Yucca Mountain Project

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TOPICAL REPORT

YMP/TR-004Q

Revision 02

November 2003

U.S. Department of Energy
Office of Civilian Radioactive Waste Management
Las Vegas, Nevada

INTENTIONALLY LEFT BLANK

Preparation:

11/5/03

Joseph D. Ziegler
Director, Office of License Application and Strategy

Date

Approval:

11/5/03

W. John Arthur III
Deputy Director, Office of Repository Development

Date

R Dennis Brown

11/5/03

R. Dennis Brown
Director, Office of Quality Assurance

Date

Originator:

John A McClure

11/03/2003

John A. McClure
Engineered Systems - Risk and Criticality

Date

Checker:

FOR CWM

11/03/2003

Claude W. Mays
Engineered Systems - Risk and Criticality

Date

Quality Engineering Representative:

11/03/2003

Darrell K. Svalstad
Quality Assurance – Quality Engineering – Science Projects

Date

Responsible Manager:

11/3/03

Robert W. Andrews
Acting Manager, Engineered Systems

Date

INTENTIONALLY LEFT BLANK

CHANGE HISTORY

REV. NO.	ICN NO.	EFFECTIVE DATE	DESCRIPTION OF CHANGE
00	00	11/30/1998	Initial issue
01	00	11/16/2000	Revisions to incorporate commitments made in answering NRC requests for additional information, addressing open items from the Safety Evaluation Report for Revision 0 of the Topical Report, and providing updates to the methodology. Former Chapters 3 and 4 have been combined and reordered. Appendices C and D have been removed.
02	00	11/05/2003	Complete revision to update the approach used in the methodology to maintain consistency with NRC's 10 CFR Part 63 final rule and current model validation reports. Revision 02 supercedes and replaces all prior revisions of this document, i.e., Revisions 00 and 01.

INTENTIONALLY LEFT BLANK

ABSTRACT

This topical report describes the approach to the risk-informed, performance-based methodology to be used for performing postclosure criticality analyses for waste forms in the Monitored Geologic Repository at Yucca Mountain, Nevada. The risk-informed, performance-based methodology will be used during the licensing process to demonstrate how the potential for postclosure criticality will be limited and to demonstrate that public health and safety are protected against postclosure criticality. The report describes the overall approach used in the methodology, presents performance criteria, and describes the general criticality scenarios. The details of the methodology and modeling approach are documented in separate model reports. The overall validation methods employed for the methods and models used for determining critical configurations, evaluating criticality, estimating probabilities, estimating criticality consequences, and estimating criticality risk are described in this report with the details included in the individual model reports.

The disposal criticality analysis methodology provides a systematic means for evaluating the following through the entire postclosure period of the repository.

(1) The combined system of a waste form, waste package, engineered barrier, and repository for effectiveness in limiting the potential for criticality in the repository

(2) The consequences of any such criticalities

(3) The impact of any consequences on the regulatory performance objectives for the repository.

The design parameters and environment within which the waste forms will reside are currently not fully established and will vary with the detailed waste package design, engineered barrier design, repository design, and repository layout. Therefore, it is not practical to present the full validation of the methodology in this report. The methodology will be fully developed and validated for design applications to which it will be applied for the repository License Application and applicable documents developed in support of licensing activities.

Revision 02 of the topical report was undertaken to incorporate the licensing requirements for disposal of spent nuclear fuel and high-level radioactive wastes in geologic repository at Yucca Mountain identified in the U.S. Nuclear Regulatory Commission's 10 CFR Part 63 rule *Disposal of High-Level Radioactive Wastes in a Proposed Geologic Repository at Yucca Mountain, Nevada*, revisit *Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report*[1] open items addressed in Revision 01, and to update the documentation of the approach used in the disposal criticality methodology. The U.S. Department of Energy will use the accepted methodology in reports developed in support of licensing activities for the Monitored Geologic Repository at Yucca Mountain, Nevada, to demonstrate the acceptability of proposed systems for limiting the potential for postclosure criticality.

[1] Reamer, C.W. 2000. "Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0." Letter from C.W. Reamer (NRC) to S.J. Brocoum (DOE/YMSCO), June 26, 2000, with enclosure. ACC: MOL.20000919.0157.

Any sample results presented in this report that were derived from analyses based on specific features of the repository design or performance, which may be subject to change, should not be taken as final. Such sample results are, however, consistent with the present state of knowledge on this subject and neither the analyses nor the sample results are expected to change significantly.

CONTENTS

Page

FIGURES

Page

TABLES

Page

INTENTIONALLY LEFT BLANK

1. INTRODUCTION

The U.S. Congress charged the U.S. Department of Energy (DOE) with managing the geologic disposal of high-level radioactive waste and spent nuclear fuel (SNF) through the Nuclear Waste Policy Act of 1982 and the Nuclear Waste Policy Amendments Act of 1987. An important objective of geologic disposal is keeping the fissionable material in a condition such that there is limited potential for a self-sustaining nuclear chain reaction (criticality) to occur in the disposal site.

This report describes the approach used in the methodology for evaluating the criticality potential for SNF[2] and high-level radioactive waste (HLW), referred to collectively as the waste form, after the Monitored Geological Repository (repository) is sealed and permanently closed (postclosure phase). This report focuses on providing an overview (i.e., approach) of the methodology and the models that are an integral part of it. The criticality-related model development and validation activity planned for use in support of the licensing activities for the repository at Yucca Mountain, Nevada, will follow the methodology approach described in this report. Details of the models (i.e., methodology) and their validation activities will be documented in separate reports.

In addition to this chapter, which presents the background, objective, scope, and quality assurance controls, the report is divided into four other chapters. Chapter 2 discusses applicable U.S. Nuclear Regulatory Commission (NRC) regulations and addresses the regulatory framework within which the topical report is developed. NRC guidance documents and industry standards used in developing the approach used in the methodology are also discussed.

Chapter 3 describes the disposal criticality analysis methodology approach. This description includes the approach for building hypothetical scenarios that lead to degraded configurations, defining parameters for such configurations, evaluating criticality potential of the configurations for the applicable range of parameters, and estimating the probability of achieving critical configurations. The approach used in the methodology for estimating configuration reactivities and evaluating consequences of potential criticalities is also provided. The chapter concludes by discussing the process for combining probability and consequence estimates with total system performance assessment (TSPA) radionuclide transport modeling to obtain an estimate of the overall risk, which is determined, in part, by the calculated annual dose received in the accessible environment due to the combined nominal radionuclide source and probability weighted incremental source from potential criticalities. The modeling and validation approaches for the analysis models are discussed for each analysis component of the criticality analysis methodology.

[2] The approach used in the methodology presented in this report will be applied to commercial SNF [including pressurized water reactor, boiling water reactor, and mixed oxide fuels], U.S. Department of Energy SNF, and vitrified HLW. The methodology used for criticality analyses for naval SNF in the disposal container prior to container degradation and for naval SNF after container degradation, but before the loss of cladding integrity and fission product and uranium release is described in "Transmittal of the Naval Nuclear Propulsion Program Addendum to the Yucca Mountain Site Characterization Office 'Disposal Criticality Analysis Methodology Topical Report'" (Mowbray 1999).

Chapter 4 summarizes the methodology approach presented and provides conclusions regarding the purpose, potential uses, and limitations on its use. Chapter 5 lists the document references. Listings of acronyms and abbreviations are presented in Appendix A. A glossary of terms used in the report is provided in Appendix B.

1.1 BACKGROUND

This report describes the process and analytical tools planned for use in evaluating the acceptability of natural and engineered systems for limiting the potential for, and any subsequent consequences of, postclosure criticality in the repository. The risk-informed, performance-based methodology approach presented in this report is consistent with the regulatory requirements for disposal of spent nuclear fuel and high-level radioactive wastes in geologic repository at Yucca Mountain, Nevada (10 CFR Part 63). The regulatory requirements include, among other things, the 10 CFR Part 63 regulatory performance objectives of the repository at Yucca Mountain prior to closure and during postclosure. Requirements for the overall postclosure performance of the repository in 10 CFR 63.113 include the use of multiple barriers, limits on the expected annual dose to the reasonably maximally exposed individual, limits on the release of radionuclides to the accessible environment, and a limit on individual radiological exposures in the event of human intrusion. There are no specific design criteria for postclosure criticality control in 10 CFR Part 63. These requirements are consistent with a risk-informed, performance-based regulation, which treats criticality as one of the features, events, and processes (FEP) that must be considered for the overall system performance assessment.

Features are defined as topographic, stratigraphic, physical, or chemical characteristics of the site. They may influence the configuration parameters, and thereby influence outcome of the criticality analysis. Examples of features are faults that may focus or block the flow of groundwater, or topographic lows in geologic strata that may provide locations where fissionable solutes can accumulate. Processes are natural or anthropogenic phenomena that have potential to affect a disposal system performance and that operate during all or a significant part of the period of performance. Examples of processes include groundwater flow, corrosion, and precipitation. Events are similar to processes, but have a short duration compared to the period of performance. Events can possibly have a more disruptive effect on the emplaced material than processes. Examples of events would be the sudden collapse of a basket due to the corrosion of structural members, seismic events, or rock-fall onto a waste package.

Limiting the potential for criticality (as well as any subsequent consequences) during the postclosure phase of the repository relies on multiple barriers, both natural and engineered. The natural barrier system consists of the rock formations and the climate around the repository, and includes the geologic, mechanical, chemical, and hydrological properties of the site. As defined within 10 CFR 63.2, the engineered barrier system is comprised of the waste packages and the underground facility in which they are emplaced. A waste package is the generic term for describing the waste form (radioactive waste and any encapsulating or stabilizing matrix) and any containers, shielding, packing, or other neutron absorbent materials immediately surrounding an individual package. The underground facility consists of the underground structure and openings that penetrate the underground structure (e.g., ramps, shafts, and boreholes, including their seals). The engineered barrier system will work in concert with the natural barrier system to minimize the potential for conditions that would be conducive to a criticality event after the repository has been permanently closed.

The design for the repository will incorporate multiple barriers that are both redundant and diverse to minimize the potential for conditions conducive to criticality. This is referred to as the defense-in-depth concept; should one system fail, another exists to provide adequate protection. Separate barriers that act to isolate the fissionable material from water (moderator) accumulation and/or contact provide an example of redundant barriers. SNF with fuel pin cladding within waste packages designed with an outer corrosion-resistant barrier and covered by a drip shield provides such a function. The combination of a barrier that impedes or limits the amount of water ingress into a waste package and a barrier that contains neutron-absorbing materials provides diverse barriers (e.g., borated stainless steel plates inside the waste package absorb neutrons while the waste package prevents water from entering the waste package).

The purpose of analyzing the potential for criticality of waste forms is to estimate the effectiveness of measures implemented before closure of the repository designed to minimize the criticality potential of waste forms. These measures must maintain their effectiveness over thousands of years as the waste package/waste form configurations change due to degradation as the environment changes in the repository.

This type of analysis differs from conventional analyses for criticality. The primary differences result from the nature and timing of events that may lead to criticality. For conventional criticality analysis, the events are primarily attributed to short-term equipment failure and human error. However, the events in the repository that may lead to a criticality are related to both short term and long-term processes. Short-term effects (e.g., human error during the preclosure period) can exacerbate long-term effects (e.g., corrosion) that influence potential criticalities.

The approach to the methodology described in this report addresses the design features of the engineered barrier system and how various processes in the repository (e.g., groundwater flow and corrosion) affect these features. The principal components of the engineered barrier system are the waste packages, which are designed to preclude criticality occurring in sealed, undamaged packages. During design, criticality analyses will be performed to demonstrate that the initial emplaced configuration of the waste form will remain subcritical even under flooded conditions. Therefore, for criticality to occur, a waste package must fail (barriers breached), the materials inside the package must degrade, the absorber material must either be lost or become ineffective, and for thermal systems, moderator material must accumulate within the waste package.

Deterministic analyses are used to evaluate the various long-term processes, the combination of events, and any potential criticality. Similarly, the analysis of any potential consequence resulting from a criticality (e.g., increase in radionuclide inventory) is a deterministic analysis. However, it is not possible to state with certainty what will actually happen, which events will occur, and what actual values the parameters will have, so the individual deterministic calculations must be applied in a probabilistic context. In addition, the potential for criticality is related to various processes and events that take place over long periods of time and have associated uncertainties that must be considered. Therefore, establishing the likelihood of a criticality occurring involves probabilistic analyses. Hence, the disposal criticality analysis methodology is a blend of deterministic and probabilistic aspects.

The consequence of a potential criticality along with the probability of occurrence is used in establishing the risk to the health and safety of the public from the release of radioactive material. This approach treats postclosure criticality as a disruptive event or process in the performance assessment conducted for the repository at Yucca Mountain.

As previously stated, the risk-informed, performance-based methodology approach presented in this topical report is consistent with the regulatory requirements for disposal of spent nuclear fuel and high-level radioactive wastes in a geologic repository as promulgated in 10 CFR Part 63. The existing regulations are discussed in further detail in Chapter 2 of this report.

