticality events (or probability-consequence pairs). The performance assessment model evaluates the perturbation in dose attributable to the criticality and evaluates potential impact on repository performance objectives.

The methodology relies on probabilistic evaluations for identifying configurations with a potential for criticality. Criticality evaluations are performed for three regions or locations within the repository; internal (to waste package), near-field external, and far-field external. Thus, the areas of applicability for the neutronics models range from intact configurations of SNF (inside the waste package) to configurations of neutronically significant species of SNF materials in the host rock of the repository (far-field locations). Validation of the neutronics models is performed using commercial reactor criticality (CRC) data, laboratory criticality experiments (LCEs), and chemical assay data. Analysis of the CRC data addresses both isotopic model validation and criticality model validation with a single class of experiments. Chemical assay data are being analyzed to augment the CRC evaluations and establish the uncertainty in k_{eff} associated with the integral method used in the CRC analyses for isotopic model validation. Analysis of the LCEs are used to augment validation of the criticality analysis model for intact

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

fuel and configurations of fissionable material representing various degraded states. The recommendations presented in NUREG/CR-6361 are followed in the selection of experiments for validating the neutronics model for disposal criticality evaluations and for the determination of bias and subcritical limits. Subcritical limit values will be determined, as appropriate based on applicability of experimental data, to represent various degraded states of SNF.

As indicated in this report, the development and validation of the models supporting the disposal criticality analysis methodology is a continuing process that has not been completed. Therefore, it is premature to draw specific conclusions concerning these models. Over the next year this effort will be completed and documented in a topical report. The topical report will then present specific conclusions relative to the accuracy and applicability of the models for disposal criticality evaluations.

In Chapter 1, the Yucca Mountain Project planning assumption was presented. This assumption states that the risk-based approach to dealing with disposal criticality is not only the best approach, but also that it is the only feasible approach. This assumption will be validated during the completion of the development of the disposal criticality analysis methodology. Conclusions relative to this risk-based approach will be presented in the topical report.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

7.0 LIST OF APPENDICES

| The following is a list of the appendices for the technical report.

A. Acronyms and Glossary

A.1 List of Acronyms and Abbreviations (4 pages)

| A.2 Glossary of Terms (8 pages)

| B. Sample of Design Process and Methodology Application

| C. Sample Application of the Methodology to DOE SNF

| [Note: The information presented in Appendix B and Appendix C is preliminary and is provided to illustrate the current status of the methodology. This information will be updated as the methodology is finalized.]

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

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Disposal Criticality Analyses Methodology Technical Report

APPENDIX A

ACRONYMS AND GLOSSARY

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Appendix A.1: List of Acronyms and Abbreviations

ACD	Advanced Conceptual Design
ACE	Type of nuclear data library used in the MCNP computer program
Ag	Silver
Al	Aluminum
ALARA	As Low As Reasonably Achievable
Am	Americium
ANS	American Nuclear Society
ANSI	American National Standards Institute, Inc.
AREST-CT	Name of a computer code for combined transport and chemistry
ARO	All Rods Out
AROCBC	All Rods Out Critical Boron Concentration
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
ATM	Approved Test Material
AUCF	Advanced Uncanistered Fuel waste package design
AVEL	Average lethargy of the neutron causing fission
B	Boron
B&W	Babcock and Wilcox or B&W Fuel Company
BNL	Brookhaven National Laboratory
BOC	Beginning of Cycle
BOL	Beginning of Life
BONAMI-S	Name of a computer program, part of SCALE
BPR	Burnable Poison Rod
BPRA	Burnable Poison Rod Assembly
BWR	Boiling Water Reactor
C	Carbon
°C	Degrees Centigrade
CASMO	Name of a computer program
CDF	Cumulative Distribution Function
CE	Combustion Engineering
CERES	Name of an International Collaborative Program
Cf	Californium
CF	Canistered Fuel
CFR	Code of Federal Regulations
CH	Calico Hills
CHn1v	Calico Hills nonwelded unit 1 vitric
CHn1z	Calico Hills nonwelded unit 1 zeolitized
Cm	Curium
COUPLE-S	Name of a computer program, part of SCALE
CRA	Control Rod Assembly
CRC	Commercial Reactor Critical
CRWMS	Civilian Radioactive Waste Management System
Cs	Cesium

Appendix A.1: List of Acronyms and Abbreviations

CSAS	Name of a computer program sequence, part of SCALE
DC	Disposal Container
DHLW	Defense High-Level Waste
DI	Document Identifier
DOE	U. S. Department of Energy
EBS	Engineered Barrier System or Segment
EFPD	Effective Full Power Days
ENDF	Name of a nuclear cross section library set (Evaluated Nuclear Data File)
EOC	End of Cycle
EPA	U. S. Environmental Protection Agency
EPRI	Electric Power Research Institute
EQ3/6	Name of a computer program
ESF	Exploratory Studies Facility
Eu	Europium
Fe	Iron
Fe _n O _m	Iron oxide (n and m are integers less than 4)
FEP	Features, Events, and Processes
FEHM	Name of a computer program
FMEA	Failure Modes and Effects Analysis
FSAR	Final Safety Analysis Report
Gd	Gadolinium
GE	General Electric
GROA	Geologic Repository Operations Area
GWd/MTU	Gigawatt-Day per Metric Ton of Uranium
HEU	Highly Enriched Uranium
HFP	Hot Full Power
HLW	High-level Waste
H/X	Water-to-fuel volume ratio
HZP	Hot Zero Power
I	Iodine
I _c	Number of source cycles that are skipped before data accumulation begins in an MCNP calculation
ID	Inside Diameter
IOC	Interoffice Correspondence
ISO-9000	Name of the International Standards Office's Quality Assurance Program
K _d	Sorption (or distribution) coefficient
k _{eff}	Effective neutron multiplication factor
k _∞	Infinite neutron multiplication factor
KENO	Name of a computer program
kW	Kilowatt
LA	License Application
LANL	Los Alamos National Laboratory
LBL	Lawrence Berkeley Laboratory

Appendix A.1: List of Acronyms and Abbreviations

LCE	Laboratory Critical Experiment
LLNL	Lawrence Livermore National Laboratory
LWR	Light Water Reactor
MCC	Material Characterization Center
MCNP	Name of a computer program (Monte Carlo N-Particle)
M&O	Management and Operating Contractor
MeV	Million Electron Volts
MGDS	Mined Geologic Disposal System
MIT	Massachusetts Institute of Technology
Mo	Molybdenum
MOC	Middle of Cycle
MOX	Mixed Oxide
MPa	Megapascals
MPC	Multi-Purpose Canister
MTU	Metric Tons of Uranium
MWd	Megawatt Days
Nd	Neodymium
NEMO	Name of a computer program
NLP	Nevada Site Administrative Line Procedure
NITAWL-S	Name of a computer program, part of SCALE
Np	Neptunium
NQA-1	ASME Standard on Nuclear Quality Assurance
NRC	U.S. Nuclear Regulatory Commission
NUREG	Designator for an NRC Document
O	Oxygen
OCRWM	Office of Civilian Radioactive Waste Management
OD	Outside Diameter
ORIGEN-S	Name of a computer program, part of SCALE
ORNL	Oak Ridge National Laboratory
ORR	Oak Ridge Research
Pa	Protactinium
PDF	Probability Density Function
ppm B	Parts per million of boron
Pm	Promethium
PNL	Pacific Northwest Laboratory
PRA	Probabilistic Risk Assessment
PTn	Paintbrush Tuff Non-welded
Pu	Plutonium
PWR	Pressurized Water Reactor
Q	Quality Affecting (A classification of information)
QA	Quality Assurance
QAP	Quality Administrative Procedure
QARD	Quality Assurance Requirements and Description

Appendix A.1: List of Acronyms and Abbreviations

R ²	The fraction of the variation explained by the regression
REV	Revision of a document
Rh	Rhodium
RIP	Name of a computer program (Repository Integration Program)
RSIC	Radiation Shielding Information Center
Ru	Ruthenium
RW	Radioactive Waste (referring to DOE/RW)
SAS2H	Name of a computer code sequence, part of SCALE
SCALE	Name of a computer program (Standardized Computer Analysis for Licensing Evaluations)
SIP	Scientific Investigation Plan
SL	Subcritical Limit
Sm	Samarium
SNF	Spent Nuclear Fuel
SNL	Sandia National Laboratories
SRP	Savannah River Plant
SRS	Savannah River Site
SS-B	Stainless Steel Boron
S _w	Water saturation in the porespace
SZ	Saturated-Zone
t	Time
TBD	To Be Determined
TBR	To Be Resolved
TBV	To Be Verified
Tc	Technetium
TCw	Tiva Canyon welded
TOUGH2	Name of a computer program (Transport of Unsaturated Groundwater and Heat)
TS	Topopah Spring
TSPA	Total System Performance Assessment
VA	Viability Assessment
TSw	Topopah Spring welded
TSw2	Topopah Spring welded unit 2
TSw3	Topopah Spring welded unit 3 (Vitrophyre tuff)
TUFF	Name of a computer program
U	Uranium
U _n O _m	Uranium Oxide (n and m are numbers)
UCF	Unclustered Fuel
UCRL	University of California Research Laboratory
UNS	Unified Numbering System for Metals and Alloys
USL	Upper Subcritical Limit
UZ	Unsaturated-Zone
W	Westinghouse
WIPP	Waste Isolation Pilot Plant
WP	Waste Package
WTAL	WIPP Technical Assistance Contractor

Appendix A.1: List of Acronyms and Abbreviations

wt. %	Weight Percent
Xe	Xenon
XSDRNPM-S	Name of a computer program, part of SCALE
YMP	Yucca Mountain Site Characterization Project
ZAID	Name of a isotope identifier for cross section libraries
ZP	Zero Power
α	Reciprocal of the minimum transport time to the accessible environment
β	Bias or the reciprocal of the time duration over which there is a significant probability of criticality occurrence
ϕ	Porosity of the rock
ρ_{bd}	Dry bulk density
τ	Time, primarily as variable of integration ($d\tau$)

Appendix A.1: List of Acronyms and Abbreviations

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Appendix A.2: Glossary of Terms

This glossary contains the meaning of the specialized terms used in the report. The references in square brackets at the end of a definition are the highest level document which contains that definition verbatim.

Accessible environment means: (1) The atmosphere, (2) the land surface, (3) surface water, (4) oceans, and (5) the portion of the lithosphere that is outside the controlled area. [10 CFR 60.2] ^{A.2-1}

Anticipated processes and events are those natural processes and events that are reasonably likely to occur during the period the intended performance objective must be achieved. To the extent reasonable in the light of the geologic record, it shall be assumed that those processes operating in the geologic setting during the Quaternary Period continue to operate, but with the perturbation caused by the presence of emplaced radioactive waste superimposed thereon. [10 CFR 60.2] ^{A.2-1}

As low as is reasonably achievable means making every reasonable effort to maintain exposures to radiation as far below the dose limits in 10 CFR 20 as is practical consistent with the purpose for which the licensed activity is undertaken, taking into account the state of technology, the economics of improvements in relation to state of technology, the economics of improvements in relation to benefits to the public health and safety, and other societal and socioeconomic considerations, and in relation to utilization of nuclear energy and licensed materials in the public interest. [10 CFR 20.1003] ^{A.2-2}

Backfill is a material used to fill the space previously created by excavation or drilling, such as in a shaft or borehole.

Barrier is any material or structure that prevents or substantially delays movement of water or radionuclides. [10 CFR 60.2] ^{A.2-1}

Burnup credit is an approach used in criticality evaluations which accounts for the reduction in criticality potential associated with spent nuclear fuel relative to that of fresh fuel. Burnup credit reflects the net depletion of fissionable isotopes and the creation of neutron absorbing isotopes during reactor operations. Burnup credit also accounts for variations in the criticality potential of spent nuclear fuel produced by radioactive decay since the fuel was discharged from a reactor. Burnup credit is one of the licensing issues which will be addressed in the Topical Reports submitted to the U.S. Nuclear Regulatory Commission. For geologic disposal, burnup credit accounts for the reduction in reactivity associated with 29 isotopes (Principal Isotopes) from commercial light water reactor spent nuclear fuel. This credit applies specifically to the ceramic form of commercial spent nuclear form.

Canister is a metal receptacle with the following purpose: (1) for solidified high-level radioactive waste, its purpose is a pour mold, and (2) for spent fuel, it may provide structural support for loose rods, nonfuel components, or confinement of radionuclides during preclosure operations.

Appendix A.2: Glossary of Terms

Cask is a container for shipping or storing spent nuclear fuel and/or high-level waste that meets all applicable regulatory requirements.

Canistered Fuel Disposal Container, CI BBAAB0000. The Canistered Fuel Disposal Container component includes all items that form a disposal container for a canistered SNF waste form which is a small CF or a large CF. This component includes the small CF disposal container component and the large CF disposal container component. The CF disposal container includes but is not limited to multiple containment barriers including multiple closure lids.

Civilian Radioactive Waste Management System is the composite of the sites, and all facilities, systems, equipment, materials, information, activities, and the personnel required to perform those activities necessary to manage radioactive waste disposal.

Cladding is the metal cylinder that surrounds the uranium pellets.

Container is the component of the waste package that is placed around the waste form or the canistered waste form to perform the function of containing radionuclides.

Containment is the confinement of radioactive waste within a designated boundary. [10 CFR 60.2]^{A.2-1}

Criticality control is the suite of measures taken to maintain fissionable material, including spent fuel, in a subcritical condition during storage, transportation and disposal, so that no self-sustaining nuclear chain reaction can occur. Subcriticality is assured by loading spent fuel that meets certain requirements related to fuel age, enrichment, and reduction in nuclear fuel reactivity through burnup.

Degraded Basket is a waste package system state in which the basket has lost the original geometric separation between spent fuel assemblies and/or lost any neutron absorbing materials integral to the basket. There are 3 subcategories:

Partially Degraded Basket. Partially degraded baskets still maintain the geometric separation between spent fuel assemblies but have lost any neutron absorbing materials integral to the basket.

Collapsed Basket. Collapsed baskets have lost the geometric separation between spent fuel assemblies but maintains some of the original neutron absorbing materials integral to the basket.

Fully Degraded Basket. System state such that the baskets no longer exists.

Appendix A.2: Glossary of Terms

- | **Disposal** is the isolation of radioactive wastes from the accessible environment. [10 CFR 60.2] ^{A.2-1}
Disposal means the emplacement in a repository of high-level radioactive waste, spent nuclear fuel, or other highly radioactive material with no foreseeable intent of recovery, whether or not such emplacement permits the recovery of such waste. [10 CFR 961.11] ^{A.2-3} [NWPA Section 2(9)] ^{A.2-4}

Disposal container is a vessel consisting of the barrier materials and internal components designed to meet disposal requirements, into which the uncanistered or canistered waste form will be placed.

- | **Disposal system** is any combination of engineered and natural barriers that isolate spent nuclear fuel or radioactive waste after disposal. [40 CFR 191.12(a)] ^{A.2-5}

Drift is a nearly horizontal mine passageway driven on or parallel to the course of a vein or rock stratum or a small crosscut in a mine.

- | **Emplacement Drift Backfill Materials Subsystem Element, CI BBDB00000** includes all backfill materials placed in the waste emplacement drifts as an engineered barrier for the purpose of containing and isolating the waste from the accessible environment. Backfill will be used to retard the migration of radionuclides from the waste package to the geologic setting. It may also be placed in peaked layers to provide a barrier which prevents water from contacting the waste package.

- | **Emplacement Drift Invert Subsystem Element, CI BBDC00000** consists of the material or inverted arch placed at the bottom of the emplacement drift to provide a floor with a flat surface. The Invert includes the invert materials placed in the waste emplacement drifts as an engineered barrier for the purpose of containing and isolating the waste from the accessible environment. The invert will retard the migration of radionuclides from the waste package to the geologic setting.

Engineered Barrier Segment, CI BB0000000. The Engineered Barrier Segment includes the Waste Package Subsystem and the Underground Facility Subsystem. The major components of the Engineered Barrier Segment shall contribute to the assigned function, Isolate Waste, by containing waste in the waste packages during the prescribed containment period, and then by limiting the release of radionuclides during the post-containment period.

The Waste Package Subsystem includes the uncanistered fuel, canistered fuel, and defense high-level waste disposal containers, filler materials, shielding, packing and absorbent materials, and waste package support subsystem elements. The Underground Facility Subsystem includes the emplacement drift openings, emplacement drift backfill materials, and emplacement drift invert subsystem elements.

- | **Engineered barrier system (EBS)** is the waste packages and the underground facility. [10 CFR 60.2] ^{A.2-1}

- | **EBS Near-Field.** For purposes of the disposal criticality analysis methodology, near-field is the volume inside an emplacement drift, excluding the interior of the waste package.