1.2 OBJECTIVE

The objectives of this topical report are to present the principles of the risk-informed, performance-based disposal criticality analysis methodology approach to the NRC, identify those parts of the approach previously accepted, and to seek acceptance of the remaining aspects of the approach. The methodology and applications will be discussed in detail in model and analysis reports developed in support of licensing activities.

For certain fuel types, any processes, criteria, codes or methods different from those presented in this report will be described in separate addenda (e.g., Mowbray 1999 [for Naval Nuclear Propulsion Project SNF]). These addenda will employ the principles of the methodology approach described in this report as a foundation. Departures from the specifics of the approach used in the methodology presented herein will be described in the addenda.

This topical report discusses the following aspects of the approach used in the methodology for performing criticality analyses for the geologic disposal of the waste forms and seeks acceptance of those parts not previously accepted in *Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0* (Reamer 2000b).

A. The following performance criteria presented in Figure 3-1 (discussed in Sections 3.1 and 3.2) are acceptable for ensuring that design options are properly implemented for minimizing the potential for, and subsequent postulated consequences of, criticality:

   1. The *Probability Screening Criterion* discussed in Section 3.2.1: The probability screening criterion is defined to be well below (a minimum of two orders of magnitude) the 10 CFR 63.114(d) probability criterion for exclusion of events from TSPA that is one chance in 10,000 of an (criticality) event occurring in the repository over 10,000 years. This screening level is set such that, if satisfied, no single configuration class would be a significant contributor to the total probability of criticality for the repository.

   2. The *Criticality Potential Criterion* discussed in Section 3.2.2: The maximum calculated effective neutron multiplication factor (k_{eff}) for subcritical systems (configuration classes) for postclosure will be less than the critical limit. The critical limit is the value of k_{eff} at which the system is considered potentially critical as

characterized by all the appropriate biases and associated uncertainties for each internal and external configuration class analyzed for the repository. Configuration classes satisfying this criterion have an insignificant potential for criticality and can be excluded from further consideration. (accepted subject to implementation, [Reamer 2000b, Section 3.2.1])

3. The *Design Probability Criterion* discussed in Section 3.2.3: The probability of one criticality occurring will be less than one over the entire repository for the first 10,000 years. This probability includes all combinations of waste packages and waste forms. This probability criterion is used to define a waste package criticality control limit in support of defense-in-depth with respect to the repository criticality performance objectives discussed in Section 2.2.2. If the calculated probability of criticality exceeds this design criterion, implementation of criticality mitigating strategies will be required. (self-imposed criterion, no NRC objections to its use [Reamer 2000b, Section 3.2.3])

B. The list of Master Scenarios, presented in Section 3.3 and summarized in Figures 3-2a, 3–2b, 3-3a, and 3-3b, comprehensively identifies degradation scenarios associated with the repository at Yucca Mountain that may significantly affect the potential for, and the subsequent postulated consequences of, criticality. The degradation processes of interest for criticality are related to a combination of FEPs that result in configuration classes that have the potential for criticality requiring further evaluation of this potential. Generic degradation scenarios and potential critical configuration classes have been identified by considering the features of the site and the characteristics of the waste form and other waste package internal components. Potential critical configuration classes are states of a degraded waste package defined by a set of parameters characterizing the quantity and physical arrangement of the materials that have a significant effect on criticality. (Internal Criticality Scenarios accepted subject a proviso on seismic events [Reamer 2000b, Section 3.3.1], External Criticality Scenarios accepted subject to contingencies [Reamer 2000b, Section 3.3.2])

C. The portion of the approach used in the methodology for developing internal and external configurations discussed in Section 3.4 is acceptable in general for developing a comprehensive set of potentially critical postclosure configurations for disposal criticality analysis. Acceptance is sought for the part of the methodology approach, described in Sections 3.4.1.1 and 3.4.2.1, for evaluating the parameter ranges of configuration classes over the range of environmental conditions currently postulated for the repository at Yucca Mountain. Specifically, the 14 steps in the approach specified for internal configurations in Section 3.4.1.1 and the five steps in the approach specified for external configurations in Section 3.4.2.1 are acceptable and sufficiently comprehensive. (degradation approach provisionally accepted for internal configurations, [Reamer 2000b, Section 3.4.1.1], accumulation approach accepted for external configurations [Reamer 2000b, Section 3.4.2.1]).

D. The methodology approach based upon event tree/fault tree sequences for estimating the probability of postclosure critical configuration classes discussed in Section 3.6 is acceptable in general for disposal criticality analysis. The applicability of the method for postclosure conditions in the repository will be demonstrated in model reports that will be developed in support of licensing activities. NRC acceptance of probability values for the occurrence of critical configurations over the period of regulatory concern obtained from the model and their applicability for postulated postclosure conditions will be sought in analyses developed in support of licensing activities.

E. The portion of the approach used in the methodology for estimating consequences of potential postclosure criticality events (as discussed in Section 3.7) is acceptable in general for disposal criticality analysis. Specifically, that technical reviews of the consequence models and, as available, comparisons of specific experimental results with simulation results are sufficient to demonstrate the acceptability of the criticality consequence models for postulated internal and external criticality and for transient as well as for steady-state criticality events.

F. The methodology approach for the isotopic and criticality models is acceptable in general for disposal criticality analysis. Specifically:

1. For commercial SNF, acceptance is sought for use the reduced reactivity (burnup credit) associated with the net depletion of fissile isotopes and the creation of neutron-absorbing isotopes during reactor operations as discussed in Sections 3.5.1 and 3.5.2. Acceptance is sought for the use of the principal isotope selection process for burnup credit in criticality analyses of intact commercial SNF discussed in Section 3.5.2.1.1.

2. The approach to the methodology described in Section 3.5.3.1 for the isotopic model is acceptable for establishing the isotopic bias in k_{eff} to be used for commercial spent nuclear fuel burnup credit. The applicability of this bias in critical limit values for postulated postclosure conditions in the repository will be demonstrated in model reports that will be developed in support of licensing activities. NRC acceptance of isotopic bias and uncertainty values for k_{eff} and their applicability for postclosure conditions will be sought in analyses supporting the licensing activities. (approach for evaluating the uncertainties associated with isotopic decay and branching ratios provisionally accepted for internal and external waste forms [Reamer 2000b, Section 3.5.3.1])

3. The approach to criticality modeling process described in Section 3.5.3.2 is acceptable in general for disposal criticality analysis. Specifically, the process presented for calculating the critical limit values and the process presented for establishing the Range of Applicability of the critical limit values is acceptable. This process will be followed to calculate critical limit values and/or functions for specific waste forms and waste packages as a function of degradation conditions. The applicability of the critical limit values for postulated postclosure conditions in the repository will be demonstrated in model reports that will be developed in support of licensing activities. NRC acceptance of critical limit values and their applicability for postclosure repository conditions will be sought in analyses supporting licensing activities. (k_{eff} evaluation approach provisionally accepted for internal and external waste forms [Reamer 2000b, Section 3.5.2.2])

4. The approaches for estimating the bias and uncertainty in the critical limit calculation and establishing the lower bound tolerance limit functions for a waste form discussed in Section 3.5.3.2 are acceptable. (approach to evaluating the statistical uncertainty portion of Δk_c accepted subject to contingencies [Reamer 2000b, Section 3.5.3.2])

G. The methodology approach for the degradation and release model and the external accumulation model (as presented in Sections 3.4.1.3 and 3.4.2.3) is acceptable in general for disposal criticality analysis. (degradation approach provisionally accepted for internal configurations, [Reamer 2000b, Section 3.4.1.1], accumulation approach accepted for external configurations [Reamer 2000b, Section 3.4.2.1])

H. The proposed requirements presented in Section 3.5.3.1.2 for modeling burnup of commercial SNF for design applications are sufficient to ensure adequate conservatism in the isotopic concentrations used for burnup credit. These requirements describe acceptance criteria for confirmation of this conservatism. The confirmation of the conservatism in the application model used for burnup credit for commercial SNF will be demonstrated in model reports that will be developed in support of licensing activities. NRC acceptance of the confirmation of the conservatism in the application model for postulated postclosure conditions in the repository will be deferred until required for the License Application process.

I. The approach for selecting principal isotopes to model burnup in intact (non-leakage) commercial SNF, resulting in the set presented in Table 3-1 (Section 3.5.2.1.1), is acceptable for disposal criticality analysis provided that the bias in k_{eff} associated with predicting the isotopic concentrations is established in the model reports as described in Section 3.5.3.1. The applicability of the principal isotopes selected for intact commercial SNF will be demonstrated in model reports that will be developed in support of licensing activities.

   The k_{eff} values from criticality evaluations of breached commercial SNF will reflect both the isotopic bias in k_{eff} established from radiochemical assay analysis and the changes in the principal isotope concentrations established by the geochemical analysis.

J. The selection process for identifying isotopes from the list of principal isotopes for degraded commercial SNF presented in Section 3.5.2.1.5 is acceptable for disposal criticality analysis. The applicability of isotopes selected from the list of principal isotopes for degraded commercial SNF configurations will be demonstrated in model reports that will be developed in support of licensing activities. NRC acceptance of the use of selected isotopes in postulated postclosure conditions in the repository will be sought in activities supporting the licensing process.

K. Verified burnup values are recorded for each commercial nuclear fuel assembly in reactor records kept by each utility. Consistent with other NRC regulated operations, DOE is seeking acceptance for using reactor records as the primary basis for commercial nuclear fuel assembly burnup values to be used for disposal criticality analyses with on-site measurements required only under special circumstances. Uncertainties in burnup values will be addressed in applications of the criticality methodology. Acceptance is sought that the requirements discussed in Section 3.5.3.1 are sufficient to ensure adequate conservatism in the isotopic model for burnup credit.

The methodology approach outlined above will be used for the following waste forms: commercial SNF, DOE SNF, and vitrified HLW with the exception of the determination of isotopic inventories and burnup credit which is inappropriate for DOE SNF and vitrified HLW.

1.3 SCOPE

Waste packages for the repository are designed such that criticality is precluded for undegraded configurations, even under flooded conditions. This report describes the approach used in the methodology for estimating the potential for postclosure criticality events under degraded conditions and their subsequent consequences. The approach makes use of various processes and tools for identifying potentially critical configurations (including probability of occurrence), calculating the configuration reactivity, estimating the direct consequences of potential criticality events, and evaluating the risk of any potential criticalities (in terms of risk relative to dose at the accessible environment). The methodology provides a means to evaluate potential postclosure criticality events for the full range of waste form conditions (intact, degraded, and degradation products), for postulated conditions of impairment to the engineered systems (waste package and other engineered barriers), and for the range of possible locations (in-package, near-field, and far-field).

A brief overview of the methodology is presented in Figure 3-1 and discussed in Section 3.1 of this report. Section 3.2 presents performance criteria imposed to ensure appropriate criticality controls are implemented in the waste package design. A standard set of degradation scenarios that may lead to configurations of material with the potential for criticality is presented in Section 3.3. A detailed description of the criticality analysis methodology approach is presented in Sections 3.4 through 3.8.

The analytical tools are the models developed to implement the approach used in the methodology. These models include degradation analysis, neutronic analysis, probability estimation, consequence estimation of any potential criticality, and TSPA dose estimation at the accessible environment. The modeling approach and the validation approach for these analysis models are also presented in Sections 3.4 through 3.8 of this report. The process described will be followed for model validation and documented in model reports that will be developed in support of licensing activities. Because of their classified nature, analytical models for the Naval Nuclear Propulsion Program are described in "Transmittal of the Naval Nuclear Propulsion Program Addendum to the Yucca Mountain Site Characterization Office 'Disposal Criticality Analysis Methodology Topical Report'" (Mowbray 1999).

1.4 QUALITY ASSURANCE

The DOE quality assurance program applies to the development of this topical report. The report was prepared in accordance with Office of Civilian Radioactive Waste Management (OCRWM) procedures and *Technical Work Plan for: Risk and Criticality Department* (BSC 2003a, Section 2.1.22). Approved quality assurance procedures identified in the technical work plan (BSC 2003a, Section 3) have been used to conduct and document the activities described in this report. The technical work plan also identifies the methods used to control the electronic management of data (BSC 2003a, Section 8) during the documentation activities. The methodology approach described in this report is related to the evaluation of the repository's engineered barrier system (10 CFR 63.115). Components of the engineered barrier system have been identified as items important to radiological safety and waste isolation in a number of classification analyses (e.g., BSC 2003b, Appendix A).

Any computer software results reported in this topical report are example applications of the methodology developed under this approach and include references to the supporting documents where descriptions of the software, its use, and software control procedures are provided.

Work supporting licensing activities using the methodology developed under this approach will be performed in accordance with current versions of *Quality Assurance Requirements and Description* (DOE 2003) and procedures and with applicable NRC regulatory guidance. Information developed by such work will meet the level of detail and accuracy consistent with Section 2 of *Yucca Mountain Review Plan, Final Report* (NRC 2003).

INTENTIONALLY LEFT BLANK

2. REGULATORY PERSPECTIVE

The purpose of this topical report is to present the approach used in the methodology for analyzing the potential for criticality during the postclosure phase of the repository at Yucca Mountain. This chapter discusses applicable NRC regulations along with the regulatory framework within which the topical report is developed. Application of the methodology will provide input to TSPAs that will determine if the repository will meet its overall postclosure performance objectives (10 CFR 63.113).

This topical report is being submitted in accordance with *Topical Report Review Plan* (Holonich 1994) issued by the NRC Division of High-Level Waste Management. Consistent with the purpose of a topical report as described in that plan, this topical report focuses on the postclosure disposal criticality methodology approach under evaluation during the pre-licensing phase, as applied specifically to the Yucca Mountain site. Those portions of the approach in the topical report accepted by the NRC staff and documented in Safety Evaluation Reports will be used in support of licensing activities for the repository at Yucca Mountain.

The existing disposal criticality regulations and the approach to postclosure criticality analysis are discussed in Sections 2.1 and 2.2, respectively.

Potential criticality during the postclosure period is only one of numerous scenarios that might affect the repository's ability to isolate waste from the accessible environment and protect the health and safety of the public. This topical report, however, only addresses the approach used in the methodology for estimating the likelihood of postclosure criticality events occurring in the repository and the subsequent consequences of any potential criticality events.

Revision 0 of this topical report (YMP 1998) was submitted to the NRC in January 1999. The NRC staff reviewed the document and issued a request for additional information, "*U.S. Nuclear Regulatory Commission Request for Additional Information on the U.S. Department of Energy Topical Report on Disposal Criticality Analysis Methodology*" (Reamer 1999), that contained questions and comments on a number of aspects of the methodology approach as described in the topical report. The DOE responded in writing (Brocoum 1999), providing clarifications and corrections as appropriate to address the NRC questions and comments.

After submittal of the Revision 0 topical report, it became evident that some discussions in Revision 0 of the topical report pertained to applications of the methodology rather than to the approach itself. These aspects of the methodology are more properly addressed in documents supporting licensing activities and were thus removed from the topical report.

The NRC staff reviewed the DOE response and issued "*Draft Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0*" (Reamer 2000a), which stated that the staff accepted certain aspects of the methodology approach (in some cases subject to verification of DOE plans described in its response to the Request for Additional Information). Other aspects of the approach used in the methodology for which the NRC staff believes the DOE has not provided sufficient justification or detailed information were carried as open items.

The NRC and DOE staffs held a technical exchange in March 2000 to discuss the draft safety analysis report (Reamer 2000a). Subsequent to the meeting, the DOE provided comments

(Brocoum 2000) on the NRC's draft safety evaluation report (Reamer 2000a). The NRC then issued their final report, "*Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0*" (Reamer 2000b) for Revision 0 of the topical report. Like the draft safety evaluation report, the final safety evaluation report accepted certain aspects of the methodology approach while leaving other aspects the subject of open items.

For reasons discussed above, and to fully address the NRC request for additional information (Reamer 1999), the DOE agreed to revise the topical report (Reamer and Williams 2000, Attachment 1), which was subsequently reissued as Revision 01, *Disposal Criticality Analysis Methodology Topical Report* (YMP 2000). Revision 02 of the topical report was undertaken to incorporate references to the NRC requirements for disposal of spent nuclear fuel and high-level radioactive wastes in geologic repository at Yucca Mountain, Nevada (10 CFR Part 63), revisit the open items from "Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0" (Reamer 2000b) addressed in Revision 01 of the topical report, and to update documentation of the approach used in the disposal criticality methodology.

2.1 REGULATORY FRAMEWORK

The existing regulations pertinent to the Yucca Mountain Project are promulgated in the NRC final rule 10 CFR Part 63. The regulations focus on risk-informed, performance-based criteria for a Yucca Mountain facility for a definitive measure of repository postclosure performance.

To ensure that the DOE develops and supports a defensible and rigorous performance assessment, 10 CFR 63.114(f) requires the DOE to:

> Provide the technical basis for either inclusion or exclusion of degradation, deterioration, or alteration processes of engineered barriers in the performance assessment, including those processes that would adversely affect the performance of natural barriers. Degradation, deterioration, or alteration processes of engineered barriers must be evaluated in detail if the magnitude and time of the resulting radiological exposures to the reasonably maximally exposed individual, or radionuclide releases to the accessible environment, would be significantly changed by their omission.

Postclosure criticality is an alteration process for the waste form, which, by definition in 10 CFR Part 63, is part of the waste package and thus part of the engineered barriers. Therefore, postclosure criticality is an alteration process of the engineered barriers. It is also potentially a degradation or deterioration process of the engineered barriers (due to the possibility of pressure increases, thermal effects, radiolysis, and possibly other potential effects).

10 CFR 63.102(j), in discussing "concepts" of the performance assessment regulations, states in part:

> The features, events, and processes considered in the performance assessment should represent a wide range of both beneficial and potentially adverse effects on performance (e.g., beneficial effects of radionuclide sorption; potentially adverse effects of fracture flow or a criticality event). Those features, events, and

processes expected to materially affect compliance with § 63.113(b) or be potentially adverse to performance are included, while events (event classes or scenario classes) that are unlikely (less than one chance in 10,000 over 10,000 years) can be excluded from the analysis.

It is expected that the methodology developed under the approach described in this topical report can and will be used to demonstrate that the probability of criticality is very unlikely during the period of regulatory concern. Therefore, it is expected that postclosure criticality events will be screened from further consideration in the nominal scenario for the performance assessment as allowed by 10 CFR Part 63. However, if criticality events cannot be screened from consideration, it is expected that the application of the methodology will be used to demonstrate that the consequences of one or more potential criticalities would have a negligible impact on the radionuclide inventory available as an external source even if such events were to occur.

The approach discussed in this topical report to the disposal criticality analysis methodology is based on risk-informed, performance-based analyses. This approach is fully consistent with 10 CFR Part 63. Revisions to the topical report will be made as necessary to comply with any future revisions to applicable regulatory requirements, conditions of the license, or additional requirements imposed by the applicant.

2.2 USE OF THE CRITICALITY METHODOLOGY APPROACH IN DEMONSTRATING COMPLIANCE

This section discusses the risk-informed approach taken in this topical report to support analyses demonstrating that potential postclosure criticality events will not add any significant risk to the accessible environment by compromising the repository performance objectives (10 CFR 63.113). It also describes in general terms the planned approach to providing defense-in-depth against postclosure criticality.

Approaches to demonstrating that public health and safety are protected against potential hazards posed by nuclear facilities are generally deterministic or probabilistic; criticality safety evaluations for non-reactor facilities in the United States have all been deterministic.

The approach to addressing postclosure criticality described in this topical report is intended to provide a rigorous method of demonstrating that public health and safety are protected against the consequences of any potential postclosure criticality. That approach avoids the drawbacks of the exclusive use of a deterministic approach and is consistent with 10 CFR Part 63. As discussed in the sections that follow, the approach combines probabilistic analysis with defense-in-depth against potential postclosure criticality.

2.2.1 Risk-Informed, Performance-Based Analysis

The analysis methodology approach presented in this topical report does not attempt to support a demonstration that postclosure criticality either will not occur or is totally incredible (that is, guaranteed to have a probability below the threshold of concern). Instead, the approach used in the methodology focuses on evaluation of the probability of occurrence of configurations and, for configurations with potential for criticality, the probability of criticality for those configurations. Additionally, if the total probability of criticality for the repository exceeds the

10 CFR 63.114(d) probability criterion for exclusion of events from TSPA, criticality consequences must be evaluated for those configurations contributing to the potential for criticality. Such consequences are input into an evaluation of the repository performance parameters for assessing compliance with the 10 CFR 63.113 performance objectives. The use of risk-informed, performance-based analyses in regulatory matters is consistent with the NRC policy statement 60 FR 42622. It is likewise consistent with correspondence among the NRC commissioners on risk-informed, performance-based regulation (Jackson 1998).

The analysis methodology is a combination of:

- An evaluation of the probability of occurrence of the various configurations that span the range of possible waste package/waste form configurations
- An evaluation of the probability of criticality for configurations that have potential for criticality
- An estimation of consequences for those potential critical configurations that cannot be screened from further consideration by low probability
- An estimation of the impact on repository performance objectives from any such consequences
- An identification of candidates for additional criticality control measures if the 10 CFR 63.113(b) criteria for risk to the accessible environment cannot be met.

Risk posed by criticality will be determined by analyzing criticality as a potential detractor to the repository's overall performance using the methodology approach described in this report. The probabilities and consequences of potential criticality events will then form a part of the repository performance assessment. Thus, the overall postclosure risk will be evaluated with input from consequence analyses of configurations that have a probability of criticality above the probability screening criterion. Redesign of the waste package/engineered barrier system to mitigate public health and safety risks due to postulated criticality consequences is anticipated only if the estimated overall performance exceeds the regulatory performance objectives[3].

It is recognized that defense-in-depth is needed against criticality events even if the probability of occurrence and subsequent consequences of such events for the repository's performance and for the health and safety of the public would be below regulatory performance objectives. This approach, in combination with other defense-in-depth measures, is expected to allow demonstration that public health and safety are protected against postclosure criticality. The overall approach to defense-in-depth against postclosure criticality is discussed in Section 2.2.2. This approach is called risk-informed because the results of the risk evaluations are used in conjunction with other measures to guide the implementation of defense-in-depth against criticality.

[3] The total probability of all analyzed waste forms is also checked against the self imposed design probability criterion and if the total probability is above the design probability criterion of less than one criticality over 10,000 years, then implementation of criticality mitigation strategies would be necessary.

2.2.2 Defense-in-depth Against Postclosure Criticality

The NRC rule 10 CFR Part 63 captures the concept of defense-in-depth in terms of "multiple, diverse barriers that comprise the engineered and geologic systems." As previously noted, the risk-informed approach to postclosure criticality includes both probabilistic analysis and defense-in-depth. This section discusses the approach to defense-in-depth against postclosure criticality and the role of the disposal criticality analysis methodology in that approach. The approach includes, but is not limited to, the following aspects.

One aspect of the defense-in-depth philosophy involves taking advantage of the many natural and engineered features of the site and repository that contribute to minimizing the probability of postclosure criticality events and subsequent consequences of any such events. For a criticality to occur, multiple changes in conditions must occur (e.g., waste package breach, water intrusion with retention, and removal of neutron absorbers). Should a criticality occur, however, barriers will also protect against its consequences by protecting against release of energy and radionuclides to the accessible environment. The engineered features eventually implemented are expected to provide barriers to postclosure criticality that are both diverse (dissimilar methods to limit susceptibility to common-mode failures) and redundant (multiple barriers performing the same function that reduce the probability of criticality). Examples of diverse barriers are the waste package, neutron-absorbing materials in the basket, and iron based alloys (that, together with their degradation products, displace moderator) in the basket materials. Similarly, the use of two separate barriers (waste package and drip shield) to impede entry of water into the waste form is an example of the use of redundant barriers. The waste package itself impedes entry of water into the waste form locale, and the drip shield limits or prevents damage to the waste package from dripping water or rockfall. The result is expected to be a repository with a low probability for the occurrence of any postclosure criticality event or, in the unlikely occurrence of a criticality event, maintaining the overall dose to the public below the regulatory performance objectives. Because a detailed description of the specific site and engineered features (DOE 2001) are outside the scope of this topical report, design of the repository and exploitation of the site features to provide defense-in-depth are not discussed further in the report.

Another aspect of the defense-in-depth philosophy is the imposition of an upper bound on the probability associated with potential criticality events that will be implemented in conjunction with the methodology approach presented, as discussed earlier in this section. The approach used in the methodology includes evaluation of the probability of the events and the contributing factors to their potential for occurrence. This analysis will identify processes, conditions, and events most likely to lead to criticality. With this information, reasonable and feasible approaches to reducing the probability of occurrence of potential criticality events will be sought.

One other aspect of the defense-in-depth philosophy is the use of appropriate conservatism in the analyses, although inclusion of conservatism is notably outside the requirements of 10 CFR Part 63. The approach to conservatism is discussed in various sections of this topical report.

2.3 APPLICATION OF NRC GUIDES AND INDUSTRY CODES AND STANDARDS

Guidance documents from the NRC and various applicable industry standards have been used in developing the methodology approach. Additional guidance may be used to further refine the approach.

2.3.1 NUREGs

The information and guidance contained in NUREG/CR-2300, *PRA Procedures Guide, A Guide to the Performance of Probabilistic Risk Assessments for Nuclear Power Plants* (NRC 1983), have been reviewed for application to the postclosure criticality analysis methodology approach. This guide provides methods and information for performing the three levels of probabilistic risk assessment (PRA) for a nuclear power plant. In general, much of the information contained in NUREG/CR-2300 (NRC 1983) is specific to the analysis of nuclear power plants, and not directly applicable to disposal criticality analysis. However, the philosophy and general flow of the methodology approach presented in this topical report is consistent with the objectives of the three levels of a PRA described in NUREG/CR-2300 (NRC 1983).