Appendix A.2: Glossary of Terms

| **Far-Field.** For purposes of the disposal criticality analysis methodology, far-field is the volume
| outside the emplacement drifts and extends to the accessible environment.

| **Filler Materials, CI BBAAD0000.** The Filler Materials component includes all filler materials used
| to fill the free space remaining in disposal containers after loading the high-level nuclear waste.
| Filler materials may be used for neutron absorption, moderator displacement, chemical buffering, or
| radionuclide retardation. The most likely application would be the addition of filler material to
| selected SNF waste package disposal containers, i.e., UCF, CF, or dual purpose canisters, for the
| purpose of moderator displacement to aid in criticality control. Filler material may also be added
| to DHLW waste package disposal containers. Filler materials, if used, will be added to the waste
| packages disposal containers only at the repository.

| **Fissile materials** are those materials which will fission with slow neutrons (e.g., U-235, Pu-239).
|

| **Fissionable materials** are those materials which will fission if neutrons have enough energy. Note
| all fissile materials are fissionable, but not all fissionable materials are fissile. "Fissionable" is used
| in most places in this report instead of "fissile", although fissile may be applicable for most
| configurations from commercial SNF.
|

| **Fragmented fuel.** See Spent nuclear fuel.

| **Geologic repository** is a system which is intended to be used for, or may be used for, the disposal
| of radioactive wastes in excavated geologic media. A geologic repository includes (1) the geologic
| repository operations area, and (2) the portion of the geologic setting that provides isolation of the
| radioactive waste. [10 CFR 60.2] ^{A.2-1}

| **Geologic repository operations area (GROA)** is a high-level radioactive waste facility that is part
| of a geologic repository, including both surface and subsurface areas, where waste handling activities
| are conducted. [10 CFR 60.2] ^{A.2-1}

| **High-level radioactive waste (HLW)** means (1) the highly radioactive material resulting from the
| reprocessing of spent nuclear fuel, including liquid waste produced directly in reprocessing and any
| solid material derived from such liquid waste that contains fission products in sufficient
| concentrations; and (2) other highly radioactive material that the Nuclear Regulatory Commission,
| consistent with existing law, determines by rule requires permanent isolation. The CRWMS will
| only accept solidified HLW. For the purposes of this document, HLW is vitrified borosilicate glass
| cast in a stainless steel canister. [NWSA Section 2(12)] ^{A.2-4} [10 CFR 72.3] ^{A.2-6} [10 CFR 960.2]
| ^{A.2-7} [10 CFR 961.11] ^{A.2-3} [MGDS-RD] ^{A.2-8}

| **HLW Disposal Container, CI BBAAC0000.** The High-Level Waste (HLW) Disposal Container
| component includes all items which form a disposal container for high-level process waste forms
| packaged in waste canisters originating from Savannah River, Hanford, Idaho National Engineering
| Laboratory, West Valley, and any other designated locations supplying process waste for disposal.

Appendix A.2: Glossary of Terms

| The HLW disposal container includes but is not limited to multiple containment barriers including multiple closure lids, and internal structure. HLW disposal container is also referred to as defense HLW or DHLW disposal container.

| (Items) **Important to Waste Isolation** means the natural and engineered barriers that are relied on for achieving the postclosure performance objectives in 10 CFR 60 Subpart E.

| **Institutional Barrier System** consists of the active and passive institutional controls. Active institutional controls include (1) controlling access to the MGDS by any means other than passive institutional controls, (2) performing maintenance operations or remedial actions at a site, (3) controlling or cleaning up releases from a site, or (4) Monitoring parameters related to disposal system performance.

| Passive institutional controls include (1) permanent markers placed at a disposal site, (2) public records and archives, (3) government ownership and regulations regarding land or resource use, and (4) other means of preserving knowledge about the location, design, and contents of a disposal system. (TBR) [40 CFR 191.02]^{A.2-3}

| **Intact Baskets** are waste package baskets that still maintain the original geometric separation between spent fuel assemblies and still maintain any neutron absorbing materials in the basket.

| **Intact Fuel.** See Spent nuclear fuel.

| **Invert** is the level bottom placed in the drifts.

| **Isolation** is inhibiting the transport of radioactive material so that amounts and concentrations of this material entering the accessible environment will be kept within prescribed limits. [10 CFR 60.2]^{A.2-1}

| k_{eff} is the effective neutron multiplication factor for a system. It is a measure of the reactivity or criticality potential of a system.

| k_{∞} is the infinite neutron multiplication factor. It is the multiplication factor for an infinite lattice (i.e., no leakage from the system).

| **Multi-purpose canister** refers to a sealed, metallic container maintaining multiple spent nuclear fuel assemblies in a dry, inert environment and over packed separately and uniquely for the various system elements of storage, transportation, and disposal. (See definition of waste form.)

| **Near-field.** See EBS Near-field

| **Neutronically significant species** are the principal fissionable and absorber isotopes/elements.

Appendix A.2: Glossary of Terms

Off-normal are abnormal or unplanned events or conditions that adversely affect, potentially affect, or are indicative of degradation in, the safety, security, environmental or health protection performance or operation of a facility.

Package means the packaging together with its radioactive contents as presented for transport. [10 CFR 71.4] ^{A.2-9}

Packaging means the assembly of components necessary to ensure compliance with the packaging requirements of 10 CFR 71. It may consist of one or more receptacles, absorbent materials, spacing structures, thermal insulation, radiation shielding, and devices for cooling or absorbing mechanical shocks. The vehicle, tie-down system, and auxiliary equipment may be designated as part of the packaging. [10 CFR 71.4] ^{A.2-9}

Packing and Absorbent Materials, CI BBAD00000. The Packing and Absorbent Materials Subsystem Element includes any items or materials immediately surrounding an individual waste container that inhibit the release of radionuclides to the accessible environment.

Performance assessment means any analysis that predicts the behavior of a system or a component of a system under a given set of constant or transient conditions.

Permanent closure is final backfilling of the underground facility and the sealing of shafts and boreholes. [10 CFR 60.2] ^{A.2-1} [Note: A decision on backfilling the emplacement drifts has not been finalized at this time.]

Postclosure means the period of time after the permanent closure of the geologic repository.

Preclosure means the period of time before and during the permanent closure of the geologic repository.

Radioactive waste or waste is HLW and other radioactive materials other than HLW that are received for emplacement in a geologic repository. [10 CFR 60.2] ^{A.2-1}

Repository is any system licensed by the Commission that is intended to be used for, or may be used for, the permanent deep geologic disposal of high-level radioactive waste and spent nuclear fuel, whether or not such system is designed to permit the recovery, for a limited period during initial operation, of any materials placed in such system. Such term includes both surface and subsurface areas at which high-level radioactive waste and spent nuclear fuel handling activities are conducted. [NWSA] ^{A.2-4}

Retrieval is the act of intentionally removing radioactive waste from the underground location at which the waste had been previously emplaced for disposal. [10 CFR 60.2] ^{A.2-1}

Risk is the product of the probability of a given process or event and a measure of its consequences.

Appendix A.2: Glossary of Terms

Shielding, CI BBAC00000. The Shielding Subsystem Element includes any material that provides radiation protection, beyond the limited shielding inherently provided by the disposal container, which will be disposed of as part of the waste package. This configuration item excludes any shielding that is not an integral part of the waste package (i.e., over packs necessary for transport or for use within containment buildings where waste containers are handled or stored).

Spent nuclear fuel (SNF) is fuel which has been withdrawn from a nuclear reactor following irradiation, the constituent elements of which have not separated by reprocessing. [Specifically in this document, SNF includes (1) intact, non-defective fuel assemblies; (2) failed fuel assemblies in canisters; (3) fuel assemblies in canisters; (4) consolidated fuel rods in canisters; (5) non-fuel assembly hardware inserted in PWR fuel assemblies, including, but not limited to, control rod assemblies, burnable poison assemblies, thimble plug assemblies, neutron source assemblies, instrumentation assemblies; (6) fuel channels attached to boiling water reactor fuel assemblies; and (7) non-fuel assembly hardware and structural parts of assemblies resulting from consolidation in canisters.] [NWPA Section 2(23)]^{A.2-4} [10 CFR 961.11]^{A.2-3} The specific types of SNF discussed in the disposal criticality analysis methodology include:

Intact Fuel. Intact fuel is the category of SNF that is still in a ceramic form (e.g., UO_2) and still maintains its regular lattice geometry.

Fragmented Fuel. Fragmented SNF has been degraded to fragments, but still retains its as-replaced chemical composition (modified by radioactive decay).

SNF Dissolution Products. The chemical species or elements that were formerly components of SNF. These elements could be in solution or precipitates.

Subcritical Limit is the value that the calculated k_{eff} for a system/configuration of fissionable material must be shown to be below to be considered subcritical. The subcritical limit is dependant upon the computer system being used to calculate k_{eff} , the configuration being evaluated, and the regulatory margins specified for the application.

Unanticipated processes and events mean those processes and events affecting the geologic setting that are judged not to be reasonably likely to occur during the period the intended performance objective must be achieved, but which are nevertheless sufficiently credible to warrant consideration.

UCF Disposal Container with Basket, CI BBAAA0000. The Uncanistered Fuel (UCF) Disposal Container with Basket component is a disposal container containing a fuel basket. The UCF disposal container is employed only at the repository for the disposal of uncanistered (bare) commercial PWR and BWR spent nuclear fuel assemblies. Such assemblies would originate from either SNF sent to the repository in bare fuel transportation casks, or the contents of any dual purpose canisters which are determined to be unsuitable for disposal. The UCF disposal container includes but is not limited to multiple containment barriers including multiple closure lids, basket members, optional neutron absorber material, optional thermal shunts, and internal supports for the basket. The containment

Appendix A.2: Glossary of Terms

barriers consist of corrosion-allowance and/or corrosion-resistant materials. Criticality control alternatives include but are not limited to neutron absorber material alloyed with the basket material, addition of neutron absorbing panels or control rods, and/or addition of filler material for moderator displacement to aid in criticality control.

Underground facility is the underground structure, including openings and backfill materials, but excluding shafts, boreholes, and their seals. [10 CFR 60.2] ^{A.2-1}

Underground Facility, CI BBD000000. The Underground Facility Subsystem is that portion of the Engineered Barrier Segment that has been allocated the primary function of limiting radionuclide transport.

The Underground Facility Subsystem includes the following Subsystem Elements: Emplacement Drift Openings, Emplacement Drift Backfill Materials, and Emplacement Drift Invert.

Unrestricted area means any area, access to which is not controlled by the licensee for purposes of protection of individuals from exposure to radiation and radioactive materials, and any area used for residential quarters.

Waste container is a sealed disposal container with the uncanistered or canistered waste form (and possibly filler material) placed therein.

Waste form is the radioactive waste materials and any encapsulating or stabilizing matrix. [10 CFR 60.2] ^{A.2-1} A loaded multi-purpose canister is a canistered waste form. [MGDS-RD] ^{A.2-8}

Waste package means the waste form and any containers, shielding, packing and other absorbent materials immediately surrounding an individual waste container. [10 CFR 60.2] ^{A.2-1}

Waste Package, CI BBA000000. The Waste Package Subsystem includes any waste form containers, shielding, and packing and absorbent materials immediately surrounding an individual disposal container. The multibarrier disposal containers will be used for geologic disposal of high-level radioactive waste forms, limited to intact irradiated reactor fuel assemblies from pressurized water reactors, boiling water reactors, and vitrified glass or other solid process high-level waste forms in canisters. The multibarrier disposal containers will consist of multiple layers of corrosion-allowance and/or corrosion-resistant materials.

The Waste Package Subsystem includes the following Subsystem Elements: UCF Disposal Container and Basket, Canistered Fuel Disposal Container, DHLW Disposal Container, Filler Materials, Shielding, Packing and Absorbent Materials, and Waste Package Support.

Waste Package Support, CI BBAB00000. The Waste Package Support Subsystem Element includes the components necessary to support and stabilize the waste container when emplaced in the repository. These components are those items which (1) are in immediate contact with the

Appendix A.2: Glossary of Terms

emplaced disposal container (or shield, if included), and (2) will remain permanently emplaced in the drift with the waste package. The items in this subsystem include but are not limited to cradles used to support the disposal container/shield and any associated items to restrain movement of the disposal container/shield.

Appendix A.2: Glossary of Terms

References:

- | A.2-1 *Disposal of High-Level Radioactive Wastes in Geologic Repositories*, 10 CFR 60, NRC, January 1995.
- | A.2-2 *Standards for Protection Against Radiation*, 10 CFR 20, NRC, January 1994.
- | A.2-3 *Standard Contract for Disposal of Spent Nuclear Fuel and/or High-Level Radioactive Waste*, 10 CFR 961, NRC, January 1994.
- | A.2-4 *Nuclear Waste Policy Amendments Act of 1987, Public Law 100-23*. December, 1987.
- | A.2-5 *Environmental Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes; Final Rule*, 40 CFR 191 (currently remanded), EPA (Environmental Protection Agency), 1985.
- | A.2-6 *Licensing Requirements for the Independent Storage of Spent Nuclear Fuel and High-Level Radioactive Waste*, 10 CFR 72, NRC, January 1995.
- | A.2-7 *General Guidelines for Recommendation of Sites for Nuclear Waste Repositories*, 10 CFR 960, NRC, January 1994.
- | A.2-8 *Mined Geologic Disposal System requirement Document*, DOE/RW-0404P, DI:B00000000-00811-1708-00002 REV 02, DCN 02, OCRWM.
- | A.2-9 *Packaging and Transportation of Radioactive Materials*, 10 CFR 71, NRC, January 1995.

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

APPENDIX B

Sample of the Design Process and Methodology Application

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

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APPENDIX B: Sample of the Design Process and Methodology Application

Table Of Contents

Section	Page
1.0 Disposal Criticality Control Design	B-1
1.1 Design Concepts Considered for Disposal Criticality Control	B-1
1.2 Burnup Credit	B-9
1.3 Design Concepts Selected for Disposal Criticality Control	B-10
1.4 Description of Sample System Design	B-11
2.0 Sample Determination of Potentially Critical Configurations	B-22
2.1 Sample Internal Waste Package Configurations	B-22
2.2 Sample EBS Near-Field Configurations	B-23
2.3 Sample Far-Field Configurations	B-24
3.0 Sample Criticality Evaluations	B-25
3.1 Sample Waste Package Criticality Evaluations	B-26
3.2 Sample EBS Near-Field Criticality Evaluations	B-28
3.3 Sample Far-Field Criticality Evaluations	B-28
4.0 Sample Criticality Consequence Evaluations	B-30
5.0 Sample Risk Evaluation	B-33
6.0 Sample Total System Performance Consequence Evaluation	B-38
7.0 Conclusions	B-42
8.0 References	B-43

APPENDIX B: Sample of the Design Process and Methodology Application

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APPENDIX B: Sample of the Design Process and Methodology Application

LIST OF FIGURES

Figure Title	Page
Figure B-1. B&W 15×15 Fuel Assembly	B-14
Figure B-2. 21 PWR UCF Disposal Container	B-16
Figure B-3. Engineered Barrier Segment	B-18
Figure B-4. WP Emplacement Concept	B-20
Figure B-5. Sample Repository Layout	B-21
Figure B-6. Increase in Isotopic Inventory from 10,000 year Criticality	B-32
Figure B-7. Normalized Additional Dose Due to a Single Internal Criticality Event	B-37
Figure B-8. Normalized Additional Dose Due to a Single External Criticality Event	B-37
Figure B-9. Expected-Value Dose History at Assessable Environment Including Criticality	B-41
Figure B-10. Expected-Value Dose History at Assessable Environment Only From Criticality	B-41

APPENDIX B: Sample of the Design Process and Methodology Application

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APPENDIX B: Sample of the Design Process and Methodology Application

LIST OF TABLES

Table Name	Page
Table B-1. Mechanical Parameters of B&W 15×15 Fuel Assembly	B-13
Table B-2. Progressive Degradation of Borated Stainless Steel Control Panels	B-22
Table B-3. Basket Structure Gone, Uniform Iron Oxide and Boron Concentration	B-23
Table B-4. Sample Subcritical Limits for Potential Configurations	B-25
Table B-5. Percentage Increase in Total Curies of the 36 TSPA-95 Isotopes in a Single Waste Package	B-31
Table B-6. Criticality Effect on Radionuclides Determined to be Important to Total Performance	B-39

APPENDIX B: Sample of the Design Process and Methodology Application

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APPENDIX B: Sample of the Design Process and Methodology Application

This appendix provides a sample of the design process used to develop the disposal criticality control system and the application of the disposal criticality analysis methodology for a waste package/EBS design in a repository. Refer to Appendix A for the list of acronyms and abbreviations, and glossary of terms.