Section 2.1.3 of NUREG/CR-2300, *Scope and Results of Analysis* (NRC 1983), describes PRA Levels 1, 2, and 3. As stated in this section, a Level 1 PRA "consists of an analysis of plant design and operation focused on the accident sequences that could lead to core melt, their basic causes, and their frequencies." The emphasis is on developed event sequences and understanding how core melt can occur. The disposal criticality analysis methodology approach identifies a sequence of events and/or processes that may lead to criticality and determines the probability of each sequence. The development and use of a list of Master Scenarios (Section 3.3) and associated configuration classes, as discussed in Chapter 3 of this report, emulates the purpose of a Level 1 PRA.

Section 2.1.3 of NUREG/CR-2300, *Scope and Results of Analysis* (NRC 1983), describes a Level 2 PRA as "an analysis of the physical processes of the accident and the response of the containment … (and) predicts the time and the mode of containment failure as well as the inventories of radionuclides released to the environment." The disposal criticality methodology approach to criticality consequence analysis estimates the power, duration, and increasing radionuclide inventory resulting from each criticality. Essentially, this portion of the analysis estimates a source term to be used in a Level 3 analysis (or in a TSPA, in the case of the methodology approach presented in this topical report).

Section 2.1.3 of NUREG/CR-2300, *Scope and Results of Analysis* (NRC 1983), says that a Level 3 PRA "analyzes the transport of radionuclides through the environment and assesses the public-health and economic consequences of the accident …". For postclosure criticality analysis as described in this topical report, the source term (from "Level 2") is used as input to the TSPA, which determines the consequences of criticality sequences on the performance of the repository.

The methodology approach presented in Chapter 3 of this topical report is intended to provide a rigorous and systematic approach similar to that provided in a nuclear power plant PRA to ensure completeness and comprehensiveness, including the alignment of the analytical tasks. For example, in a PRA for a nuclear power plant, a complete list of initiating events that consider both industry and plant-specific experience must be developed. The approach described in this topical report starts with a list of Master Scenarios (Section 3.3), developed and refined with consideration of the ways a waste package can be affected by each scenario.

However, although there are similarities between the approaches to nuclear power plant PRA and the analysis described in this topical report, many of the tools and techniques used to evaluate a nuclear power plant are not directly applicable to a long-lived repository because the problem being solved is different. A PRA for a nuclear power plant looks at an initiating event, followed by the success or failure of a variety of actively or passively functioning mitigating systems, to determine the likelihood of core damage. Many of the considerations important to a power plant PRA (such as operator actions and active mitigating systems) do not apply to the approach to the disposal criticality analysis methodology. The mitigating systems in the postclosure repository are all passive. Unlike the case for reactor systems, which are maintained to a certain state of readiness as required by technical specifications, there will be no maintenance in the postclosure repository. Therefore, many aspects of the tool set of NUREG/CR-2300 (NRC 1983) are not explicitly used in the postclosure disposal criticality analysis methodology approach. However, the general philosophy for performing a PRA for a nuclear power plant, and the systematic and rigorous approach used in them, have been incorporated into the methodology approach described in Chapter 3.

Guidance from NUREG/CR-6361, *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages* (Lichtenwalter et al. 1997), has been used in selecting benchmark cases to validate the criticality model in the methodology and in establishing a critical limit (an upper subcritical limit is not used in this approach). This NUREG references American National Standards Institute and American Nuclear Society standard ANSI/ANS-8.17-1984, *Criticality Safety Criteria for the Handling, Storage, and Transportation of LWR Fuel Outside Reactors* (discussed in the following section) as the recommended method for establishing subcriticality.

NUREG/CR-5661, *Recommendations for Preparing the Criticality Safety Evaluation of Transportation Packages* (Dyer and Parks 1997), has been used for guidance on how to extend a defined Range of Applicability for the establishment of a critical limit. The NUREG references an industry standard discussed in the following section (ANSI/ANS-8.1-1998, *Nuclear Criticality Safety in Operations with Fissionable Material Outside Reactors*).

2.3.2 Industry Standards

Five industry standards have been considered in developing the approach used in the methodology:

1. ANSI/ANS–8.1-1998. *Nuclear Criticality Safety in Operations with Fissionable Material Outside Reactors*.

2. ANSI/ANS-8.15-1981 (Reaffirmed in 1995). *Nuclear Criticality Control of Special Actinide Elements*.

3. ANSI/ANS-8.17-1984 (Reaffirmed in 1997). *Criticality Safety Criteria for the Handling, Storage, and Transportation of LWR Fuel Outside Reactors*.

4. ANSI/ANS-8.10-1983 (Reaffirmed in 1999). *Criteria for Nuclear Criticality Safety Controls in Operations with Shielding and Confinement*.

5. ANSI/ANS-8.21-1995. *American National Standard for the Use of Fixed Neutron Absorbers in Nuclear Facilities Outside Reactors*.

Each is briefly discussed in the following paragraphs.

ANSI/ANS-8.1-1998. This standard provides guidance for preventing criticality accidents in the handling, storing, processing, and transporting of certain fissionable material, specifically ^{233}U, ^{235}U, and ^{239}Pu. 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 approach described in the topical report for criticality analyses external to a waste package (both near field and far field locations) either uses or is consistent with much of the guidance for prevention of criticality accidents provided in this standard. The guidance in this standard is followed in establishing critical limits[4]. 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 in the development of the disposal criticality analysis methodology approach. Guidance from this standard has also been used for developing trends in the bias to extend the range of applicability of the calculational method. However, the single-parameter limits (such as limits on mass, enrichment, volume, and concentration) in the standard are not applied because the complexity and variety of possible degraded configurations, with various blends of isotopes, cannot be addressed by the single-parameter limits.

The standard describes use of the double-contingency criterion, which states that two unlikely and independent events are required for a criticality to occur. This criterion is considered inappropriate for application to the repository postclosure period, as discussed in Section 2.2 above. The risk-informed postclosure criticality analysis approach described in this report will comprehensively address FEPs that pose the potential for criticality but will not do so using the double-contingency criterion.

ANSI/ANS-8.15-1981. This standard addresses isotopes of actinide elements that are capable of supporting a chain reaction, other than those isotopes addressed in ANSI/ANS−8.1-1998, and that may be encountered in sufficient quantities to be of concern for criticality. It addresses these isotopes in a similar manner to that used in ANSI/ANS−8.1-1998 to address ^{233}U, ^{235}U, and ^{239}Pu. The single-parameter limits of ANSI/ANS-8.15-1981 are not applied to disposal

[4] It should be noted that this topical report does not make use of a "subcritical limit" as discussed in several standards. It is considered inappropriate, as part of a risk-informed criticality analysis methodology, to attempt to specify an amount by which the repository system must be subcritical. Rather, the term "critical limit" is used. This term accounts for uncertainties in a similar manner to their treatment in the standards for storage facilities, but it accounts for them in the probabilistic analysis rather than through use of deterministic analysis compared to a subcritical limit. The concepts are similar but the applications necessarily different.

criticality analysis for the same reason as discussed above for ANSI/ANS-8.1-1998. Because ANSI/ANS-8.15-1981 refers to the methodology approach discussed in ANSI/ANS-8.1-1998, the methodology approach in this topical report is consistent with ANSI/ANS-8.15-1981 to the same extent it is consistent with ANSI/ANS-8.1-1998, as previously described.

ANSI/ANS-8.17-1984. This standard provides guidance for criticality safety for a specific light water SNF waste form as opposed to the more general scope of ANSI/ANS-8.1-1998. ANSI/ANS-8.17-1984, which is intended to provide supplemental guidance for ANSI/ANS-8.1-1998, allows neutron absorbers to be relied on for controlling criticality. In addition, it allows credit to be taken for burnup through reactivity measurements or through analysis and verification of exposure history. It also provides criteria to establish subcriticality, though it does not require that a specific margin to criticality be maintained.

The methodology approach used for criticality analyses internal to a waste package and the approach to establishing neutron absorber credit through the use of material degradation and transport models is consistent with the guidance in this standard. In addition, the standard's guidance is used in establishing the critical limit (the section of the standard titled "Criteria to Establish Subcriticality"). The approach for establishing criticality prescribed in Section 5.1 of this standard is similar to the approach recommended in NUREG/CR-6361 *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages* (Lichtenwalter et al. 1997) for establishing subcriticality, with certain differences reflecting the differences between the deterministic storage analyses and risk-informed disposal analyses.

The risk-informed, performance-based methodology approach described in this topical report defines a critical limit that is used to identify systems that have the potential to become critical. Past applications of ANSI/ANS-8.17-1984, which were deterministic, defined an upper subcritical limit that used an arbitrary subcritical margin. The critical limit values described in this report do not include an arbitrary subcritical margin (i.e., Δk_m as defined in ANSI/ANS-8.17-1984), but set it to zero for postclosure applications. Setting this value to zero for applications that follow the topical report methodology approach is consistent with the absence of the requirement in 10 CFR Part 63. That rule, like DOE's proposed criticality analysis method, focuses on risk and not on arbitrary margins. Imposition of an arbitrary margin would constitute a subsystem performance objective, which is inconsistent with the NRC approach in the regulation. DOE's disposal criticality method is intended to address the 10 CFR Part 63 performance objectives. DOE's proposed method will contain appropriate conservatisms for a risk-informed, performance-based approach. Therefore, DOE believes that its method adequately accounts for uncertainties such that an arbitrary margin is not needed. This judgement concerning the adequacy of the margin for this approach will be confirmed after the repository and design models are developed.

ANSI/ANS-8.10-1983. 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 to criticality design and analysis described in ANSI/ANS-8.10-1983 requires designing for one, rather than two, unlikely events as required by ANSI/ANS-8.1-

1998 and ANSI/ANS-8.17-1984. The methodology approach presented in this topical report is consistent with the approach described in ANSI/ANS-8.10-1983.

ANSI/ANS-8.21-1995. This standard provides guidance for the use of fixed neutron absorbers as an integral part of nuclear facilities and fissionable material processing equipment outside reactors, where such absorbers provide criticality safety control. The methodology approach described in this report makes use of fixed absorbers as described in this standard but the verification and inspection standards, due to the long time periods of concern, cannot be implemented.

2.3.3 Regulatory Guides

NRC Regulatory Guide 3.71, *Nuclear Criticality Safety Standards for Fuels and Material Facilities*, was used in developing this methodology approach. This regulatory guide endorses 15 ANSI/ANS standards, including the five identified in the previous section, as useful in development of disposal criticality analysis methodology approaches.

However, the regulatory guide takes exception to certain aspects of the standards. The exception pertinent to the approach used in the methodology described in this topical report is the requirement for accepting burnup credit. The Regulatory Guide states that credit for fuel burnup may be taken only when the amount of burnup is confirmed by physical measurements that are appropriate for each type of fuel assembly in the environment in which it is to be stored. With the exception of physical measurements of burnup, the planned implementation of the methodology approach presented in this report is consistent with Regulatory Guide 3.71 to the same extent it is consistent with the five ANSI/ANS standards discussed in Section 2.3.2.

Interim Staff Guidance - 8, Revision 2. Burnup Credit in the Criticality Safety Analyses of PWR Spent Fuel in Transport and Storage Casks (NRC 2002), was used in developing the approach in the methodology for estimating burnup values and their uncertainties for commercial spent nuclear fuel (CSNF). This guidance document provides recommendations for utilization of burnup credit in criticality safety analyses. The planned implementation of the approach for verification of assembly burnup values presented in this report is consistent with appropriate recommendations in Interim Staff Guidance-8 (NRC 2002).

3. METHODOLOGY APPROACH

This chapter presents the methodology approach for performing criticality analyses for waste forms emplaced in the repository at Yucca Mountain for long-term disposal. This methodology applies to the time period of regulatory concern after the repository is permanently closed. Although the methodology will apply to the entire postclosure period, the application of the individual models will vary as postulated conditions, events of interest, and levels of uncertainty change. Provisional acceptance of the principles of the risk-informed, performance-based approach discussed in this chapter was provided in *Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0* (Reamer 2000b, Section 3.1). In addition, specific aspects of the approach used in the methodology are noted throughout Chapter 3. The full list of items for which acceptance has been documented or is being sought can be found in Section 1.2.

Chapter 3 is divided into 8 sections. An overview of the overall methodology approach is provided in Section 3.1. Section 3.2 discusses performance criteria imposed by the methodology to ensure appropriate criticality controls are implemented in the waste package design. Section 3.3 describes how degradation scenarios are built from FEPs. These include scenarios that lead to potentially critical configurations inside the waste package, outside of the waste package in the near field environment, and outside the waste package in the far field environment. It also describes how these configurations are grouped into standard classes to make the problem manageable, while also ensuring that a comprehensive set of configurations is considered.