1.0 Disposal Criticality Control Design

The first section of this appendix discusses the design process and concepts considered for disposal criticality control. Burnup credit, the concepts selected, and a sample WP/EBS are described.

1.1 Design Concepts Considered for Disposal Criticality Control

Criticality control methods are required to ensure compliance with regulatory requirements. There are some well defined design concepts for providing criticality control for a low enriched system, such as commercial light water reactor (LWR) spent nuclear fuel (SNF). The next section will discuss the design concepts considered for SNF waste package disposal criticality control.

1.1.1 Waste Package Criticality Control Concepts

The design concepts for providing criticality control for waste packages containing commercial LWR SNF are listed below along with a discussion of their applicability for disposal criticality control.

1.1.1.1 Basket Design

Geometry restrictions are implemented in the waste package through the use of a basket, which restricts the arrangement of fuel within the canister or container. The amount of fissionable material (number of fuel assemblies) in the waste package is also limited by the basket design. (Limiting the amount of fissionable material is the ultimate criticality control method.) The basket design controls the number of fuel assemblies and their arrangement within the waste package, and therefore affects the criticality potential of the system.

APPENDIX B: Sample of the Design Process and Methodology Application

The degradation of the basket over time (and the potential loss of geometry control) is an important consideration when using this concept. The disposal criticality analysis methodology, as described, will account for the geometry of materials and amounts of fissionable material in systems being analyzed.

Package basket is one design concept to be used to contribute to waste package disposal criticality control.

1.1.1.2 Neutron Absorbers

Neutron absorbers are materials that capture neutrons to prevent them from participating in the fission chain reaction. The use of supplemental neutron absorber materials is an accepted method for criticality control. Neutron absorber credit is routinely used as a criticality control measure in reactors, spent fuel pools, and cask systems.

Neutron absorber materials placed in control panels and control rods provide a significant amount of negative reactivity, thus lowering the system's potential for criticality. The amount of criticality control is dependent upon the type and amount of neutron absorber present. Some of the neutron absorbers used by the nuclear industry are boron, cadmium, gadolinium, hafnium, and silver-indium-cadmium. The neutron absorbers are normally alloyed or mixed in small amounts within carrier materials.

Maintaining criticality control with a neutron absorber depends upon retaining the absorber in the carrier material and retaining the carrier material. (The methodology addresses cases where the absorber and carrier material are separated.). Potential mechanisms for loss of the absorber material through physical removal (e.g., leaching or preferential corrosion) must be considered. Material performance and neutron depletion evaluations must be made for the neutron absorber material loaded into a control system (e.g., panel or rod). This will determine the amount of absorber available for criticality control at future times during disposal in the repository.

The disposal criticality analysis methodology, as described, will account for the material performance of neutron absorber and carrier materials in systems being analyzed.

Neutron absorbers (in the form of panels and/or rods) are another design concept to be used to contribute to waste package disposal criticality control.

APPENDIX B: Sample of the Design Process and Methodology Application

1.1.1.3 Moderator Displacement: Filler Materials

The presence of moderator material in a waste package containing commercial LWR SNF increases the reactivity of the package. Since the engineered barrier system is designed to reduce the presence of moderating material, the only source of moderator of concern for criticality control internal to the waste package results from the condition in which water enters and remains within the waste package. The inclusion of additional (filler) material to limit the amount of water that can enter and remain within the waste package is referred to as moderator displacement. Moderator displacement is an effective criticality control mechanism. Use of a particular filler material for criticality control requires quantification of the amount of the filler material that can be loaded in the package, the reactivity effect of displacing an equivalent amount of moderator, and the impact on waste package mass due to the addition of the filler material. Evaluations and experiments are being performed (TBD) to ensure that the material performance characteristics of the filler will permit it to last over the time period of criticality control during isolation.

In addition to the specific criticality control requirements for filler material, the following issues concerning degradation must also be considered when using a filler material (TBV):

- a. Chemical interactions between the filler and waste must not compromise the function of the waste package,
- b. Filler materials with explosive, pyrophoric or chemically reactive characteristics are precluded,
- c. Filler materials that are liquid under ambient repository conditions are precluded,
- d. Galvanic interactions between the filler material and other components must not compromise the function of the waste package, and
- e. Filler materials or their decomposed/reacted components must not accelerate the transport of radionuclides through any of the barriers.

APPENDIX B: Sample of the Design Process and Methodology Application

The disposal criticality analysis methodology, as described, will account for the material performance of filler materials (if present) in systems being analyzed.

Filler materials is another design concept which is being considered as a alternative to contribute to waste package disposal criticality control.

1.1.1.4 Moderator Exclusion: Barriers and Seals

The presence of moderator material in a waste package containing commercial LWR SNF increases the reactivity of the package. Water is the major moderator of concern for commercial LWR SNF emplaced in a deep geological repository. The engineered barrier system is designed to reduce the presence of water near the waste packages and prevent it from contacting the waste forms for as long as reasonably possible. Thermal loading strategies, emplacement drift design, and water diverters (TBD) are being designed to reduce the presence of water near the waste package. The waste package barriers and seals (welds) are design to prevent water from contacting the waste forms inside for as long as is reasonably possible (times in excess of 3,000 years). Due to the long time period of disposal, the failure of the waste package's moderator excluding barriers and seals is eventually expected to occur.

The disposal criticality analysis methodology, as described, will account for the performance of waste package barriers and seals in systems being analyzed. Slow (aqueous and two-phase corrosion/degradation modes) and fast (rockfalls, drift collapse, and other seismic events) breaching mechanisms along with the presence of undetected defects (manufacturing and closure) are all considered together in the methodology.

Barriers and seals are a design concept which will be accounted for, but not relied upon to contribute to waste package disposal criticality control.

1.1.1.5 Small Capacity Waste Packages

As stated earlier, limiting the amount of fissionable material is the ultimate criticality control method. Limiting the capacity (number of fuel assemblies) in a waste package limits the amount of fissionable material, and therefore limits the criticality potential of the system. Waste packages with one pressurized water reactor (PWR) SNF assembly or two boiling water reactor (BWR) SNF assemblies will not go critical as long as the assemblies are intact.

APPENDIX B: Sample of the Design Process and Methodology Application

The disadvantage of small capacity waste packages for criticality control is a total system issue. Disregarding the huge cost impact resulting from an order of magnitude more packages and a much larger emplacement area, the performance benefits of the "thermal umbrella" (heat driving water away from emplacement drifts) with the higher thermal loading is lost with a repository filled entirely with small capacity packages.

A small number of SNF assemblies may have sufficiently high reactivity or other concerns to require a small capacity waste package. A small number of small capacity waste packages will not adversely impact the total system. The disposal criticality analysis methodology, as described, will account for the small capacity waste package design concept.

The small capacity waste package design concept may be used as an alternative design to contribute to waste package disposal criticality control for very high reactivity fuel.

1.1.1.6 Flux Traps

Flux traps are a type of basket design which combines geometry and neutron absorbers. Flux traps used the geometry of the basket to provide a separation gap between neutron absorber plates. The gap, when filled with water, increases the effectiveness of the neutron absorber plates, thereby creating a "trap" for neutrons traveling between assemblies.

The major concern/disadvantage of flux traps for disposal applications is that the reactivity/criticality potential of the flux trap significantly increases when the trap structure degrades (the effectiveness of the neutron absorbers in the flux trap is lessened). For long term disposal applications, flux traps will degrade. For flux trap systems to be disposable, there must be sufficient criticality control without accounting for the flux trap. Therefore, there is no advantage for using flux traps for disposal. Flux trap designs are expected for some canistered wastes (multipurpose canisters containing commercial SNF for example).

The disposal criticality analysis methodology, as described, can account for the presence of flux trap designs. Flux traps will represent a slightly different start point for the configuration generators.

Flux traps do not contribute to long-term waste package disposal criticality control and therefore are not a design concept being used for disposal.

APPENDIX B: Sample of the Design Process and Methodology Application

1.1.1.7 Rod Consolidation

Rod consolidation is a form of moderator displacement. The fuel rods in commercial LWR fuel are less reactive when there is no water between the rods. The concept of rod consolidation involves removing the rods from their original spacing array and placing them together in a tightly packed array. The tightly packed array reduces the amount of moderator between fuel rods, and reduces the reactivity of the bundle.

The major concerns with rod consolidation are operational and performance. The operational concerns have been identified in test programs which removed and consolidated fuel rods from SNF assemblies at different utilities. The operation of removing rods from their spacer grids has been shown to be damaging to the fuel rods, and to cause high radiation exposure to workers. The operation of bundling the fuel rods together has been shown to be much less efficient than envisioned and also further damaging to the rods. The performance concerns comes from the more ready availability of radionuclides from the damaged rods. The Department of Energy has made the decision to dismiss rod consolidation as a major mode of criticality control for disposal.

The fuel assemblies which have been consolidated in the test programs will need to be disposed of. Special waste package designs will need to be developed to accommodate this existing consolidated fuel. The disposal criticality analysis methodology, as described, can account for the presence of consolidated bundles of fuel rods.

The rod consolidation design concept for criticality control will not be used as a means of waste package disposal criticality control.

1.1.2 External Near-Field Criticality Control Concepts

The design concepts for providing criticality control in the engineered barrier system (EBS)/near-field containing commercial LWR SNF debris and/or the fissionable materials from commercial LWR SNF are listed below along with a discussion of their applicability for disposal criticality control.

APPENDIX B: Sample of the Design Process and Methodology Application

1.1.2.1 Invert Design: Particulate Trap/Core Catcher

The primary location for EBS/near-field criticalities is expected to be in the invert underneath the waste package. The Particulate Trap/Core Catcher design concept controls the location of LWR SNF debris and fissionable material when they leave the waste package. The design, if working correctly, retards the flow of fissionable material and controls the geometry or shape of the fissionable material mass in the invert, thereby controlling the criticality potential of the material. There are questions of how effective the concept would be under some conditions and how it would last over time.

The disposal criticality analysis methodology, as described, will account for the presence of a particulate trap/core catcher (if used) in the EBS invert design.

Particulate Trap/Core Catcher is a design concept which will be accounted to contribute to, but not relied upon, for disposal criticality control in the EBS/near-field.

1.1.2.2 Invert Design: Depleted Uranium Dilutant

The formation of critical masses of fissionable material from commercial LWR SNF outside of the waste packages is considered highly unlikely (improbable) but possible. The design concept of depleted uranium dilutant involves the addition of large quantities of depleted uranium to lower the effective enrichment of LWR SNF fissionable materials so that criticality is no longer possible. The use of depleted uranium raises important health and safety issues for workers emplacing the depleted uranium and for ventilation of the drifts in possible retrieval scenarios (preclosure).

The disposal criticality analysis methodology, as described, will account for the presence of a depleted uranium dilutant (if used) in the EBS invert design.

Depleted uranium dilutant is a design concept which may be used as an alternative design for very high reactivity fuel, but is not to be relied upon to contribute to disposal criticality control in the EBS/near-field for normal commercial LWR SNF.

APPENDIX B: Sample of the Design Process and Methodology Application

1.1.2.3 Water Diverter/Waste Package Drip Shield

The water diverter/drip shield concept would limit corrosion of the waste package and waste form to very slow two-phase (water vapor) based corrosion. The slow degradation rate of the waste form under these conditions could allow for significant decay of fissile isotopes and extend the time when sufficient fissionable material could be available in the near-field for criticality. The lack of liquid water would also slow the transport of materials (fissile and absorber) from the expected slumped subcritical mass (the degraded waste package and waste form). The long term performance of a water diverter/drip shield is questionable. Feasible designs are still to be determined.

The disposal criticality analysis methodology, as described, will account for the presence of a water diverter/waste package drip shield (if used) in the EBS design.

The water diverter/waste package drip shield design concept will be accounted for (if present), but not relied upon to contribute to disposal criticality control in the EBS/near-field.

1.1.2.4 Backfill

The addition of a backfill material (such as crushed tuff) into the emplacement drifts is intended to function similarly to the water diverter/drip shield concept for criticality control purposes, limiting water contact and fissionable material transport. The operation of emplacing a backfill that would perform these functions, and the long term performance of any backfill emplaced, are questionable. The presence of a backfill may even enhance degradation of some barriers.

The disposal criticality analysis methodology, as described, will account for the presence of backfill (if used) in the EBS design.

The backfill design concept (if used) will be accounted for, but not relied upon to contribute to disposal criticality control in the EBS/near-field.

1.1.3 External Far-Field Criticality Control Concepts

Far-field criticalities by definition take place outside the engineered barrier system, so design concepts do not directly provide any criticality control. All the engineered barrier features that

APPENDIX B: Sample of the Design Process and Methodology Application

act to divert water away, and retard radionuclide release also help to prevent far-field criticalities. The one design concept that may assist in providing criticality control in the repository far-field is the use of depleted uranium in the invert.

The depleted uranium, as for the invert case described above (Section 1.1.2.2), would dilute any potential stream of fissile materials (U-235) from dissolved SNF. The hope would be that the depleted uranium would be transported with the fissile material to any potential far-field site where a criticality might occur. The development of depleted uranium which has similar chemical transport properties to the spent fuel, having the depleted uranium retain those properties over long periods of time in the drift invert environment, and having a sufficient amount of depleted uranium in the drift to perform the criticality control task are all still being addressed.

The intrinsic properties of commercial LWR SNF (low enrichment) and of the nature of the potential repository site being evaluated make far-field criticality event exceedingly unlikely. The use of depleted uranium as a dilutant is not currently considered necessary nor cost effective for commercial SNF.

[The use of depleted uranium for HEU fuels is still in consideration to assist disposal far-field criticality control.]

1.2 Burnup Credit

In addition to these design concepts, burnup credit (taking credit for fuel depletion and the generation of neutron absorbers in spent nuclear fuel assemblies) may be used to assist in meeting regulatory requirements. Although burnup credit is not a design concept that is implemented for criticality control, burnup is an intrinsic property of spent nuclear fuel that may be considered in designing criticality control systems.

Burnup credit is the process of accounting for the reduced reactivity of spent nuclear fuel (commercial LWR SNF) as compared to fresh fuel of the same initial enrichment. The approach recognizes that the fuel has been irradiated and accounts for the net depletion of fissile material and for the creation of neutron-absorbing isotopes as a result of fission in an operating reactor. The criticality potential of SNF also varies with cooling time (the time since removal from the

APPENDIX B: Sample of the Design Process and Methodology Application

reactor core) as radionuclides are created and subsequently decay. Neutronics models used to estimate the criticality potential of SNF show that the reduced reactivity (criticality potential) due to burnup is a valuable contributor to long-term criticality control.

Evaluation of an engineered barrier system design using the burnup credit approach requires a reasonable and conservative prediction of the isotopic composition of the SNF and analysis of the system reactivity based on these isotopes. The burnup credit methodology is validated using experimental data. This includes fresh fuel criticality experiments, commercial LWR criticality data, and chemical assay data for commercial spent nuclear fuel. Analysis of this data establishes the biases and uncertainties in the methodology and extends these biases and uncertainties to the range of applicability for long-term waste disposal in a repository. The burnup credit methodology presented in this report is applicable for configurations internal to waste packages. For external configurations, the material separation, transport, and deposition processes are such that credit cannot be taken for some species of neutron absorbers which were formerly present in the SNF (TBV).

The methodology described in this report references the data and parts of the methodology presented to the NRC in the "Topical Report on Actinide-Only Burnup Credit for PWR Spent Nuclear Fuel Packages"^{B-11}.

The disposal criticality analysis methodology must be able to evaluate the effectiveness of burnup credit and the design methods used for controlling criticality. Validation of the methodology used to evaluate the criticality control potential of these concepts and the range-of-applicability of this methodology are addressed in Section 4.1 of the main body of the report.

1.3 Design Concepts Selected for Disposal Criticality Control

The various criticality control design concepts and burnup credit were evaluated for use in disposal criticality control. In addition to burnup credit, the general disposal criticality control waste package/EBS design concepts selected include basket design, neutron absorber, and the invert particulate trap/core catcher design. The filler material and small capacity waste package concepts are held as alternatives. The use of the depleted uranium dilutant design concept is to be evaluated for higher enriched fuels.

APPENDIX B: Sample of the Design Process and Methodology Application

The design concepts selected were incorporated into the waste package design during the Advanced Conceptual Design (ACD) phase. The design concepts selected were evaluated with the preliminary disposal criticality analysis methodology. The preliminary evaluations indicated that the design concepts should work. The selection and evaluation of the waste package disposal criticality control design concepts is documented in the MGDS Advanced Conceptual Design Report^{B-1}.