The individual components of the analysis methodology approach are described in the remaining sections of this chapter. Each section is divided into subsections that present the analysis process or methodology approach, the modeling approach, and the validation approach for the various models. Section 3.4 discusses the steps in the methodology approach for identifying the parameters associated with configuration classes using environmental properties of the repository and output from a non-equilibrium geochemistry model as the principal information sources. The modeling approach for the degradation analysis model (consisting of corrosion and geochemistry models) and the validation approach for the model are also presented. The neutronic methodology approach for evaluating the criticality potential of configuration classes (k_{eff}) once the configuration has been specified is described in Section 3.5.

The last three sections are concerned with estimating the probability of occurrence of critical configuration classes (Section 3.6), their subsequent consequences (Section 3.7), and associated risk Section 3.8). In this context, risk is evaluated, in part, from the probability of occurrence for the overall radionuclide concentrations and annual dose in the accessible environment. The risk is acceptable for values that do not exceed the regulatory performance objectives. For the repository, the most appropriate measure of consequence is the incremental radionuclide inventory resulting from a potential criticality event. Other effects from a potential criticality may exacerbate the effect of the incremental radionuclide inventory on risk by modifying engineered barriers to the nuclide transport sequences. If there are several possible scenarios leading to criticality, then the risk is evaluated from the probability-weighted sum of the individual consequence contributions.

Section 3.6 gives the approach used in the methodology for estimating the probability of occurrence of potentially critical configuration classes. The approach is described with respect to probability distributions of the repository environmental parameters discussed in Section 3.3 and the waste form/waste package configuration-related parameters discussed in Section 3.4. The methodology approach for estimating the consequences of criticality is presented in Section 3.7. Section 3.8 describes the methodology approach for combining probability and consequence estimates, which is part of the general TSPA methodology approach, including the modeling of radionuclide transport to develop an estimate of dose at the accessible environment.

3.1 OVERALL METHODOLOGY APPROACH

An overview of the disposal criticality analysis methodology approach is provided in Figure 3-1. This figure illustrates the flow process of major analysis components and shows the input required, as well as the decision points in the process. Dashed lines within Figure 3-1 indicate major evaluation categories. As shown in Figure 3-1, the input data includes the design of the waste package/engineered barrier system (including the waste form characteristics), the site characteristics, and the degradation characteristics of the waste package materials. In addition, a list of Master Scenarios (Section 3.3) with associated configuration classes is provided as input.

The approach to the disposal criticality methodology begins with a configuration class and evaluates the ranges that parameter values would be required to have in order to be in that class. The probability of these values can then be evaluated. These configuration classes are the states at the end of the scenario chains associated with the Master Scenarios. Thus, the parameter range associated with a configuration class is determined from geochemistry degradation analyses that permit the configuration class to develop within a designated time interval.

The list of Master Scenarios, as discussed in Section 3.3, represents a comprehensive set of degradation scenarios that must be considered as part of the criticality analysis for any waste form. These scenarios were developed at a workshop on postclosure criticality for the Total System Performance Assessment for the Viability Assessment abstraction/testing effort (CRWMS M&O 1997a). This Master Scenario List is believed to be comprehensive with respect to the spectrum of scenarios that might occur in the repository and might affect criticality risk. The degradation scenarios in this set help define the different configuration classes that result from the effects of FEPs that affect the containment capability of waste packages and the integrity of their contents.

The decision points shown in Figures 3-1 indicate tests against performance criteria that are imposed by the methodology to ensure sufficient measures are implemented to meet the 10 CFR Part 63 postclosure probability criterion for exclusion of events from TSPA or, if not met, then to meet the overall regulatory performance objectives. These measures include analyzing the significant factors contributing to the probability of criticality and implementing design enhancements to reduce the overall risk, if those particular objectives are not met.

The process represents a logical, systematic approach. Moving through Figure 3-1, the process evaluates how the waste package may degrade by tracking the types of possible conditions and anticipated interactions that could take place based upon repository design and performance characteristics. Geochemical performance evaluations (Section 3.4) include input from both the system characteristics and from the Master Scenario List for configuration classes. The process identifies applicable scenarios that result in degraded configuration classes that may have potential for criticality. Potential critical configuration classes are states of a degraded waste

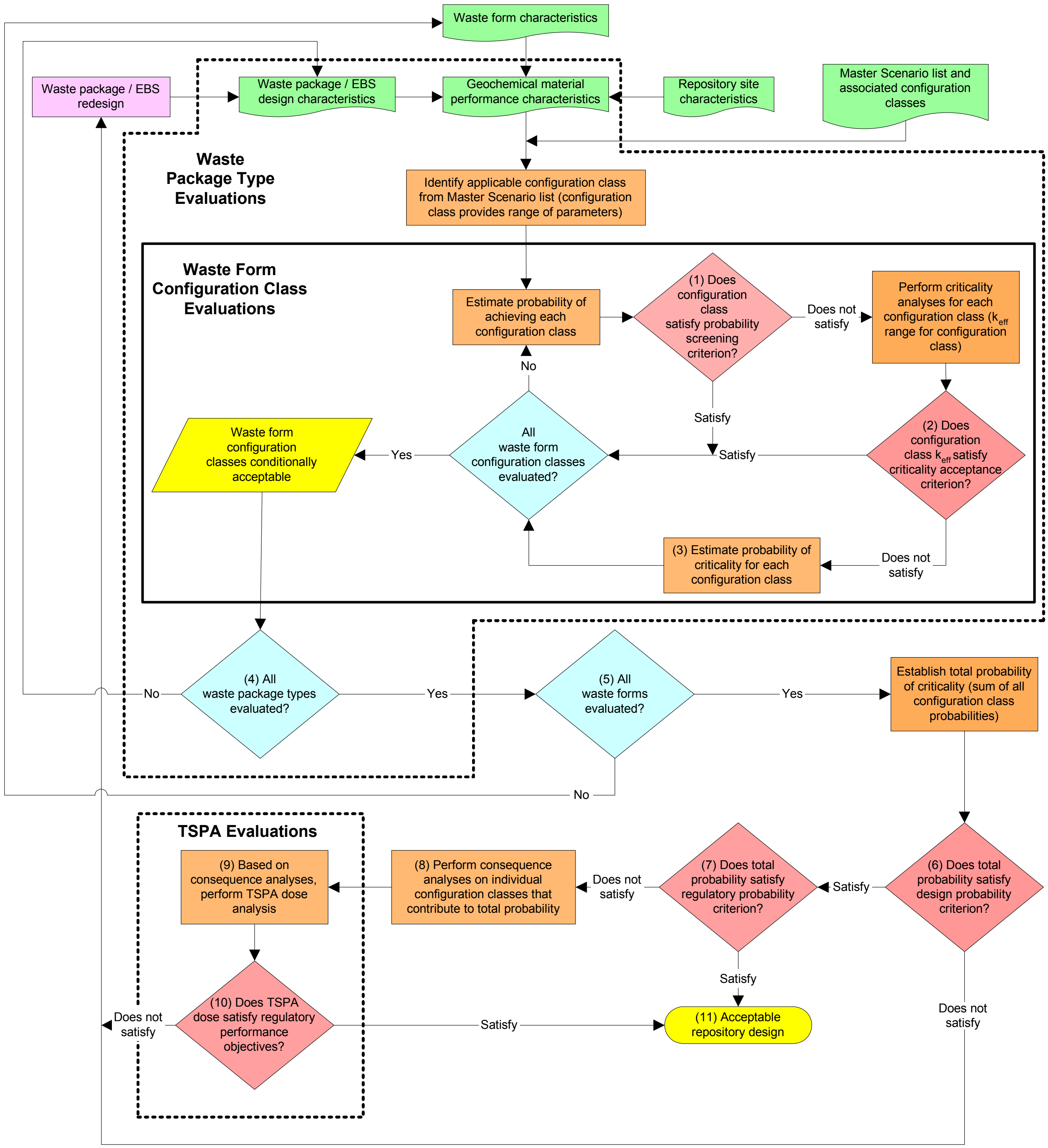


Figure 3-1. Overview of Disposal Criticality Analysis Methodology Approach

package defined by a set of parameters characterizing the quantity and physical arrangement of the materials that have a significant effect on criticality. These parameters include, among other things, the quantities of fissionable material, neutron absorber material, corrosion products, reflecting material, and moderator that are assembled in some arrangement.

After the applicable scenarios are identified, analyses (Section 3.4) of the possible degradation sequences are performed to define the specific parameter ranges of the end-states for each waste form/waste package configuration class. This information is used by the configuration generator and criticality calculations. For example, the specifics of a degradation sequence (event tree sequence) will depend, in part, upon climatic input (repository input) and composition of the waste package/engineered barrier system structural materials. Probability values associated with fault tree inputs to top events in the event tree provide the information for estimating the probability of occurrence of the configuration classes. The Range of Parameters derived from the degradation analyses are input to the criticality model (Figure 3-4) for calculations of the criticality potential of configuration classes as necessary.

As noted in Figure 3-1, postclosure criticality evaluations are performed only for those degraded configuration classes of the waste form/engineered barrier system for which the probability of the occurrence of the configuration class exceeds the probability screening criterion (Box 1). This predetermined probability screening criterion is defined to be well below (a minimum of two orders of magnitude) the 10 CFR 63.114(d) regulatory criterion of one chance in 10,000 of occurring over 10,000 years. The probability of occurrence for a configuration class is used as an upper bound for the probability of criticality for that configuration class if the screening criterion is satisfied and thus excluded from further consideration. If the probability screening criterion is not satisfied, then a criticality analysis of the configuration class is performed. These criticality evaluations are performed for the configuration classes in each waste form over the Range of Parameters for the particular class. Configurations both inside and outside of the waste package that may have the potential for criticality are considered. The approach used in the methodology for estimating the probability of achieving a critical state for configuration classes with criticality potential is presented in Section 3.6.

The second decision point in Figure 3-1 is a test on the criticality potential criterion (Box 2) that is based upon the critical limit for the waste form. The critical limit is the value of k_{eff} at which the configuration class is considered potentially critical as characterized by statistical tolerance limits. Critical limit values are obtained by analysis of experimental systems with a range of neutronic parameters that are representative of the configuration parameters expected for the repository. Further description of the critical limit criterion is given in Section 3.2.2. A discussion of the approach for developing the critical limit criterion is presented in Section 3.5 with an overview in Figure 3-4. The process for calculating the critical limit is described in Section 3.5.3.2.

Configuration classes that satisfy the criticality potential criterion (k_{eff} < waste form critical limit) are considered to be subcritical and their probability of criticality is insignificant (i.e., there is no significant contribution to the total probability of criticality for the repository). Configuration classes that do not satisfy the criticality potential criterion for the waste form require further analysis to estimate their probability of criticality (Box 3). The approach used for criticality analyses is discussed in Section 3.5. The probability of criticality is estimated for each configuration class as a function of the characteristics of the waste form (i.e., based upon the probability of the parameter values that result in critical configurations). Since it is likely that a finite parameter space (up to the full Range of Parameters) will be associated with configuration classes that have potential for criticality, the maximal probability of criticality will be utilized. This overall process is applied to all variants of the waste package design applicable to a waste form (Box 4) and to all waste forms (Box 5). If the total probability of criticality for the repository does not satisfy the repository design probability criterion (Section 3.2.3) of less than one criticality in 10,000 years (Box 6), criticality mitigation strategies must be employed that may extend to waste package/engineered barrier system redesign. If the design probability criterion is satisfied, the total probability of criticality over the repository is then tested against the 10 CFR Part 63 regulatory probability criterion (Box 7) and, if satisfied, the repository design is acceptable with respect to criticality issues without further analysis. Otherwise, criticality consequence evaluations are performed for those waste forms that contribute to the repository criticality potential (Box 8). Reactivity values from the criticality model are required only for the configuration classes marked for consequence analyses.

The criticality consequence analysis estimates the impact of potential criticality events on the radionuclide inventory, and on the integrity of the engineered barrier system in the repository. Changes in the radionuclide inventory may affect the source term considered in the TSPA risk assessment (Section 3.8). Thermal effects (temperature at the source as a function of time) may impact the ambient ground water seepage rate in the region near location of the criticality event and potentially affect the migration of radionuclides. Mechanical failures (e.g., enhanced material degradation from corrosion due to elevated temperatures) may also affect the TSPA risk assessment. The perturbations in the repository locale resulting from criticality consequence analyses are treated as disruptive scenarios within the TSPA analyses (CRWMS M&O 2000a, Section 4.5).

The TSPA estimates the dose due to the radionuclide inventory enhanced from criticality events for all waste forms and waste packages (Box 9), and determines if the dose in the accessible environment or other locations meet the regulatory performance objectives. If the regulatory performance objectives (final decision point [Box 10]) are not satisfied, additional design options must be implemented to reduce factors contributing to the dose. If the regulatory performance objectives are met, the repository design is considered to be acceptable for disposal (Box 11).