Based upon the evaluations of the ACD phase designs, modification have been made to the various waste package designs and to the EBS invert design. To provide a sample of the methodology application, evaluations performed for one waste package design will be presented. The design and system evaluated are described in the next section.

The following sections present the sample criticality control design and some sample criticality evaluations which support that design. The criticality evaluation methodology proposed by this technical report will be applied in a systematic manner to the final design with the following objectives:

- Demonstrate that the design meets regulatory requirements.
- Provide guidance for any required improvement or enhancement of criticality control designs.
- Evaluate alternative additional criticality control methods to support the overall defense-in-depth design policy.

1.4 Description of Sample System Design

The sample evaluation is performed for PWR SNF assemblies with the design basis characteristics, in a 21 PWR SNF waste package design. The waste packages are located in an EBS (subsurface) design at the sample repository. The sample repository site is the potential Yucca Mountain Site in Nevada.

1.4.1 Waste Form

The waste form used in the sample evaluations are B&W 15×15 Mark B4 PWR SNF assemblies. The mechanical parameters of the B&W 15×15 fuel assembly used for the sample evaluation are

APPENDIX B: Sample of the Design Process and Methodology Application

| listed in Table B-1. The fuel characteristics used in the sample evaluation are the design basis fuel characteristics, 3.00 weight percent initial enrichment U-235 and 20 GWd/MTU burnup, |
| from the MGDS Advanced Conceptual Design Report^{B-1}. The mechanical parameters and design |
| basis fuel characteristics are used by SAS2H^{B-2} and MCNP 4A^{B-3} to generate the SNF isotopic |
| concentrations and to calculate the reactivity of configurations containing the fissile material. A |
| graphical representation of a fuel assembly is provided in Figure B-1.

| Figure B-1 shows a B&W 15×15 fuel assembly, with a cut-away center to show the rods from a |
| control rod assembly (CRA) (labeled "Rod control cluster"). The assemblies used in the sample |
| evaluation did not include CRAs. Figure B-1 also shows a cross section cut of a fuel rod (labeled |
| "Fuel element") with a blow up of a section showing the fuel cladding, the pellet-clad gap |
| (labeled "Annulus"), and the fuel pellet.

APPENDIX B: Sample of the Design Process and Methodology Application

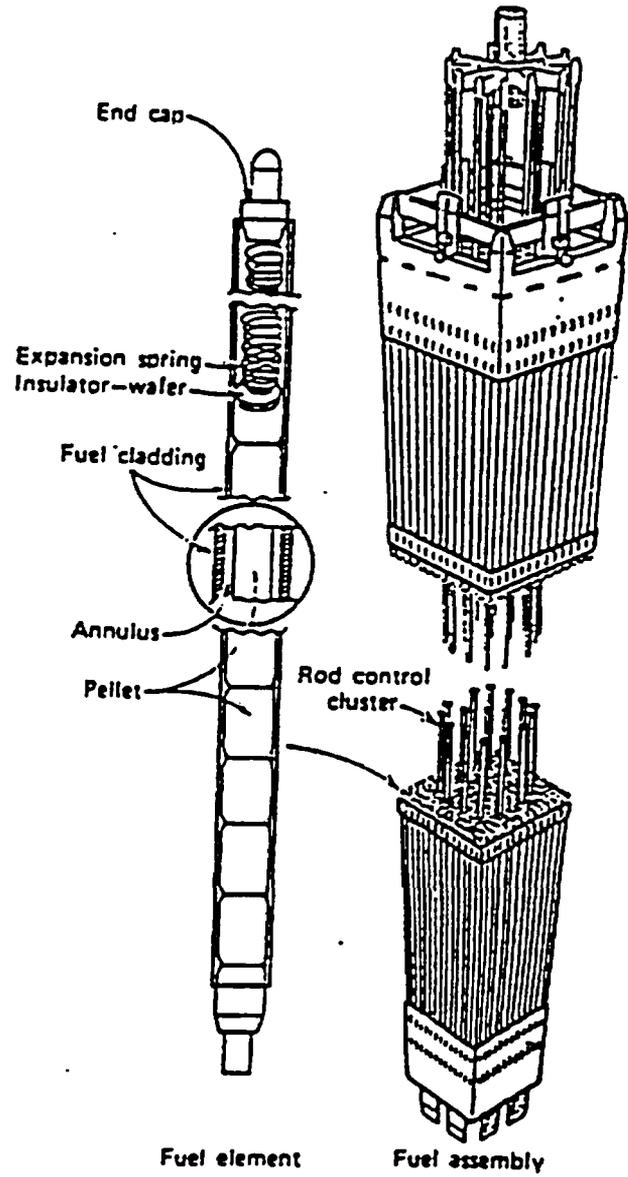
Table B-1. Mechanical Parameters of B&W 15×15 Fuel Assembly

Parameter	Value	Units	Metric	Units	Radius (cm)	Ref.
Fuel rods	208	/assembly	-	-	-	B-4
Fuel rod array	15×15	-	-	-	-	B-4
Guide tubes	16	/assembly	-	-	-	B-4
Instrumentation tubes	1	/assembly	-	-	-	B-4
Clad/tube material	Zircaloy-4	-	-	-	-	B-4
Fuel pellet OD	0.3686	inches	0.9362	cm	0.4681	B-4
Fuel stack height	141.8	inches	360.2	cm	-	B-4
Mass of U	1023	lb	464	kg	-	B-5
Mass of UO ₂	1160.64	lb	526.38	kg	-	B-4
Percent of theoretical density	95	%	-	-	-	B-4
Fuel clad OD	0.430	inches	1.092	cm	0.546	B-4
Clad thickness	0.0265	inches	0.0673	cm	-	B-4
Fuel clad ID*	0.377	inches	0.957	cm	0.479	-
Fuel rod pitch	0.568	inches	1.443	cm	-	B-4
Guide tube OD	0.530	inches	1.346	cm	0.673	B-4
Guide tube thickness	0.016	inches	0.041	cm	-	B-4
Guide tube ID*	0.498	inches	1.264	cm	0.632	-
Instrumentation tube OD	0.493	inches	1.252	cm	0.626	B-4
Instrumentation tube thickness	0.016	inches	0.041	cm	-	-
Instrumentation tube ID*	0.461	inches	1.170	cm	0.585	-
Fuel assembly envelope	8.536	inches	21.681	cm	-	B-4

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

(Reference B-4, Table 2.5) (Reference B-5, Table 2A-8)

Figure B-1. B&W 15×15 Fuel Assembly



APPENDIX B: Sample of the Design Process and Methodology Application

1.4.2 Waste Package Design

The waste package design used in the sample evaluation is the 21 PWR Advanced Unclad Fuel (UCF) waste package design. Figure B-2 provides a graphical description of the UCF design. The design relies on burnup credit and neutron absorbers to provide disposal criticality control.

Figure B-2 identifies the major components of the UCF waste package design. The material call outs for the components in the waste package are listed under the components (A 516, 316B6A, and Alloy 625). A 516 refers to the type of the carbon steel, 316B6A refers to the type of borated stainless steel, and Alloy 625 refers to the type of high nickel alloy.

APPENDIX B: Sample of the Design Process and Methodology Application

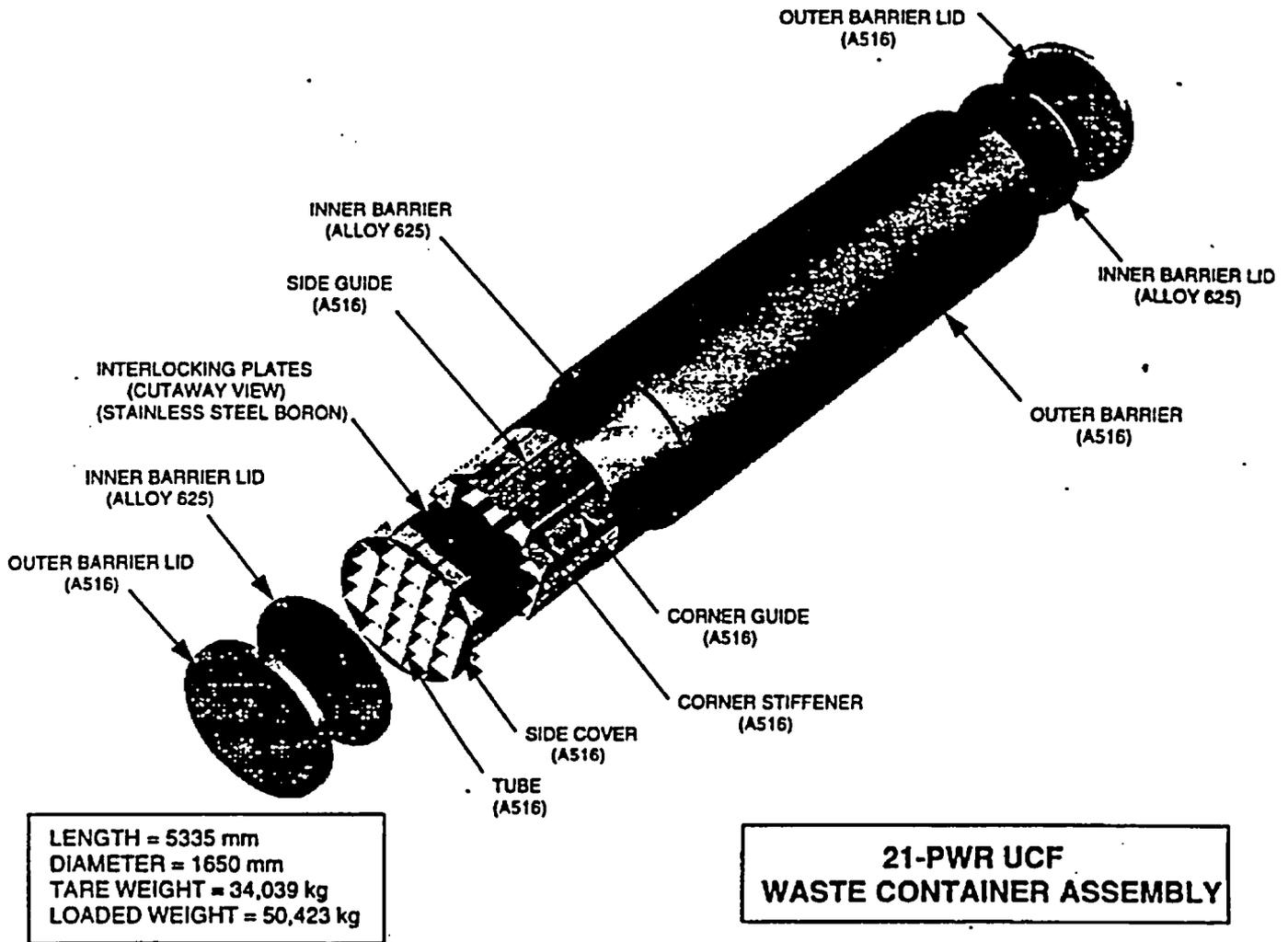
1.4.2 Waste Package Design

The waste package design used in the sample evaluation is the 21 PWR Advanced Unclad Fuel (UCF) waste package design. Figure B-2 provides a graphical description of the UCF design. The design relies on burnup credit and neutron absorbers to provide disposal criticality control.

Figure B-2 identifies the major components of the UCF waste package design. The material call outs for the components in the waste package are listed under the components (A 516, Stainless Steel Boron, and Alloy 625). A 516 refers to the type of the carbon steel, the Stainless Steel Boron is a borated Type 316 stainless steel, and Alloy 625 refers to the type of nickel-based alloy.

APPENDIX B: Sample of the Design Process and Methodology Application

Figure B-2. 21 PWR UCF Disposal Container



APPENDIX B: Sample of the Design Process and Methodology Application

1.4.3 Engineered Barrier System Design

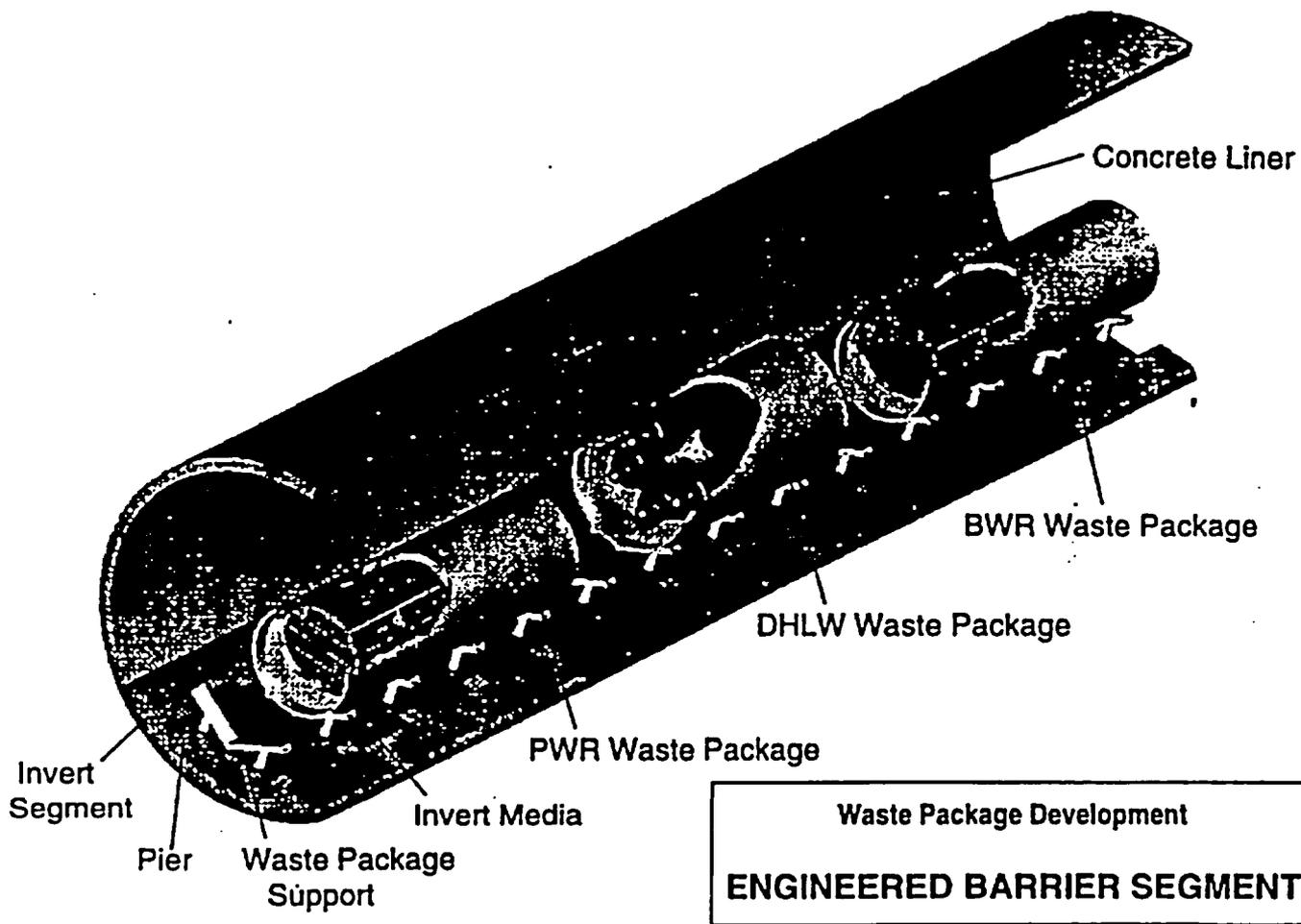
The EBS design (the underground structures) used for the sample evaluation is a modified EBS design similar to the one presented in the MGDS Advanced Conceptual Design (ACD) Report^{B-1}. Figure B-3 shows a view of the sample evaluation engineered barrier segment design. The sample EBS design has the following properties:

- 5 meter diameter emplacement drifts,
- ~2000 meter long drifts,
- Pier emplaced waste packages (instead of rail cars as used in the MGDS ACD Report^{B-1}),
- Piers consist of a carbon steel bar anchored to the steel sets with crushed tuff underneath,
- Waste package pedestal supports are made of carbon steel and are attached to the piers,
- Invert material is crushed tuff,
- 19.5 meter nominal center-to-center spacing between emplaced 21 PWR waste packages,
- 22.5 meters nominal spacing between emplacement drifts, and
- No backfill in the emplacement drifts. (Alternatives, particularly those utilizing depleted uranium, will be considered.)

Figure B-3 shows three types of waste packages in the drift; however the PWR waste package was the only type specifically addressed in the sample evaluation.

[NOTE: The current EBS Design is still evolving and may not resemble the design presented here.]

Figure B-3. Engineered Barrier Segment



APPENDIX B: Sample of the Design Process and Methodology Application

1.4.4 Repository

The sample repository site used is the proposed Yucca Mountain Site in Nevada. The repository emplacement horizon is situated in Topopah Springs welded Unit 2 tuff (TSw2). The emplacement horizon is more than 200 meters from both the ground surface and above the water table. Figure B-4 provides a sketch of the Waste Package (WP) Emplacement Concept used for the sample evaluation, including a cutaway pillar showing the different types of rock layers found between the surface and water table at the Yucca Mountain site. A detailed description of the rock layers can be found in MGDS ACD Report^{B-1}. The pillar in Figure B-4 shows only a portion of a single emplacement drift.

Figure B-5 provides a graphical representation of a sample repository layout for the potential Yucca Mountain repository. The ramps, emplacement blocks, Yucca Mountain ridge, and water table are all identified in the figure. The parallel lines shown in the areas identified as emplacement blocks are the drifts where waste packages would be emplaced. A detailed description of the conceptual repository layouts for can be found in MGDS ACD Report^{B-1}.

Figure B-4. WP Emplacement Concept

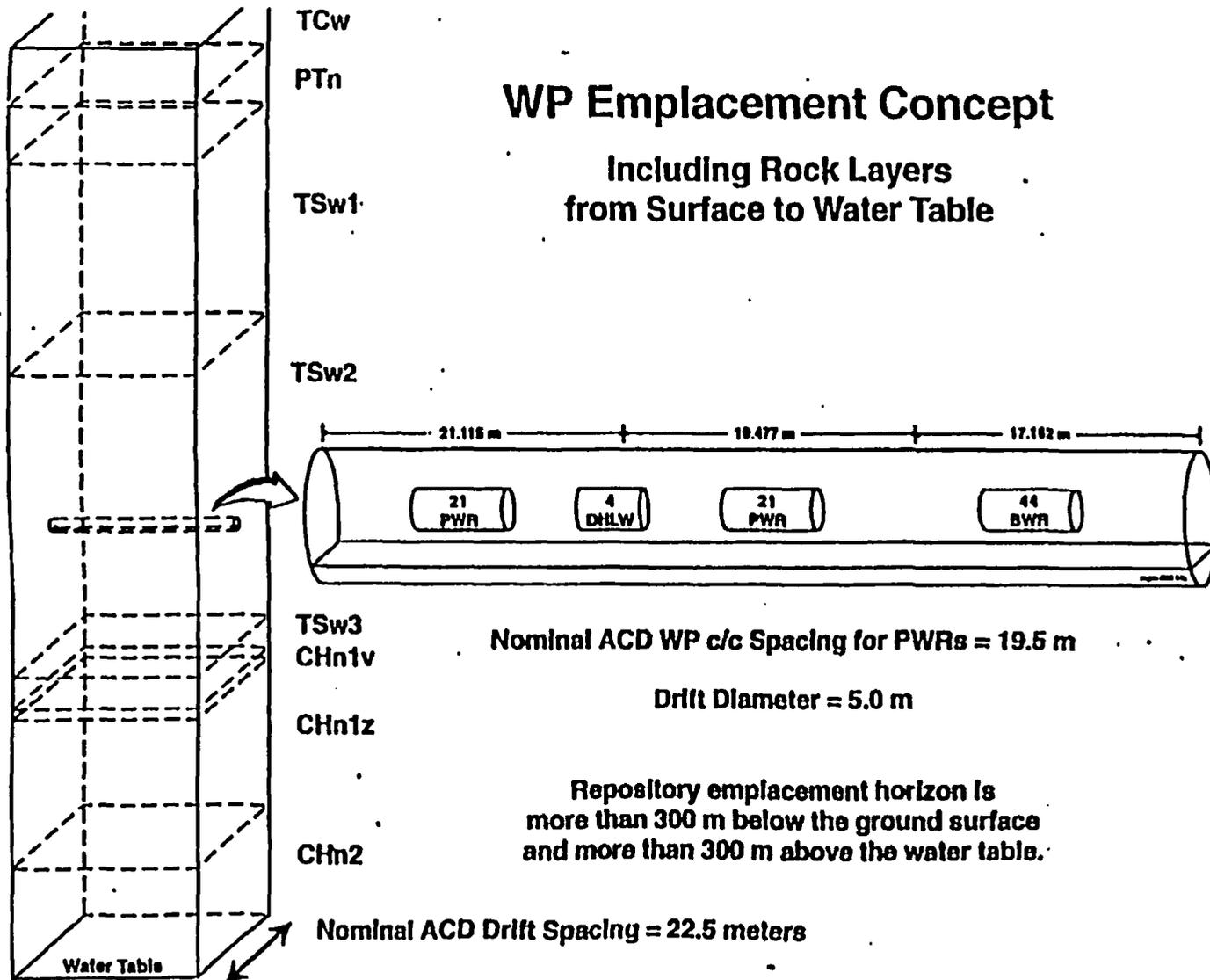
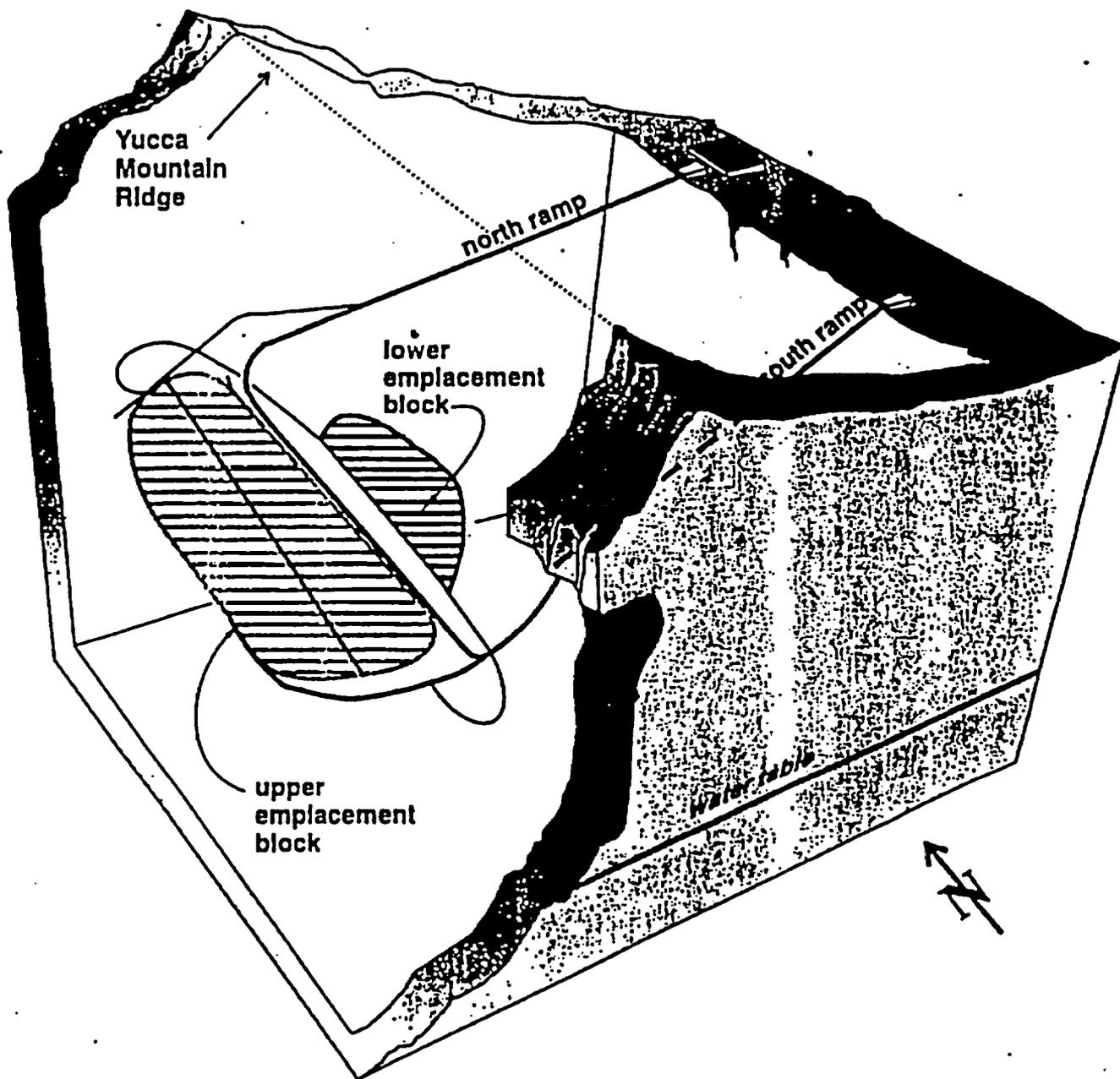


Figure B-5. Sample Repository Layout



APPENDIX B: Sample of the Design Process and Methodology Application

2.0 Sample Determination of Potentially Critical Configurations

The range of potential criticality configurations for the sample UCF waste package/EBS design at the potential Yucca Mountain repository site are determined using the configuration generator model described in Section 4.2 of the main report. The generation of these configurations follows the methodology described in Section 3.3.4 of the main report. Further information on the configuration generation code and on the following applications is given in Reference B-10 (TBD).

2.1 Sample Internal Waste Package Configurations

The following is a summary of the configurations which have been examined to date for internal criticality. These configurations were evaluated in the *Second Waste Package Probabilistic Criticality Analysis*^{B-6}.

- (1) The basket carbon steel tubes and basket guides have completely oxidized. The basket structure has collapsed; however, the fuel assemblies are still separated by the borated stainless steel plates between them. The borated stainless steel has partially corroded, with most of the boron from the corroded portions dissolved. Table B-2 provides the results of k_{eff} calculations for variations of this degraded configuration using the Monte Carlo neutronics code MCNP.

Table B-2. Progressive Degradation of Borated Stainless Steel Control Panels

% SS-B Plate Thickness Remaining	% of WP Void Space Filled With Fe_2O_3	k_{eff} (at 10,000 year peak)
80	0	0.894
50	0	0.917
50	10	0.851
25	20	0.857
25	15	0.880
10	25	0.887
10	20	0.908
10	10	0.944

Results in Table B-2 are TBV.

APPENDIX B: Sample of the Design Process and Methodology Application

- (2) The borated stainless steel is fully corroded, with large amounts of iron oxide still remaining from corrosion of the carbon steel tubes and guides, and the stainless steel plates. With the complete degradation of the stainless steel plates separating them, the fuel assemblies have settled through the oxides and are now touching. Only small amounts of boron remain trapped within the mass of oxides or in solution. Table B-3 provides the results of k_{eff} calculations for variations of this degraded configuration using the Monte Carlo neutronics code MCNP.

Table B-3. Basket Structure Gone, Uniform Iron Oxide and Boron Concentration

% of WP Void Filled With Fe_2O_3	% of Original B-10 Remaining In WP	k_{eff} (at 10,000 year peak)
0	0	1.093
30	0	0.928
30	2	0.913
30	5	0.890
20	0	0.979
20	5	0.941
20	10	0.902
20	15	0.872
20	25	0.812
20	100	0.572
10	10	0.947
10	15	0.909
10	20	0.879

Results in Table B-3 are TBV.

2.2 Sample EBS Near-Field Configurations

The sample configurations of degraded commercial SNF in the Engineered Barrier System Near-Field are listed below:

- Fissionable material left as a residue from evaporating water, with subsequent re-saturation to provide moderator.
- Fissionable material adsorbed by an ion-exchange process (e.g., in a zeolite).

APPENDIX B: Sample of the Design Process and Methodology Application

2.3 Sample Far-Field Configurations

Although far-field external criticality appears to have a very low probability, the following configurations appear to be among the most likely^{B-7}:

- Uranium adsorbed in a reducing mineral deposit, most likely of fossil organic origin.
- Fissionable material adsorbed in a zeolite material.
- Fissionable material (uranium or plutonium) precipitated on the walls of fractures.

The first two have been analyzed in the *Probabilistic External Criticality Evaluation*^{B-7}, in which it was shown that there is very small probability of accumulating a critical mass with commercial SNF (TBV). It was also shown that the second configuration could not possibly produce a critical mass with commercial SNF. The third configuration will be analyzed in the near future.

[Note: Analysis of these far-field configurations with highly enriched uranium waste forms is expected to show larger probability of accumulation of a critical mass. The highly enriched uranium waste forms requires less mass, and therefore less material transport, to form critical masses. The larger probability of these far-field configurations with highly enriched waste forms may still be insignificant. (TBV)]

APPENDIX B: Sample of the Design Process and Methodology Application

3.0 Sample Criticality Evaluations

The sample criticality evaluation performed for each of the configurations in the three different regions are discussed in this section. The MCNP 4A^{B-J} computer code with point-wise continuous energy spectrum cross sections is the criticality model being used to calculate reactivity (k_{eff}) for the configurations. The subcritical limit values used for the criticality analysis were determined by analyzing the various benchmark cases specified in Section 4.1.2 of the main report. From the benchmark analyses, the subcritical limits for the different ranges of configuration were determined for the MCNP code system. A summary of the sample results are presented in Table B-4.

Table B-4. Sample Subcritical Limits for Potential Configurations

Configurations	Subcritical Limit
Moderated intact fuel lattice inside waste package, intact-to-degraded waste package basket array	0.93 (TBD)
Moderated degraded fuel (non lattice) inside waste package, degraded waste package basket	0.92 (TBD)
Moderated fissile actinides outside waste package in the near-field	0.92 (TBD)
Moderated fissile actinides outside waste package in the far-field	0.92 (TBD)

[Note: The sample Subcritical Limits shown in this table include a 5% margin. It is intended that the margin will be reduced, if not dropped (TBV), for the probabilistic based evaluations concerned with system performance (e.g., in consequence evaluations).]

APPENDIX B: Sample of the Design Process and Methodology Application

3.1 Sample Waste Package Criticality Evaluations

The following steps were performed for the sample waste package criticality evaluation:

1. The configurations internal to the waste package determined in Section 2.1 were modeled with the criticality model (MCNP 4A).
2. Conservative SNF isotope concentrations from the SNF isotopics model (ORIGEN-S/SCALE 4.3) at the appropriate cooling times (modified according to the applicable degradation and transport models) were entered into the criticality models. The accuracy of isotopic model results for long decay times is discussed in Section 4.1.3.1 of the main report.
3. Criticality analyses of the configurations were performed and the appropriate subcritical limits were applied to the results. The results are listed in Tables B-2 and B-3 (TBV). The details of the calculations are listed in Reference B-10 (TBV).
4. For the current model, the percentages of materials remaining for the k_{eff} data sets from each of the two configurations discussed above were converted into masses of boron and iron (oxide) remaining in the flooded waste package. These masses were uniformly throughout the water in the waste package. [This is recognized to be non-conservative with respect to the iron oxide, which is highly insoluble and would be expected to settle leaving some fraction of the fuel rods without the benefit of the iron neutron absorption. Future analyses will include cases with an appropriate range of settled volumes.] A linear regression was then performed with the data sets for each configuration to develop equations describing k_{eff} as a function of the mass of boron and iron remaining. The purpose of this model is to facilitate the screening of the multitude of potential configurations (i.e., remove configurations with k_{eff} less than the subcritical limit from further consideration). The regression lines for the two configurations are given by the following equations (where Fe is in metric tons and B is in kilograms):

- (1) Collapsed basket:
 $k_{eff} = 1.026 - 0.0242*Fe - 0.00645*B, \quad R^2=0.91$

APPENDIX B: Sample of the Design Process and Methodology Application

(2) Assemblies touching:

$$k_{eff} = 1.068 - 0.0221 * Fe - 0.0236 * B, \quad R^2 = 0.99$$

Pooled data sets:

$$k_{eff} = 0.989 - 0.0132 * Fe - 0.00679 * B, \quad R^2 = 0.54.$$

(Where R^2 is the fraction of the variation explained by the regression.)

The complete calculations are described in Reference B-10. It should be noted that the collapsed basket regression implicitly incorporates the effect of decreasing basket thickness, which is generally proportional to the explicitly decreasing amounts of boron and iron. The fact that the pooled data set has such a small R^2 indicates that the two sets represent somewhat different physical processes, which is consistent with the fact that the collapsed basket variation incorporates the effect of varying assembly spacing, while the assemblies touching case does not. This distinction will be reflected in further criticality analyses by switching from the collapsed basket model to the assemblies touching model when the simplified configuration generator code (discussed in Reference B-10) indicates that the stainless steel plates have completely degraded. Currently, these models also assume the configuration occurs at the time of peak postclosure k_{eff} (at approximately 10,000 years)^{B-6}. Future versions of these k_{eff} models will incorporate the effects of time, once sufficient MCNP runs have been performed to characterize this effect for each configuration.