3.2 PERFORMANCE CRITERIA

The disposal criticality analysis methodology imposes three performance criteria: a probability screening criterion, a criticality potential criterion, and a design probability criterion. These performance criteria are decision points that are applied during the analysis to ensure sufficient measures are implemented to limit the potential for, and unlikely subsequent consequences of, possible criticality events in the repository. The criticality potential and design probability criteria form design criteria for limiting the potential for criticality in the repository during postclosure. The total probability of criticality for the repository (i.e., the sum of the probabilities for all the configuration classes that can lead to a potential criticality event) is tested against the regulatory probability criterion to determine if those configuration classes require further analysis.

The primary performance objective for the repository is to ensure that the engineered barrier system is designed so that, in conjunction with the natural barriers, the expected annual dose at the accessible environment not exceed 0.15 mSv (15 mrem) (10 CFR 63 Part 311 of Subpart L) and ground water radionuclide concentrations not exceed levels specified in 10 CFR 63 Part 331 of Subpart L. The waste package criticality performance objective is to ensure that the total effect of any criticality will not significantly compromise the engineered or the natural barrier system with respect to their ability to inhibit the releases of radioactive materials to the accessible environment. Total effect will include all aspects of potential criticality events including, but not limited to, increase in radionuclide inventory, waste heat output, and any consequent degradation of the engineered barrier system. For purposes of this objective, a significant compromise would be defined as that which could result in environmental conditions exceeding the criteria in 10 CFR 63.311 and/or 10 CFR 63.331.

3.2.1 Probability Screening Criterion

The probability screening criterion provides an initial test of the estimated probability of occurrence for a configuration class (evaluated over all end states). This test is used to screen from further consideration classes that contribute insignificantly to the total probability of a criticality occurring in the repository during the period of regulatory concern. If the probability of occurrence for a class is below this screening level, then no additional evaluations are performed for this configuration class and the probability of potential criticality for the configuration class is insignificant. The probability screening criterion is defined to be well below (a minimum of two orders of magnitude) the 10 CFR 63.114(d) probability criterion for exclusion of events from TSPA that is one chance in 10,000 of an (criticality) event occurring in the repository over 10,000 years to screen out those configuration classes that provide no significant contribution to the overall probability of criticality in the repository.

3.2.2 Criticality Potential Criterion

The criticality potential criterion provides a test to evaluate the potential for criticality of configuration classes during postclosure. The maximum k_{eff} of the configuration class is evaluated over the range of parameters for the class and compared to the critical limit for the waste form. This critical limit includes the appropriate biases and associated uncertainties for each internal and external configuration class analyzed for the repository. A presentation of the approach for developing critical limit functions is provided in Section 3.5.3.2.5 and for the criticality potential criterion in Section 3.5.3.2.10. Configuration classes for which the maximum k_{eff} over the range of parameters is below the critical limit have an insignificant potential for criticality and thus make an insignificant contribution to the overall probability of criticality for the repository.

Specific critical limit values will be established by analysis of experimental systems with a range of neutronic parameters and parameter values that are representative of the configurations to be analyzed for the repository. Specific critical limit values and the accompanying range of applicability of these values for specific in-package and out-of-package configurations will be documented in analysis reports developed in support of licensing activities. The modeling approach for calculating the critical limit values is presented in Section 3.5.2.2. The validation approach for the critical limit values and establishing their range of applicability is presented in Section 3.5.3.2.

3.2.3 Design Probability Criterion

The design probability criterion for the repository is that the total calculated probability of a criticality occurrence over the entire repository be less than one for the first 10,000 years. This value provides a sufficiently large upper bound on the probability of a criticality in the repository over the period of regulatory concern that, if not satisfied, requires the engineered barrier system to be redesigned. This probability criterion is incorporated in the methodology as part of the defense-in-depth measures (Section 2.2.2) and contributes to confidence in design control measures taken to reduce the likelihood of potential criticalities.

3.3 STANDARD CRITICALITY SCENARIOS

Degradation scenarios comprise a combination of FEPs that result in degraded configurations to be evaluated for criticality. A configuration is defined (Section 3.1) by a set of parameters characterizing the amount, and physical arrangement, at a specific location, of the materials that have a significant effect on criticality (e.g., fissionable materials, neutron absorbing materials, reflecting materials, and moderators). The great variety of possible configurations is best understood by grouping them into classes. A configuration class is a set of similar configurations whose composition and geometry are defined by specific parameters that distinguish one class from another. Within a class, the configuration parameters may vary over a given range.

Scenarios based on the FEPs that may affect criticality have been reviewed as part of a workshop on postclosure criticality for the Total System Performance Assessment for the Viability Assessment abstraction/testing effort (CRWMS M&O 1997a). This workshop produced a standard set of degradation scenarios that must be considered as part of the criticality analysis of any waste form (CRWMS M&O 1997b, pp. 13 to 45). Review and acceptance of the reports cited above (CRWMS M&O 1997a; CRWMS M&O 1997b) by the expert participants in the workshop constitutes validation of the scenario definition process. The internal and external configuration classes, given in Sections 3.4.1 and 3.4.2, respectively, cover the criticality related FEPs from the comprehensive database (Freeze et al. 2001).

The scenarios are grouped according to the three general locations for potentially critical degraded configurations: (1) inside the waste package, (2) outside the waste package in the near field environment, and (3) in the far field environment.

NOTE: “Near-field” is defined as external to the waste package and inside the drift wall (including the drift liner and invert); “far-field” is defined as beyond the drift wall (i.e., in the host rock of the repository). This was the accepted definition when the scenarios and configurations were developed in 1997 (CRWMS M&O 1997b). Certain recent analyses have used a different definition, which extends the near-field several meters into the rock. However, this document will retain the earlier terminology for consistency with the safety analysis report (Reamer 2000b).

In the discussion of scenarios and configuration classes given in the following subsections, the scenarios are grouped at the highest level, with the grouping indicated by a pair of alphabetic characters (IP for internal to the package, NF for near field, and FF for far field) followed by a number. The configuration classes are identified in a similar manner, but with a lower case letter following the number. Each configuration class also serves to define the standard scenario that leads directly to it. Many of the configuration classes can be reached by indirect scenarios routed through the triangle and circle connectors described in the following paragraph.

The internal degradation scenarios are summarized in Figures 3-2a and 3-2b and the external scenarios in Figures 3-3a and 3-3b. It should be noted that each of these figures is given in two parts (a, b) to avoid the need for foldout pages. In the sequence of Figures 3-2a, 3-2b, 3-3a, and 3-3b, the first three have outgoing connectors represented by triangles, and all have incoming connectors represented by circles. In Figures 3-2a and 3-2b, the outgoing connectors labeled E, F, and I are connected to incoming connectors in Figure 3-3a. All other outgoing connectors (with the alphabetic designations A, B, and C) are reconnected to incoming connectors (represented by circles) in Figures 3-2a and 3-2b, having the same alphabetic designation. This constitutes a feedback, with the numerical subscripts on the alphabetic designations indicating that several outputs can reconnect at the same input. For example, in Figures 3-2a and 3-2b, triangles B_1, B_2, and B_3 reconnect into circle B. Examples of this feedback are discussed further in Section 3.3.1. The shaded rectangles at the end of each scenario chain are the configuration classes to be analyzed, and are explained further below.

The top-level discriminator among the possible internal criticality scenarios (Figure 3-2a) is whether there are significant penetrations of the bottom of the waste package, with the first three scenario branches belonging to the group with no penetration of the bottom, and the last three scenario branches belonging to the group with bottom penetration. The second-level discriminator is whether the waste form degrades at a rate that is greater than, less than, or approximately equal to the degradation rate of the waste package internals. The lower level discriminators are elaborated in Sections 3.3.1 and 3.3.2. Quantification of the parameters represented by the boxes in Figures 3-2a and 3-2b and 3-3a and 3-3b for individual waste forms will be developed in support of licensing activities.

All of the external scenarios may be considered continuations of one, or more, internal scenarios. As previously noted, the connections between internal and external scenarios are indicated by the alphabetic characters at the end of the extension lines in each figure, which are enclosed in triangles in Figures 3-2a and 3-2b and in circles in Figures 3-3a and 3-3b. The connections between individual internal and external scenarios are also manifested through the source term (outflow of radioactive materials from the waste package), which is discussed in Section 3.4.

The configuration classes are shown as the shaded boxes at the end of each scenario chain in Figures 3-2a and 3-2b and 3-3a and 3-3b. Using the configuration-class concept focuses the methodology on the range of configuration parameters that result from a single scenario or set of related scenarios. The configuration classes are intended to comprehensively represent in a qualitative manner the configurations that can result from physically realizable scenarios. The parameter ranges defining the configuration classes may be refined as part of the activities in support of the repository licensing process, so that this complete coverage can be demonstrated.