5. The final step is to combine the configuration dependent k_{eff} models with the configuration generator code to provide an estimate of the flooded and degraded waste package k_{eff} as a function of time. In the configuration generator code, the boron and iron concentrations are decreased at each time step to reflect the corrosion and removal process. A simple deterministic example of this process is provided in Reference B-10. In this example, five basic parameters affecting the corrosion of basket materials and the removal of boron and iron from the waste package are varied between high and low values. The minimum amount of time required to remove sufficient boron and iron such that the flooded waste package k_{eff} exceeds 0.91 (the delimitator or subcritical limit used for the analysis^{B-6}) is estimated for various combinations of these parameters. Future versions of the configuration generator code will have probability distributions assigned to these parameters so that the probability of exceeding the defined criticality limit as a function of time can be estimated.

APPENDIX B: Sample of the Design Process and Methodology Application

3.2 Sample EBS Near-Field Criticality Evaluations

Analysis of the configurations identified in Section 2.2 has not yet been completed. The following steps will be performed for the sample EBS near-field criticality evaluation:

1. The configurations in the EBS near-field determined in Section 2.2 will be modeled with the criticality model (MCNP 4A).
2. Conservative SNF isotope concentrations from the validated SNF isotopics model (ORIGEN-S/SCALE 4.3) at the appropriate cooling times will be modified by the appropriate degradation, transport, precipitation, and retardation models. The modified isotopic concentrations will be entered into the criticality models. The accuracy of isotopic model results for long decay times is discussed in Section 4.1.3.1 of the main report.
3. Criticality analyses of the configurations will be performed and the appropriate subcritical limits will be applied to the results.
4. The system configurations where the calculated k_{eff} does not exceed the subcritical limit will be dropped from further consideration.

[Note: As part of the design process (which is outside the scope of this document) any system configuration where k_{eff} does exceed the subcritical limit will be evaluated for low impact fixes (redesigns or augmented control measures).]

3.3 Sample Far-Field Criticality Evaluations

A set of 10 uranium/water concentration combinations in tuff was evaluated to determine the minimum critical mass/radius spheres. This set represented 3 SNF types, chosen to represent the 2%, 4%, and 13% most stressing fuel with respect to k_{∞} . For each of these fuel types, the analysis was a two step process. First the most critical volume percent of UO_2 (highest k_{∞}) was determined for a family of water concentrations, using MCNP to calculate k_{∞} , for a range of UO_2 volume percentages. The k_{∞} values for one fuel type (PWR, 3.00% initial enrichment, 20 GWd/MTU) are shown in Reference B-10.

APPENDIX B: Sample of the Design Process and Methodology Application

The second step was to calculate k_{eff} using MCNP, for a range of radii, and interpolate to determine the critical radius, at which the value of k_{eff} is equal to the criticality threshold^{B-7}. The most appropriate value of criticality threshold k_{eff} was 1 minus (bias and uncertainty of the computational process) minus (twice standard deviation of the specific Monte Carlo calculation).

[Note: The criticality threshold will be replaced by the upper subcritical limit (USL) in future evaluations. The applicability of the benchmarks used in determining the USL for the far-field configurations is discussed in Sections 4.1.3.3 and 4.1.3.4 of the main.] For these cases, a fresh fuel bias and uncertainty was used because only the long lived uranium isotopes (and Np-237) were included in the configurations. The conservative assumption was made that none of the fission products and shorter lived actinides from the SNF are in the uranium-bearing groundwater from the repository (TBV). The other isotopes either decayed, or were removed from the SNF matrix much earlier than the uranium, or remained in the matrix after removal of the uranium. This process is illustrated in Reference B-10 for the UO_2 concentration giving the highest peak k_{eff} for a range of water concentrations.

The critical masses calculated according to this method are then compared against information on the grade (concentration) of natural ore deposits and their frequency of occurrence to determine the probability that reducing zones capable of concentrating a critical mass will occur in the specific repository environment. This comparison is also presented in Reference B-10.

APPENDIX B: Sample of the Design Process and Methodology Application

4.0 Sample Criticality Consequence Evaluations

This section discusses the results of a sample criticality consequence evaluation. The scenarios evaluated are based upon the configurations identified in Section 3 of this appendix. The consequence of criticality events was evaluated for systems where k_{eff} exceeded the subcritical limit. The base results of these consequence evaluations are increments to the radionuclide inventory (TBV). The detailed results are shown in Reference B-10 (TBV).

The internal criticality scenarios evaluated thus far simulate a flooded waste package that is gradually approaching a critical condition ($k_{eff}=1$) as a result of positive reactivity insertions caused by a slow loss of boron and iron from the package interior. Once a waste package reaches a k_{eff} of 1, continued small positive reactivity insertions will cause the power output of the waste package to begin to slowly rise (i.e., a long reactor period). If the power exceeds a certain limit, the rate at which water is consequentially removed from the waste package will exceed the rate of input, and the resulting water level drop will provide a negative reactivity insertion driving the waste package back towards a subcritical condition. Conversely, if insufficient power is produced, the water level will be maintained and the exchange process discussed previously will continue to remove dissolved boron, thus providing a continued source of positive reactivity insertions until the point of equilibrium is achieved. The maximum steady state power can then be estimated by determining the power required to maintain the bulk waste package water temperature at the point where water is removed at the same rate that it drips into the waste package. The waste package must produce sufficient power to raise the temperature of the incoming water to this equilibrium value, as well as account for heat losses to the environment by radiation and/or conduction. Preliminary calculations, which are provided in detail in Reference B-10, have shown that at a water temperature of 57.4°C, the evaporation rate will match the maximum TSPA-95 rate at which water drips into a WP located beneath a flowing fracture. The thermal power required to raise the water temperature to 57.4°C, while at the same time compensating for heat losses to the environment, is 2.18 kW.

To evaluate the effects of a criticality on the radionuclide inventory of a waste package, the computer code ORIGEN-S was run using the PWR criticality design basis fuel^{B-1}, and the steady state power of 2.18 kW discussed above. The criticality was assumed to occur after the fuel had aged/decayed for 15,000 years and was maintained at the above mentioned power for three durations: 1,000, 5,000 and 10,000 years. The maximum duration of 10,000 years is based on the assumption (TBV) that it is the upper bound for the conditions supporting criticality (high

APPENDIX B: Sample of the Design Process and Methodology Application

infiltration, integrity of the lower part of the barrier, sufficient fissionable material and void space remaining). The output of these runs was the radionuclide inventory, in curies, at the times corresponding to the end of each criticality, and at fuel ages (time since reactor discharge) of 45,000 and 65,000 years. In addition a fourth, decay-only case was run to determine the radionuclide inventories at the above times for fuel which did not experience a criticality event. The percentage increase in the inventories of 36 of the isotopes examined in TSPA-95 is provided in Reference B-10. The overall effect of the criticality can be summarized by the percentage increase in the total curies, over that of the decay only case, for the 36 TSPA-95 isotopes. Table B-5 shows this comparison (see Table B-5 footnote). The explicitly stated times are measured from emplacement. Figure B-6 graphically shows that even the 10,000 year duration criticality does not increase the inventory of the 36 isotopes above that at the time the criticality began. In addition, the criticality appears to have no significant long-term effect on the inventory of these isotopes. Within 25,000 years the total inventory of these 36 isotopes in fuel assemblies which experienced a criticality can barely be distinguished from the inventory in fuel assemblies which did not experience a criticality.

Table B-5. Percentage Increase in Total Curies of the 36 TSPA-95 Isotopes in a Single Waste Package

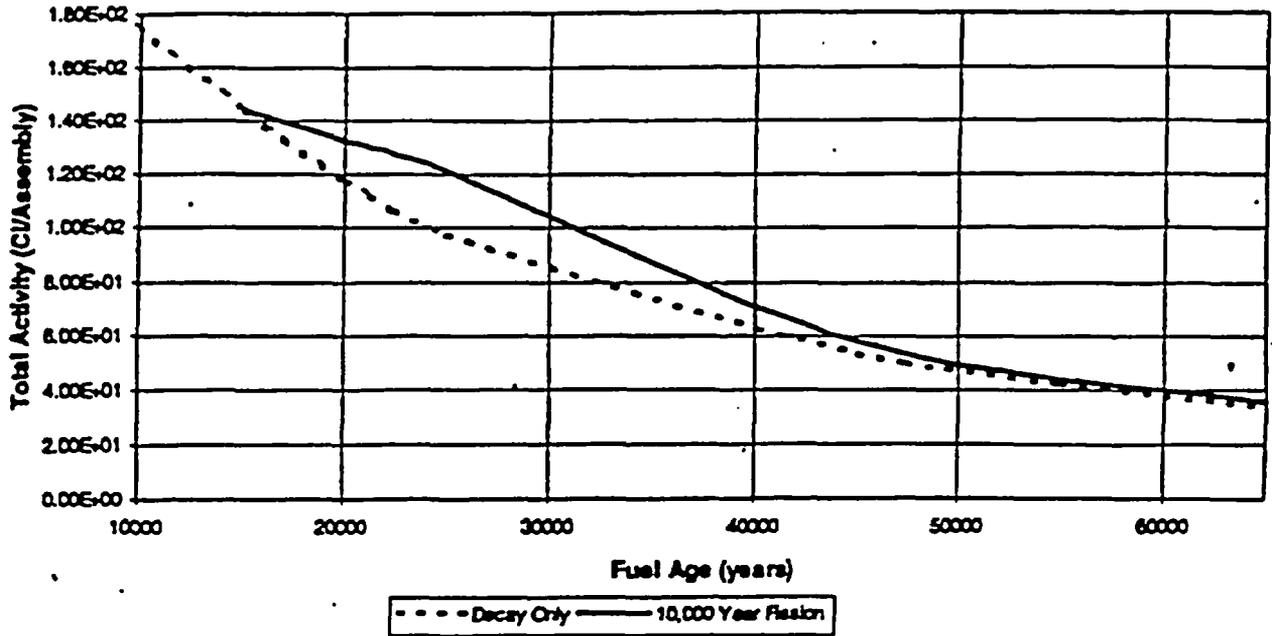
Duration of Criticality	Percent Increase at End of Criticality	Percent Increase at 45,000 years	Percent Increase at 65,000 years
1,000 years	8.5% (16k years)	0.73%	0.73%
5,000 years	15% (20k years)	4.2%	3.7%
10,000 years	24% (25k years)	9.9%	8.5%

Results in Table B-5 are TBV.

APPENDIX B: Sample of the Design Process and Methodology Application

Figure B-6. Increase in Isotopic Inventory from 10,000 year Criticality

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



APPENDIX B: Sample of the Design Process and Methodology Application

5.0 Sample Risk Evaluation

This section discusses the results of a sample Risk Evaluation performed for the potential critical events identified in Section 3. The probability of the potential critical configuration occurring (from Section 2) and the consequence of the resulting criticality (from Section 4) are combined into a risk of violating the performance objectives of the facility.

The following examples illustrate the criticality risk calculation in terms of dose at the accessible environment. When the risk-based criticality methodology is finally used in the licensing process, the expected dose rate will be computed by taking the source term from the radionuclide increase resulting from a criticality and applying the TSPA Monte Carlo analysis of the groundwater transport of this increased inventory to the accessible environment. This process must be summed over all times of occurrence of the criticality weighted by the probability of the occurrence of the criticality at that time. For purposes of this illustration, the result of the comprehensive methodology can be represented by a convolution operation which sums the product of the expected number of criticalities which occur in some time interval, $d\tau$, about a time τ , multiplied by the increase in radionuclide inventory caused by each criticality (which is generally a function of τ but will be considered to be independent of time for simplicity in this illustration), and multiplied by a transport factor which represents the fraction of radionuclide inventory mobilized from the source and traveling to the accessible environment in time $t-\tau$, over τ from 0 to t .

The transport factor represents both the length of time necessary to transport the nuclides from the source to the accessible environment once they are mobilized, and the time period over which they will be mobilizing. One extreme of the range of mobilization time periods is illustrated by the mobilization from intact SNF (assumed to have lost much of the cladding, but with the oxide matrix relatively intact), such as is shown in TSPA-95, Figure 9.3-5^{B-9}. This approximation is also appropriate following an internal criticality, since it has been shown that the most likely internal criticality (if any is possible at all) is with the assemblies reasonably intact so that the criticality can obtain the maximum benefit from the moderator between the fuel rods (*Second Waste Package Probabilistic Criticality Analysis*^{B-6}). In this case the dose rate increases with time up to 200,000 years, after which it remains relatively constant for up to 1,000,000 years, due to the long half-life of the isotopes being considered, and the slow dissolution of the SNF. At some later time the dose would decrease significantly due to the depletion of the source. For

APPENDIX B: Sample of the Design Process and Methodology Application

illustration of the relatively intact, slow dissolution case the process prior to the depletion of the source will be represented by the transport factor:

$$1 - e^{-\alpha(t-\tau)}$$

where α represents the reciprocal of the minimum transport time to the accessible environment, and an illustrative value is $\alpha = 0.75$ per 100,000 years.

It should be noted that the asymptotic value of the transport factor is normalized to 1 to represent the conservative assumption that all the nuclides will eventually reach the accessible environment; furthermore the cutoff time, after which the source depletion would diminish the dose rate, is being neglected. This approximation is probably appropriate for a criticality internal to the waste package in which the SNF remains relatively intact and will dissolve slowly.

An illustrative PDF for the time of occurrence of the criticality is:

$$\text{pdf}(\tau) = \beta^2 \tau e^{-\beta \tau}$$

where β represents the reciprocal of the time duration over which there is a significant probability of criticality occurrence, and an illustrative value is $\beta = 1.2$ per 100,000 years.

This function peaks at 83,000 years, representing two effects: 1) the conservative estimate in the *Initial Waste Package Probabilistic Criticality Analysis*^{B-8}, which showed that it took nearly 100,000 years to reach an expected number of criticalities; and 2) the fact that sometime before 500,000 years the probability of internal criticality will decrease significantly because most of the waste packages can no longer contain sufficient water to provide the moderation necessary for criticality. Forming the convolution by multiplying the PDF by the transport factor and integrating over τ from 0 to t gives the normalized (as explained below) expected dose due to a single criticality:

$$1 - e^{-\beta t} - t\beta e^{-\beta t} - \beta^2 e^{-\alpha t} \left((1 - e^{-(\beta-\alpha)t}) / (\alpha - \beta)^2 + t e^{-(\beta-\alpha)t} / (\alpha - \beta) \right)$$

This normalized expected dose is plotted in Figure B-7, along with the PDF used to generate it. To complete the risk calculation the normalized expected dose must be multiplied by: 1) the fractional increase in radionuclide inventory, 2) the fraction of waste packages achieving

APPENDIX B: Sample of the Design Process and Methodology Application

criticality, and 3) by the peak dose rate given in TSPA-95, Figure 9.3-5^{B-9}. The *Second Waste Package Probabilistic Criticality Analysis*^{B-6} shows the fractional increase in radionuclide inventory for the longest lived isotopes, due to a single waste package criticality, to be as follows: ⁹⁹Tc 4.1%, ²³⁷Np 2.1%, ¹²⁹I 4.1%. As discussed in connection with the PDF above, the expected number of criticalities in 100,000 years is only 1, while the TSPA-95 results represent the independent contributions of the number of waste packages which would have been breached in the Monte Carlo simulation of that more comprehensive methodology. Hence there is a reduction by an additional factor of up to 10,000 (the approximate total number of SNF waste packages). Since the present TSPA-95 analysis does not give this number directly, and in view of the illustrative purpose of this calculation, the explicit result of applying these factors is not presented here.

It should be noted that these fractional increases are different from the increases in total curies given in Section 4, above, because the focus here is on long lived isotopes. It is this focus on long lived isotopes which makes the fractional increase applicable to the total dose rates given in TSPA-1995, Figure 9.3-5^{B-9}.

Following an external criticality (if one could occur) the resulting increased radionuclide inventory would be much more readily mobilized, than would the relatively intact SNF in the case considered above. Therefore, the comprehensive TSPA methodology would produce a time dependent dose reflecting a transport function which peaked and declined over a time period much shorter than 1,000,000 years. Since this situation has not yet been analyzed by the TSPA methodology, the form of the transport function must be hypothesized. For this purpose, a probability density function is used:

$$\text{pdf}_1(t-\tau) = \alpha^2 t e^{-\alpha(t-\tau)}, \text{ where } \alpha = 0.75 \text{ per } 100,000 \text{ years,}$$

which has the same rising behavior as the transport function, but is normalized so that its integral is 1. The functional form for the PDF of the external criticality occurrence time is the same as for the internal criticality, but the peak is broader and occurs at 400,000 years.

$$\text{pdf}_2(t) = \beta^2 t e^{-\beta t}, \text{ where } \beta = 0.25 \text{ per } 100,000 \text{ years}$$

APPENDIX B: Sample of the Design Process and Methodology Application

In this illustration of external criticality α and β have approximately the same meaning as for the internal criticality illustration described above. The convolution of the criticality occurrence and the subsequent transport to the accessible environment is then represented by the integral:

$$pdf_c(t) = \int_0^t pdf_2(\tau) pdf_1(t-\tau) d\tau$$

which can be evaluated analytically to give:

$$pdf_c(t) = \alpha^2 \beta^2 e^{-\alpha t} \left[\frac{t^2 e^{-(\beta-\alpha)t}}{\beta-\alpha} + \frac{t(1-e^{-(\beta-\alpha)t})}{(\beta-\alpha)^2} + \frac{t^2 e^{-(\beta-\alpha)t}}{\beta-\alpha} + \frac{2te^{-(\beta-\alpha)t}}{(\beta-\alpha)^2} + \frac{2(1-e^{-(\beta-\alpha)t})}{(\beta-\alpha)^3} \right]$$

- | A graph of this normalized expected dose is given in Figure B-8, together with the $pdf_2(t)$. It should be noted that the normalization of this expected dose is different from that shown in Figure B-7 for the internal criticality. Correction factors for fractional nuclide increase and fraction of total inventory reaching criticality would be applied, but they would be different from the internal criticality case. More importantly, these correction factors would have to be applied to the short dissolution time analog of TSPA-1995, Figure 9.3-5^{B-9}.

APPENDIX B: Sample of the Design Process and Methodology Application

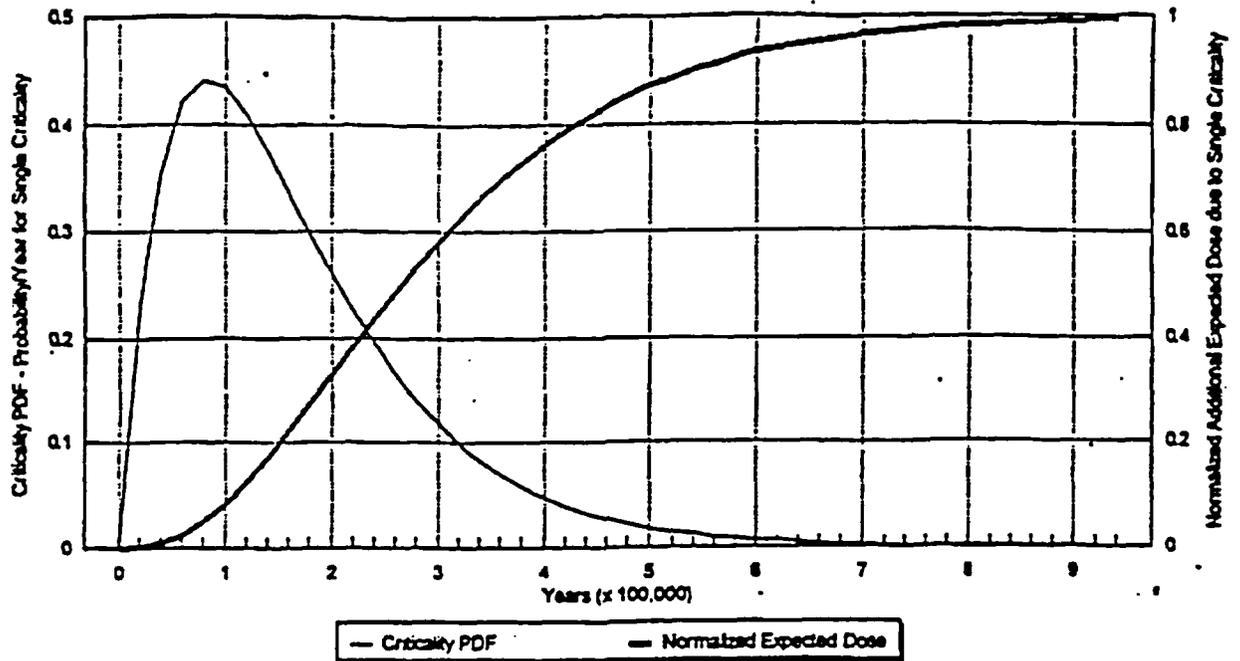


Figure B-7. Normalized Additional Dose Due to a Single Internal Criticality Event

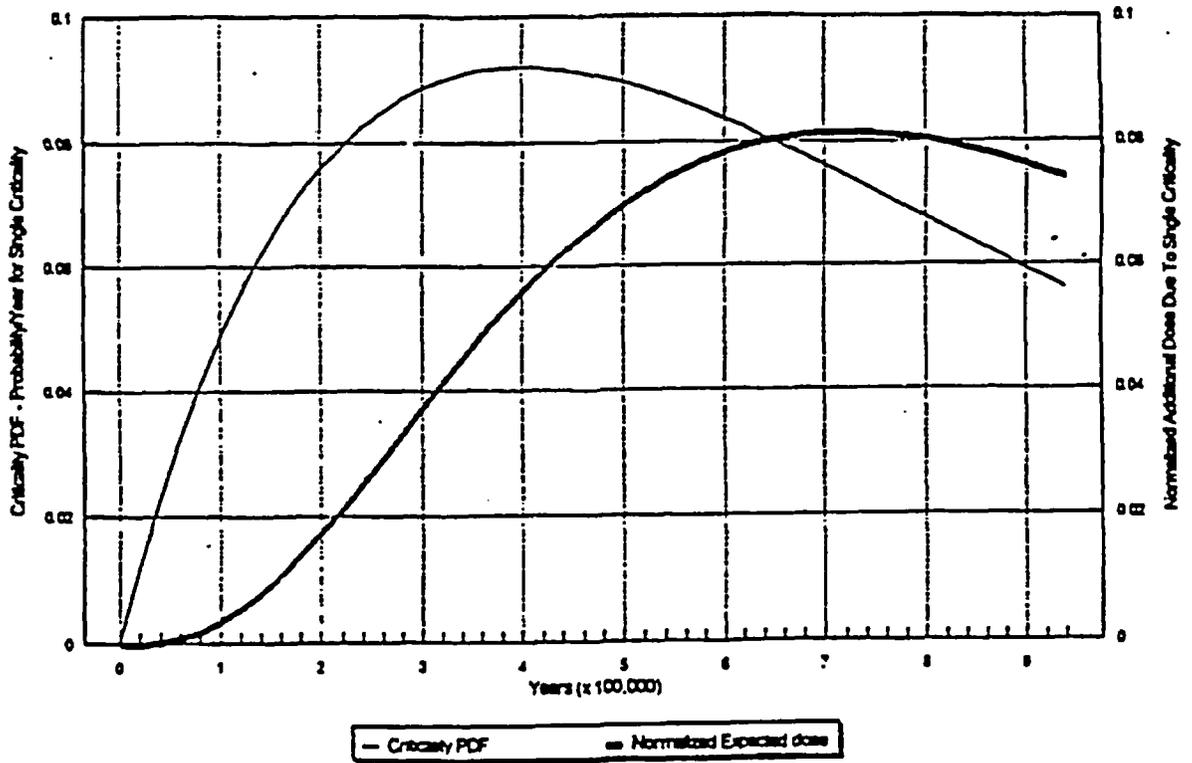


Figure B-8. Normalized Additional Dose Due to a Single External Criticality Event

APPENDIX B: Sample of the Design Process and Methodology Application

6.0 Sample Total System Performance Consequence Evaluation

| As previously discussed in Section 3.1 of the main report, a performance assessment evaluation will be conducted prior to a detailed TSPA analysis that uses an incremented source term. If the consequence is determined to be insignificant upon evaluation of the incremented source term, no criticality perturbations to TSPA analyses will be conducted. However, if detailed TSPA calculations are warranted, the approach described in Section 3.1 of the main report and using the models described in Section 4.4 of the main report will be implemented.

| An example calculation was conducted for this report using an incremented source term from an internal waste package criticality event theorized in the an earlier evaluation^{B-6}. The results of the example evaluation indicate that, for the example potential critical events, there was no significant adverse effect to the repository Total System Performance. The dose to the public was not significantly increased by the inclusion of the potential criticality events identified as part of the example evaluations. The summary of results from this evaluation are listed in Table B-6 (TBV).

| Three criticality events were defined in *Second Waste Package Probabilistic Criticality Analysis*^{B-6}. The three criticality events were:

- 1) 1,000 year criticality occurring after 15,000 years,
- 2) 5,000 year criticality occurring after 15,000 years, and
- 3) 10,000 year criticality occurring after 15,000 years.

| The inventory created by the criticality event for these three cases were presented in Tables 7.5-1, 7.5-2, and 7.5-3 in the *Second Waste Package Probabilistic Criticality Analysis*^{B-6}. The percent difference due to the criticality was also presented in these tables and gives an indication of the increase or decrease of the particular isotope inventory.

| A quantitative total system performance assessment using the perturbed radionuclide inventory is given below. The key isotopes contributing to release and dose to man were determined in TSPA-1995^{B-9} to be ¹²⁹I, ²³⁷Np, and ⁹⁹Tc. ¹²⁹I and ⁹⁹Tc provided peak release to and doses at the accessible environment at early times and ²³⁷Np provided peak, and generally, highest release at later times in the simulations conducted for TSPA-1995. The percent increase from the original inventory of each of the key radionuclides for each of the criticality events was reviewed and is

APPENDIX B: Sample of the Design Process and Methodology Application

presented in Table B-6. These data indicate that the greatest increase in source term inventory occurs for the longest criticality event (10,000 year event). However, the change is only approximately a 4 percent increase in inventory. Assuming an addition of 4 percent to the inventory of the key radionuclides as determined by TSPA-1995, the criticality would potentially produce a maximum of 4 percent increase in the simulated release or dose to man. However, the actual increase in release or dose to man is expected to be lower because the total 4 percent increase is not expected to reach the accessible environment due to dissolution rate limitations of the new source term. This increase in release is not expected to be significant to total performance.

Table B-6. Criticality Effect on Radionuclides Determined to be Important to Total Performance

Radionuclide	% Increase for 1,000 Yr Criticality	% Increase for 5,000 Yr Criticality	% Increase for 10,000 Yr Criticality
¹²⁹ I	0.45	2.0	4.1
⁹⁹ Tc	0.53	2.2	4.1
²³⁷ Np	0.26	1.0	2.1

Results in Table B-6 are TBV.

The case with a criticality event lasting 10,000 years occurring 15,000 years after closure is considered. The TSPA-1995 case of 83 MTU/acre, backfill, high infiltration, and drips on the waste package was the base case for the analyses. The criticality event was assumed to occur within a single waste package and the waste package failure was assumed to be the most conservative for the case under analysis. Dissolution rate of the source term was assumed to be the same as the initial waste form itself, since the criticality event was assumed to occur within the cladding. The inventory of the criticality source term was assumed to be increased or decreased according to the analyses presented in Table 7.5-3 of the *Second Waste Package Probabilistic Criticality Analysis*^{B-6}.

Figure B-9 shows the base case dose history at the accessible environment for the three radionuclides contributing the most to the total dose. The addition of the criticality event source term (one waste package with an inventory greater than the original inventory according to the *Second Waste Package Probabilistic Criticality Analysis*^{B-6}) does not change the results of this

APPENDIX B: Sample of the Design Process and Methodology Application

figure due to the relatively small inventory in the single waste package compared to the overall waste inventory in the potential repository.

- | Figure B-10 shows the dose history at the accessible environment for the same three radionuclides that results from the criticality event. The doses are generally several orders of magnitude below the base case and are inconsequential to performance of the repository.

APPENDIX B: Sample of the Design Process and Methodology Application

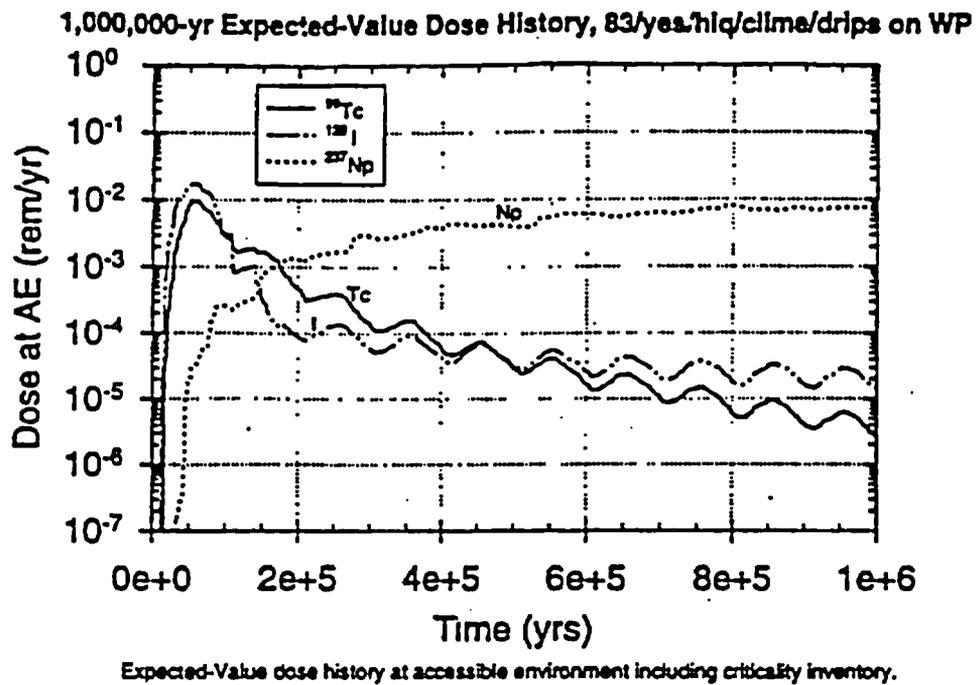


Figure B-9. Expected-Value Dose History at Assessable Environment Including Criticality

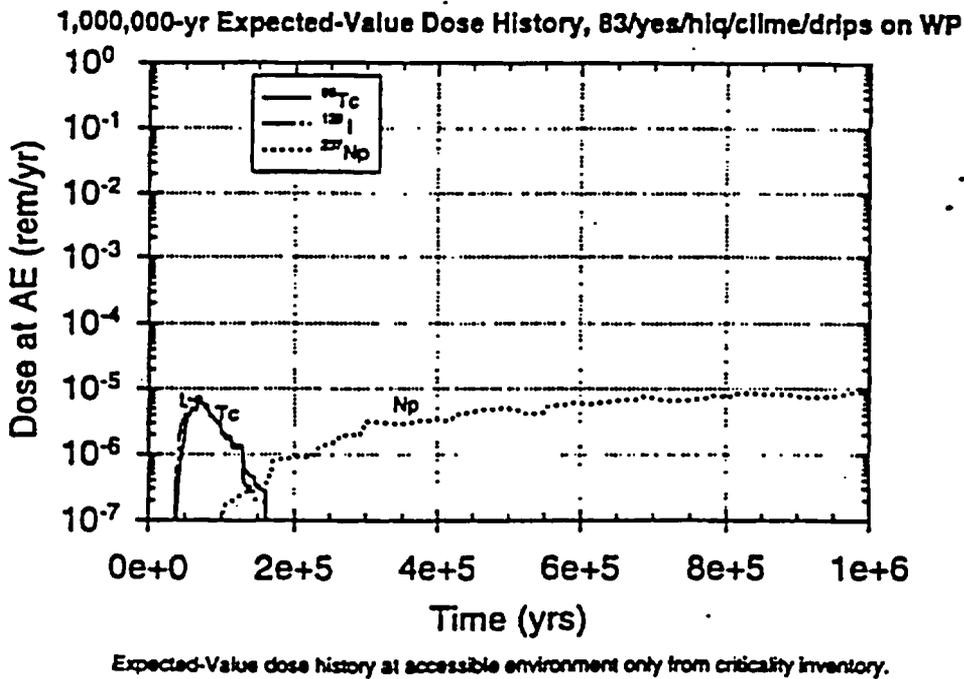


Figure B-10. Expected-Value Dose History at Assessable Environment Only From Criticality

APPENDIX B: Sample of the Design Process and Methodology Application

7.0 Conclusions

The design process in this appendix discussed the various criticality control concepts considered when selecting the disposal criticality control design concepts. A sample WP/EBS design based upon the disposal criticality control design concepts and the proposed Yucca Mountain site was then described.

The sample methodology application in this appendix presented a sample evaluation of the sample WP/EBS design. The evaluation showed little effect on the total system performance from a very conservative postulated criticality event. This sample evaluations helps form the conclusion that criticality events will not prohibit demonstrating the viability of the proposed Yucca Mountain Repository Site for a mined geological repository site for spent nuclear fuel.