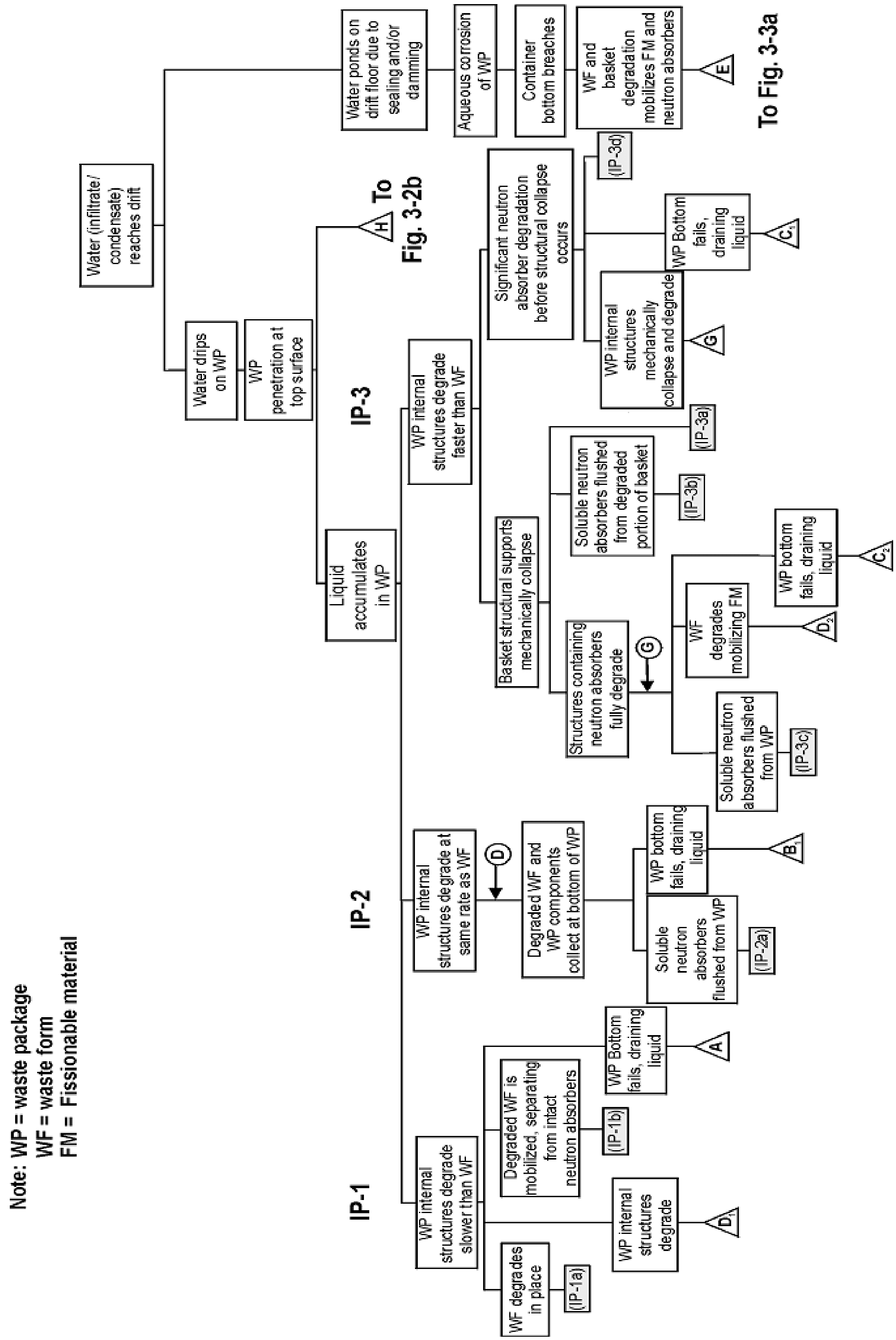


Figure 3-2a. Internal Criticality Master Scenarios, Part 1

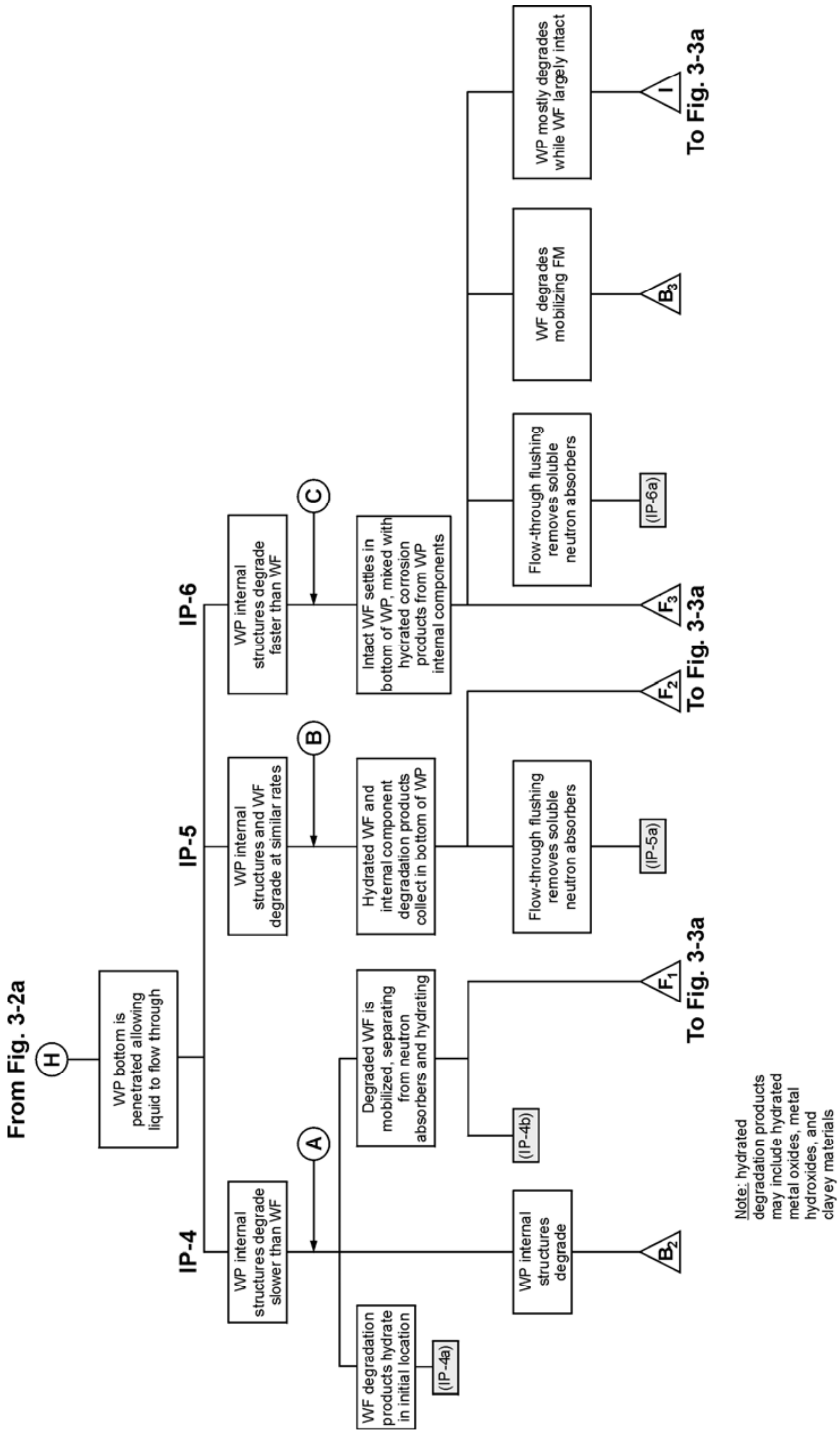


Figure 3-2b. Internal Criticality Master Scenarios, Part 2

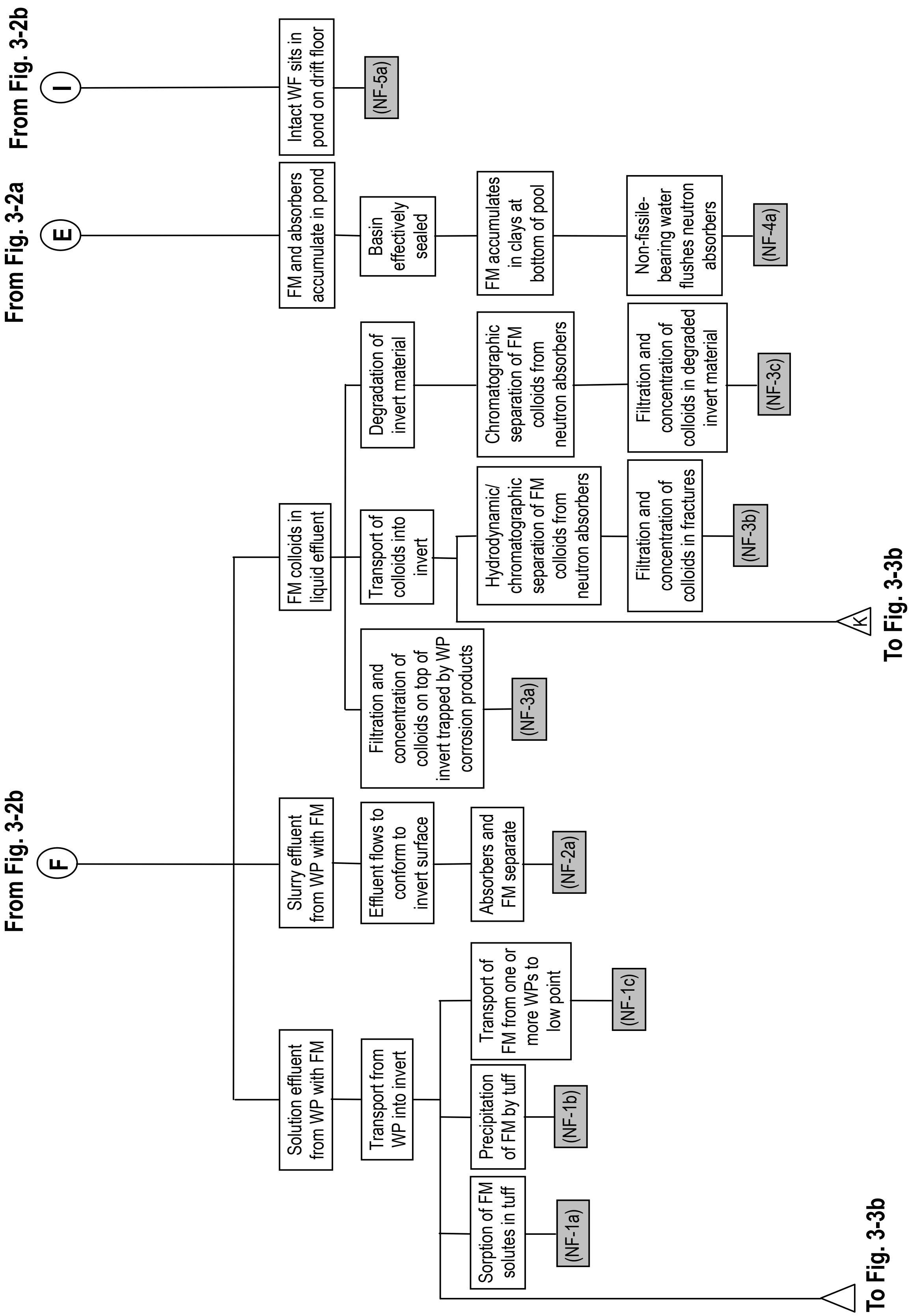


Figure 3-3a. External Criticality Master Scenarios, Part 1

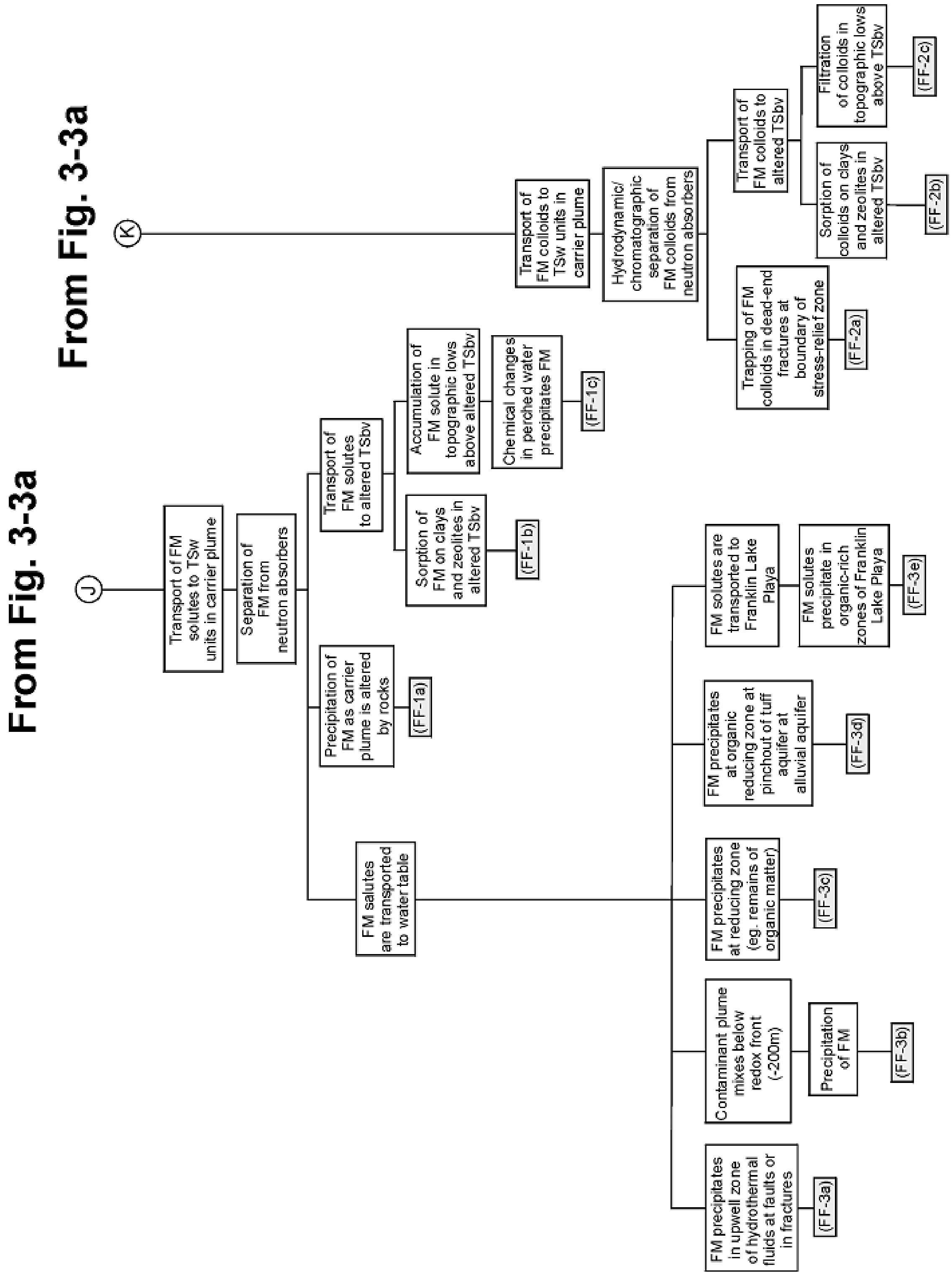


Figure 3-3b. External Criticality Master Scenarios, Part 2

The requirement for moderator (e.g., water or silica) is implied for the potentially critical configurations indicated in these figures and described in the following sections. Some of the waste form fissionable material will have sufficiently high enrichment to support unmoderated (fast) criticality if the material can be concentrated beyond its mean density in the waste form and neutron absorbing material removed. The complete analysis of these configurations will include the identification of the minimum moderator requirement for criticality in physically achievable concentrations of fissionable material, and will identify any possible fast (nonmoderated) critical configurations as part of this process.

3.3.1 Internal Scenarios

The internal degradation scenarios help define the classes of configurations that result from the effects of processes and events that degrade the contents of the waste package, after the package has been breached and the inert environment lost. The events and processes that most directly impact the potential for criticality include:

- Changes to a geometry having less neutron leakage
- Accumulation/retention of moderator
- Separation of neutron absorbers from fissionable material.

Precursors to such events and processes are also important. For convenience in this analysis, the waste-package contents are separated into two categories: the waste forms and non-SNF components in the waste package. The latter category includes various structural, thermal, and neutron absorber components of the intact basket, as well as any codisposed, non-fissionable waste forms. It should be noted that some waste forms have built-in neutron absorbers (e.g., the control rod assemblies).

How the non-SNF components in the waste package degrade is an important aspect of the evaluation since the degradation products may remain in many forms, such as insoluble neutron absorbers, insoluble corrosion products that displace water (moderator), hydrated clayey materials, or solutes affecting either the solubility or the degradation rate of the waste forms, non-SNF components in the waste package, or both. This step in the methodology approach identifies the internal configuration classes (from Figure 3-2a or 3-2b) applicable to the waste forms being evaluated. Additional information necessary to perform criticality analyses for the range of configurations in each class (i.e., the condition of the waste form; the amount of moderator; and the amount, composition, and physical distribution of the remaining waste form and other internal non-SNF corrosion products) will be determined as part of the internal-degradation-analysis step discussed in Section 3.4.