APPENDIX B: Sample of the Design Process and Methodology Application

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APPENDIX C

Sample Application of the Methodology to DOE SNF

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TECHNICAL REPORT

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APPENDIX C: Sample Application of the Methodology to DOE SNF

Table Of Contents

Section	Page
1.0 Disposal Criticality Control Design	C-1
1.1 Selected Fuel Types	C-1
1.2 Design Concepts Considered	C-2
1.3 Selected Criticality Control Concept	C-2
1.4 Waste Package Description	C-3
2.0 Degradation Scenario Leading to Potentially Critical Configuration	C-4
3.0 Sample Criticality Evaluations	C-5
3.1 MIT SNF Criticality	C-5
3.1.1 MIT SNF Intact Criticality	C-5
3.1.2 Degraded MIT SNF Within Canister	C-6
3.2 ORR SNF Criticality	C-7
3.2.1 ORR SNF Intact criticality	C-7
3.2.2 Degraded ORR SNF Within Canister	C-8
4.0 Conclusions	C-10
5.0 References	C-11

APPENDIX C: Sample Application of the Methodology to DOE SNF

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APPENDIX C: Sample Application of the Methodology to DOE SNF

LIST OF FIGURES

Figure Title

Page

None in this Appendix

APPENDIX C: Sample Application of the Methodology to DOE SNF

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APPENDIX C: Sample Application of the Methodology to DOE SNF

LIST OF TABLES

Table Name	Page
Table C-1. Intact MIT SNF Codisposal Canister Criticality Results	C-6
Table C-2. Degraded MIT SNF Codisposal Canister Criticality Calculations.	C-7
Table C-3. Intact ORR Codisposal Canister Criticality Calculations	C-8
Table C-4. Degraded ORR Codisposal Canister Criticality Calculations	C-9

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APPENDIX C: Sample Application of the Methodology to DOE SNF

This appendix demonstrates the application of the methodology to waste forms other than commercial SNF. The DOE owned research reactor fuel, which is aluminum-clad and aluminum matrix, has been designated as having a high priority for repository disposal. The M&O has performed an evaluation of the potential for criticality and developed a preliminary criticality control design for two specific fuels of this type.^{C-1} This section summarizes the methodology and results of that analysis.

1.0 Disposal Criticality Control Design

The first section of this appendix discusses those aspects of the design process and criticality control concepts which differ from those used for the commercial SNF in Appendix B. It also describes the unique features of the aluminum-based fuel selected for this analysis and the appropriate criticality control design.

1.1 Selected Fuel Types

Two DOE SNF fuel types were selected by the Alternative Technology Program of the Westinghouse Savannah River Company to be representative of the range of variations found in Al-based research reactor fuels (particularly with respect to criticality): the high-enrichment Massachusetts Institute of Technology (MIT) reactor fuel and the medium-enrichment Oak Ridge Research (ORR) reactor fuel. The MIT fuel has an initial maximum enrichment of 93.5 weight percent U-235 and the ORR fuel has an initial maximum enrichment of 20.56 weight percent U-235.

The MIT fuel assembly is constructed from 15 flat plates tilted at a sixty degree angle so that the resulting assembly has a rhomboidal (equilateral parallelogram with 60° acute angles) cross section, instead of the more common square or hexagon cross section. The MIT fuel length values used in these analyses are shorter than the original as-built length of the MIT assembly because the top and bottom ends of the assembly, which do not contain uranium materials, have been removed by cutting. The fuel plates consist of an aluminum cladding over an uranium/aluminum (U-Al_x) alloy. The maximum fuel mass for the MIT assembly is 514.25 grams of U-235 with an enrichment of 93.5 weight percent and one weight percent of U-234. The aluminum present in the U-Al_x alloy is 30.5 weight percent. The U-Al_x alloy has a significant void volume if distributed over the maximum dimensions, and thus can become

APPENDIX C: Sample Application of the Methodology to DOE SNF

waterlogged with a resultant increase in reactivity. The maximum void volume fraction in the fuel alloy is $0.6353 \text{ }^{\text{C-1}}$, so that a considerable amount of water moderator can occupy the interstices of the fuel alloy.

The ORR fuel element is constructed from 19 curved fuel plates which are held within two opposing aluminum comb plates. The ORR fuel length values used in these analyses are shorter than the original as-built length of the ORR assembly because the top and bottom ends of the assembly, which do not contain uranium materials, have been removed by cutting. The fuel plates consist of an aluminum cladding over an U-Si-Al fuel material. The maximum fuel mass for the ORR assembly is 347 grams of U-235 with an enrichment of 20.56 weight percent. The uranium present in the U-Si-Al alloy is 77.5 weight percent. There are 2 atoms of Si per 3 atoms of U, and Al fills out the bulk of the fuel material. The U-Si-Al has a significant void volume if distributed over the maximum dimensions, and thus can become waterlogged with a resultant increase in reactivity. The maximum void volume fraction in the material is $0.4064 \text{ }^{\text{C-1}}$, so that a considerable amount of water moderator can occupy the interstices of the fuel alloy.

1.2 Design Concepts Considered

The internal criticality control design concepts considered were all those considered for commercial SNF, as outlined in Appendix B, except for flux traps and rod consolidation. The flux traps were rejected because the performance degrades as the structure degrades; rod consolidation was rejected because the fuel consists of plates which have much less consolidation potential than the rod-type commercial SNF, for which the decision against consolidation has already been made.

1.3 Selected Criticality Control Concept

Analyses thus far ^{C-1} suggest that the most appropriate criticality control concept is borated stainless steel plates between fuel assemblies. As will be seen from the criticality calculations presented in Section 3, below, the high enrichment of the MIT SNF requires the borated plates between all assemblies, while the lower enrichment of ORR SNF enables a package with fewer borated plates, thereby decreasing the cost and complexity of the package. The locations of the required plates is described in Section 1.4, below.

APPENDIX C: Sample Application of the Methodology to DOE SNF

In addition to the borated stainless steel plates, there is an implicit criticality control measure: limitation of the fissile/fissionable mass per waste package. In the present waste package designs this limitation is imposed primarily by the space available for DOE SNF in the codisposal package (defined in Section 1.4, below) in which over half of the package volume is taken up by HLW glass.

1.4 Waste Package Description

The codisposal waste package design concept begins with a container loaded with 5 pour canisters (3 meters long and 30.5 cm radius) of HLW glass. The stainless steel canister containing the DOE SNF assemblies is placed in the center. This canister has an inner radius of 20.5 cm and is 1.5 cm thick; it is approximately 3 meters long. For MIT SNF the loaded canister has a cross section of 16 assemblies which are stacked in 4 axial layers, resulting in a total of approximately 33 kg of U-235 per waste package. For ORR SNF there are only 10 assemblies in cross section, also stacked in 4 axial layers, resulting in a total of only 14 kg of U-235.

The MIT SNF assemblies of nearly rhomboidal cross section are placed in a basket of 5 rows (which are actually parallelogram shaped slots to accommodate adjacent rhomboidal assemblies), the inner three rows holding 4 assemblies each and the outer two rows with 2 assemblies each. This structure is supported by carbon steel. The criticality control is provided by four sets of stainless steel/boron plates: 1) two plates between the three inner rows of assemblies, 2) two shorter plates on the inside of the two outer rows, 3) short plates between the assemblies in each row, and 4) three disk shaped separator plates between the four axial layers of assemblies. The cross section of this arrangement is shown in Figure 6.3.1-1 of Reference C-1.

The ORR conceptual basket design consists of ten square tubes (5.0 mm wall thickness) aligned so that straight structural load paths progress from one side of the basket to the other (in contrast to the zig-zag necessary to accommodate the rhomboidal shaped MIT SNF). Because of the low enrichment (relative to the MIT SNF) there is no need for axial borated steel plates (the first three types described for the MIT SNF in the previous paragraph). However, the criticality analysis shows a need for a small amount of neutron absorber which can be provided by three disk shaped separator plates (type 4 of the plate types described for the MIT SNF in the previous paragraph). The cross section of this arrangement is shown in Figure 6.3.2-1 of Reference C-1.

APPENDIX C: Sample Application of the Methodology to DOE SNF

2.0 Degradation Scenario Leading to Potentially Critical Configuration

The MIT and ORR fuel would be expected to degrade through oxidation within a few hundred years of breach of the DOE SNF canister. Uranium and aluminum oxides in water have been observed to form hydrates with a gel-like appearance and an effective solid density as low as 10%. Both flocculent and gel-like forms of aluminum have been observed in association with test coupons at SRS. The formation of these hydrated oxides has not been quantified and is not well understood. As a result, the Al-based fuel forms were assumed to degrade to a mix of hydrated Al and U oxides in water within the limits of the available volume as a bounding condition. The hydrated oxides in water mix is approximated by homogenizing the Al-based fuel and water into the basket cell resulting in a solids density of down to 35% in this analysis.

This homogenized mixture is conservative by contrast with the more likely configuration in which the fuel degradation particulates settle to the bottom of each cell.

APPENDIX C: Sample Application of the Methodology to DOE SNF

3.0 Sample Criticality Evaluations

This chapter presents the criticality results which demonstrate the sufficiency of the two criticality designs with respect to the possibility of criticality while the waste form is completely intact, or if it degrades according to the scenario described in Section 2.0, above. These results are a summarization of the criticality results in Reference C-1, which, in turn, are a summarization of the detailed calculations described in Reference C-2.

The criticality calculations used the enrichment values of the fresh fuel and took no credit for the neutron absorber fission products or actinides. This strategy was followed for two reasons: 1) it is conservative; and 2) for most of the research reactor fuel the documentation of the burnup of individual assemblies is believed to be of insufficient quality to support NRC granting of burnup credit.

As a further conservatism, the use of neutron absorber materials in transport packages is limited to a 75% credit for the minimum boron content of the absorber panels in lieu of 100% inspection of the absorber panels with a neutron transmission test. A similar design practice has been established for disposal, and the criticality analyses of this report use the 75% value.

The k_{eff} values listed in the tables of this section were determined from the output of MCNP4A ^{C-3} plus two sigma plus the 0.02 bias allowance defined in Section 5.1 of Reference C-1.

3.1 MIT SNF Criticality

The criticality of MIT SNF was evaluated for both the intact waste form and for the waste form degraded but still remaining in the SNF canister, as described in Section 2.0, above.

3.1.1 MIT SNF Intact Criticality

Results obtained in Reference C-2 for the MIT fuel in the intact configuration are provided in Table C-1. The intact configuration was evaluated for varying amounts of water moderator by varying the density of H₂O from zero to 100 percent (one gram per cubic centimeter density) in the maximum potential void volume within the fuel alloy. These calculations showed that the maximum reactivity is reached when the fuel alloy is waterlogged to the maximum extent.

APPENDIX C: Sample Application of the Methodology to DOE SNF

Table C-1. Intact MIT SNF Codisposal Canister Criticality Results

Case Name	Percent H ₂ O* in Fuel Alloy	k-calculated	sigma	k _{eff}
MITA	0	0.81181	0.00116	0.83413
MITD	25	0.83265	0.00138	0.85541
MITC	50	0.84897	0.00147	0.87191
MITE	75	0.86581	0.00150	0.88881
MITF	95	0.87857	0.00151	0.90159
MITB	100	0.88019	0.00138	0.90295

* Percentage of a maximum of 63.53 volume percent water in fuel matrix voids.

Results in Table C-1 are TBV.

3.1.2 Degraded MIT SNF Within Canister

The criticality calculations for the degraded states of the MIT SNF are documented in Reference C-2 and summarized in Table C-2. The degraded states of the MIT fuel, within the codisposal canister that are evaluated herein, are described in Section 2.0 of this appendix. MCNP calculations evaluated the reactivity of the MIT fuel as it degrades by modeling the fuel material and moderator within the codisposal basket components in successive stages of degradation. The first set of calculations, cases MITH through MITK1, show that the reactivity of the fuel is excessive if stainless steel alone is used to separate adjacent assemblies within a basket slot. The second set of calculations, cases MITL through MITO, evaluate the fuel and codisposal basket with separator plates fabricated from stainless steel/boron alloy. (SS316B2A with 0.60 wt% boron was used in the analyses, SS316B3A with nominally 0.87 wt% boron would be needed to account for 75% effectiveness of the panel without testing as described in Section 3.) In all of these cases, k_{eff} remains below the 0.95 limit.

APPENDIX C: Sample Application of the Methodology to DOE SNF

Table C-2. Degraded MIT SNF Codisposal Canister Criticality Results

Case Name	Divider Plates Between Asbls	Degraded Fuel Geometry	k-calculated	sigma	k _{eff}
MITH	Stainless	Plate Array with Comb Teeth in Asbl. Envelope	0.92513	0.00170	0.94853
MITI	Stainless	Plate Array Homogenized	0.95879	0.00119	0.98117
MITJ	Stainless	Entire Assembly (including Side Plates)	0.95779	0.00133	0.98045
MITK	Stainless	Entire Cell Homogenized	0.99362	0.00128	1.01618
MITK1	Stainless	High Boron in Divider Plates	0.95003	0.00153	0.97309
MITL	SS316B2A	Plate Array with Comb Teeth in Asbl. Envelope	0.85351	0.00158	0.87667
MITM	SS316B2A	Plate Array Homogenized	0.88749	0.00130	0.91009
MITN	SS316B2A	Entire Assembly (including Side Plates)	0.88015	0.00154	0.90323
MITO	SS316B2A	Entire Cell Homogenized	0.91557	0.00149	0.93855

Results in Table C-2 are TBV.

3.2 ORR SNF Criticality

The criticality of ORR SNF was evaluated for both the intact waste form and for the waste form degraded but still remaining in the SNF canister, as described in Section 2.0, above.

3.2.1 ORR SNF Intact criticality

The criticality calculations shown in Table C-3 below from Reference C-2 show that, due to the lower initial enrichment (only 20.56%) the ORR fuel remains subcritical regardless of the amount of water that intrudes into the fuel alloy. This is in spite of the lack of boron neutron absorber material within the basket structure in the radial direction. (Axial separators of stainless steel/boron were provided similar to those incorporated into the MIT SNF codisposal basket.)

APPENDIX C: Sample Application of the Methodology to DOE SNF

Table C-3. Intact ORR Codisposal Canister Criticality Results

Case Name	Percent H ₂ O* in Fuel Alloy	k-calculated	sigma	k _{eff}
ORR10E	0	0.84474	0.00147	0.86768
ORR10G	25	0.85567	0.00150	0.87867
ORR10H	50	0.85998	0.00154	0.88306
ORR10I	75	0.87018	0.00158	0.89334
ORR10J	95	0.87422	0.00146	0.89714
ORR10F	100	0.87446	0.00139	0.89724

* Percentage of maximum of 40.64 volume percent water in fuel matrix voids

Results in Table C-3 are TBV.

3.2.2 Degraded ORR SNF Within Canister

The calculations for the degraded ORR fuel, contained within the codisposal canister, for the various degradation stages described in Section 2.0, are presented below in Table C-4. These calculations evaluate the reactivity of the ORR fuel as it degrades by modeling the fuel material and moderator with the codisposal basket components in successive stages. The first set of calculations, cases ORRHASBL and ORRHSAB1, show that the reactivity of the fuel is excessive if the four layers of assemblies are stacked within each basket tube directly on top of one another. The second set of calculations, cases ORR1 and ORR2, evaluate the fuel and codisposal basket with axial separator plates fabricated from stainless steel/boron alloy SS316B2A. This analysis demonstrates the need for neutron-absorbing materials in the ORR axial separator plates.

APPENDIX C: Sample Application of the Methodology to DOE SNF

Table C-4. Degraded ORR Codisposal Canister Criticality Results

No Boron		k-calculated	sigma	k_{eff}
ORRHASBL	Homogenized Assembly	0.92887	0.00149	0.95185
ORRHSAB1	Homogenized Water Gap	0.94404	0.00148	0.96700
Axial SS/Boron Separator Plates				
ORR1	Homogenized Assembly	0.86127	0.00142	0.88411
ORR2	Homogenized Water Gap	0.88901	0.00140	0.91181

Results in Table C-4 are TBV.

APPENDIX C: Sample Application of the Methodology to DOE SNF

4.0 Conclusions

These designs are based on the limited degradation within the DOE SNF canister only. Several mechanisms must be evaluated with respect to the possible accumulation of a critical mass outside of the SNF canister, particularly inside the package itself or outside of the package yet remaining in the drift. If it turns out that there is a credible probability of accumulating a critical mass, and sufficient moderator, then additional criticality control measures may be needed. Two likely candidates are: 1) addition of depleted uranium (either as waste package filler or as material in the invert), or 2) reducing the fissile content per waste package.

APPENDIX C: Sample Application of the Methodology to DOE SNF

5.0 References

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APPENDIX C: Sample Application of the Methodology to DOE SNF

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