As mentioned in the previous section, the internal degradation scenarios branch into six general groups according to aspects of two processes (i.e., the accumulation of water within the waste package and the relative rates of the degradation processes affecting the waste form and the non-SNF components in the waste package). A minimum accumulation of water is important because nearly all the waste forms are incapable of criticality without moderation and water is the most effective and mobile moderator expected in the repository. Relative degradation rates of waste forms and non-SNF components in the waste package are important because different effects on the geochemistry of the system may result from a different order of degradation, altering the solubility of the corrosion products of these materials (see Section 3.4 for more detail).

Degradation scenario groups IP-1 through IP-3 (Figure 3-2a) are associated with processes that have resulted in a waste package that is penetrated only on the upper surface, so that the waste package will accumulate water if it is under a drip. The scenarios in these groups involve degradation of the material carrying the neutron absorber, release of the neutron absorber, and circulation of the solution in the waste package so that any soluble neutron absorber may be flushed through the penetration(s) near the top of the waste package. It is conservative to assume that this potential removal of the neutron absorber material occurs.

The following paragraphs list and discuss the configuration classes that have the potential for criticality, and identify the scenarios that lead to them. These class definitions encompass all of the configurations shown in Figures 3-2a and 3-2b. The more likely of these configuration classes have already been the subject of preliminary investigations. All of the configuration classes will be fully evaluated for the License Application and supporting activities.

1. The basket containing the neutron absorber is degraded, but the waste form is either intact or degraded (configuration classes IP-3a, IP-3b, IP-3c, and IP-3d). For criticality to occur, several additional conditions are required: sufficient moderator is present, neutron absorber is flushed from the waste package, and most of the fissionable material remains in the package (configuration classes IP-3b, IP-3c, and IP-3d). These configuration classes arise from scenarios in which the basket containing the neutron absorber degrades before the waste form. They result from scenario group IP-3, which involves the waste form degrading at a much slower rate than the non-SNF components in the waste package.

2. Both basket and waste form are degraded simultaneously with the same three additional conditions (water, absorber removal, and fissionable material remaining) as configuration group #1 above (configuration class IP-2a). In general, this configuration will result in the fissionable material accumulating at the bottom of the waste package. Since both waste form and non-SNF components in the waste package are fully degraded, with all the soluble degradation products removed, the only residual effect of a difference in degradation rates is the nature of any separation between the degradation products of the waste form and other internal components. The parameters of these configuration classes are determined either by the geochemistry analysis or by the evaluation of conservative alternative configurations. Therefore, this configuration class can arise directly from scenario group IP-2, or from scenario groups IP-1 or IP-3 looping to IP-2 through the D entry point fed by D_1 and D_2, respectively. Intermediate configurations in which only the basket or the waste form is degraded first are covered by configuration group #1 (above) or #3 (below).

3. The fissionable material from the waste form is mobilized and moved away from the neutron absorber, which remains in the partially degraded basket structure (configuration class IP-1b). As with configuration group #2, the fissionable material will most likely accumulate at the bottom of the waste package, but, unlike configuration group #2, the physical opportunities for this transport and accumulation are limited because the basket is only partially degraded. This configuration class results from scenario group IP-1, which involves the waste form degrading faster than the basket (non-SNF internal component in the waste package). An alternative configuration class having these

relative degradation rates is IP-1a, in which the fissionable component of the waste form does not move significantly after degradation.

4. Fissionable material accumulates at the bottom of the waste package, together with moderator provided either by water trapped in clay or by hydration of metal corrosion products, so that criticality can occur without water pooling in the waste package (configuration classes IP-4b, IP-5a, and IP-6a). The complete analysis of this configuration group will include the identification of the minimum moderator requirement for physically achievable concentrations of fissionable material, and will identify any possible fast (non-moderated) criticality as part of this process. The scenarios leading to this configuration group differ in that class IP-4b does not require the neutron absorber to be flushed from the waste package, but only that a relative displacement occurs between fissionable material at the bottom of the waste package and neutron absorber distributed throughout the container. These configuration classes can result from scenario groups IP-4 through IP-6, all of which have penetrations in the bottom of the waste package, thus preventing water from pooling in the waste package. This flow-through geometry permits removal of soluble corrosion products, but allows the insoluble corrosion products to remain within the waste package. If the penetration of the waste package bottom precedes, or directly follows, the penetration of the top, scenario groups IP-4 through IP-6 are said to be directly invoked. If there is significant degradation of waste form or non-SNF components in the waste package, then these scenarios are indirectly invoked after scenario groups IP-1, IP-2, or IP-3. In all of these scenarios, a sequence representing removal of fissionable material from the waste package through breaches in the bottom of the waste package provides a source term for the external criticality scenarios in Figures 3-3a and 3-3b.

5. As with configuration group #4 above, the moderator is provided by water trapped in clay, but in this case, the fissionable material is distributed throughout a major fraction of the waste package's volume (configuration class IP-4a). This configuration class can only be reached if the waste form degrades faster than the non-SNF components in the waste package, so that the fissionable material remains in place to be locked in by its own hydration or by the hydration of the other internal components. Therefore, it is only reached by scenario group IP-4 (direct) or indirectly after IP-1.

6. Waste form has degraded in place with non-SNF components in the waste package partially degraded (IP-1a). This configuration class is of interest if the degradation of the waste form can distribute the fissionable material into a more reactive geometry than the intact waste form.

3.3.2 External Scenarios

The scenarios leading to near field configuration classes begin with the source term consisting of the fissionable material transported out of the waste package, represented generically by the incoming connectors E and F at the top of Figure 3-3a. The only exception is the scenario leading to configuration class NF-5a (from the incoming connector I), which has the fissionable material (as degraded SNF) simply sitting on the drift floor beneath the waste package. The source term includes any fissionable material from the waste package in a form (either as solutes, colloids, or slurry of fine particulate) that can be transported into or over the invert (which may be crushed tuff) beneath the waste packages. FEPs that may act to collect the fissionable material in the near field are summarized in the upper portion of Figure 3-3a.

The external criticality configuration classes are listed below.

1. Accumulation, by chemical reduction, of fissionable material by a mass of organic material (reducing zone). Such a deposit might be located beneath the repository, at a narrowing of the tuff aquifer, or at the surface outfall of the saturated zone flow (configuration classes FF-3c, FF-3d, and FF-3e, respectively).

2. Accumulation, by sorption, onto clay or zeolite (configuration class FF-1b). Such material may be encountered beneath the repository.

3. Precipitation of fissionable material in fractures and other void spaces of the near field and the far field. This configuration is obtained from processes such as adsorption, from a reducing reaction, or from chemistry changes made possible by carrier plume interaction with surrounding rock and pore waters (configuration classes NF-1a, NF-1b, and FF-1a).

4. Accumulation of fissionable material in water that has pooled in the drift. This configuration class, NF-4a, is reached from scenario E. This scenario involves waste packages that may not have been directly subjected to dripping water but are located in a local depression so that water from other dripping sites may collect around the bottom of the package during periods of high flow. A variant of this configuration class could have the intact, or degraded, waste form in a pool in the drift (configuration class NF-5a). Such a configuration class would be evaluated for waste forms that could be demonstrated to be more robust with respect to aqueous corrosion than their waste package materials.

5. Accumulation by processes involving the formation, transport, and eventual breakup (or precipitation) of fissionable material containing colloidal particles. It has been suggested that the colloid-forming tendency of plutonium will enhance its transport capability, providing the potential for accumulation at some significant distance from the waste package. Such transport and accumulation could lead to far field configuration classes FF-2a, FF-2b, and FF-2c, for final accumulation in dead-end fractures, clay or zeolites, and topographically low regions. It could also lead to the near-field configuration classes NF-3b and NF-3c for final accumulation in the invert in open fractures of solid material or pore space of granular material, respectively.

6. Accumulation at the low point of the emplacement drift (or any connecting drift), configuration class NF-1c. The scenario leading to this configuration class must have a mechanism for sealing the fractures in the drift floor so that the effluent from individual waste packages can flow to, and accumulate at, a low point in the drift or repository, possibly in combination with effluent from other waste packages. As with the discussion of configuration class NF-4a above, such a pool would be expected to occur only within a short time (weeks or less) following a high infiltration episode.

7. Accumulation of fissionable material by precipitation in the saturated zone at the contact between the waste-package plume and a hypothetical up welling fluid or a redox front (where the plume meets a different groundwater chemistry so that an oxidation-reduction reaction can take place), configuration classes FF-3a and FF-3b, respectively.

8. Accumulation at the surface of the invert due to filtration by the degradation products, or remnants, of the waste package and its contents (configuration classes NF-2a, NF-3a, for the cases in which the fissionable material may be carried as a slurry or colloid, respectively).

9. Accumulation by precipitation from encountering perched water (groundwater deposit isolated from the nominal flow and not draining because of impermeable layer beneath) having significantly different chemistry from the fissionable material carrier plume (configuration class FF-1c).

3.3.3 Effect of Seismic Events

Configuration classes having a k_{eff} below the critical limit will also be evaluated to determine whether the critical limit can be exceeded by a sudden reactivity insertion due to a seismic disturbance. This evaluation will consist of identifying representative configuration classes (called seismic predecessor configuration classes) that could be transformed to the subject configuration by a seismic event. A representative configuration class is one that is reached from a scenario that has parameter values specified by probability distributions or taken from the conservative end of the possible range (worst case). If there are parameters that can have different worst-case values or ranges (e.g., relative corrosion rates of the waste form and potential chemistry-altering material such as stainless steel), then there will be several representative configurations. The probability of any predecessor configuration classes will be evaluated together with the probability of the seismic event having sufficient magnitude to take such a configuration class to criticality. The total probability will be summed over a representative set of seismic events, weighted by the appropriate probability for each such event.

For internal criticality, the search for predecessor configuration classes will be performed according to the following guidelines, which apply individually to each of the six internal criticality configuration classes identified in Section 3.3.1 of this document:

1. Mostly degraded basket, with only partly degraded waste form (principally spent fuel assemblies), reachable from scenario IP-3. Two types of configuration classes will be examined for predecessor configuration classes. The first type of final configuration class reachable from a higher potential energy predecessor configuration class has waste forms (e.g., assemblies) stacked in their lowest potential energy configuration with little, or no, basket material between the assemblies. The potential predecessor configuration classes to be identified are those that have some assemblies displaced vertically (upward) with support by some still-uncorroded steel basket material. The evaluation consists of calculating the Δk_{eff} between the predecessor and final configuration class and calculating the probability of occurrence of the predecessor configuration class.

   The second type of final configuration class represents a more degraded configuration class in which there is virtually no basket steel left uncorroded, and a few of the assemblies have collapsed. The collapsed waste forms may have lost some fuel pin cladding. Consequently, the fissionable material matrix may have lost some fission products, thereby compensating for some of the loss in reactivity associated with the collapse. If the collapsed waste forms are located at the bottom of the center column of assemblies, there will be a gap at the top of this column. If the water level in the predecessor configuration class is just above this gap at the top and has one or more waste forms stacked above the water level, a seismic disturbance could cause the stacked waste forms to fall into the gap, thereby increasing the number of waste forms beneath the water level and increasing the k_{eff}.

2. Both basket and waste form, mostly degraded, in a sludge of degradation products at the bottom of the waste packages reachable from all scenarios. If any configuration classes are identified as having a k_{eff} greater than the critical limit, the search for predecessor configuration classes will include two types of configuration classes. Both types of predecessor configuration classes would have the same composition of solid degradation products as the final configuration class, as determined by the geochemistry calculations. The first type of predecessor configuration class would differ from the final configuration class by having a void in the sludge. The void could be filled with water and it would be supported by some basket remnant. If the k_{eff} were increased significantly by removal of this support, the configuration class would be further evaluated as a potential sudden-insertion predecessor, including estimation of the probability of occurrence of the predecessor configuration class.

   The second type of predecessor configuration class could be conceptualized as having the same geometry as the final configuration class but lacking the optimum amount of water in the sludge. An immediate source of water would be located above the sludge in such a way that it could be immediately dumped into the sludge. At the present time this remains conceptual only because there is no known mechanism for maintaining such perched water without water leaking out as quickly as it drips in.

3. Mostly degraded (but still largely in initial position) waste form, only slightly degraded basket, reachable from scenario IP-1. Most of these configuration classes would have some neutron absorber in the basket material, and such a configuration class could not become critical until much of that basket material had corroded or fallen to a configuration removed from the SNF itself. Analyses thus far have not identified any configurations in this class having k_{eff} greater than the critical limit. If such configurations are identified, the search for predecessor configuration classes will include configuration classes for which less basket material had fallen away from the waste form. The disruption would then drop additional basket material away from the waste form. The actual occurrence of such configurations would require that sufficient absorber plate be removed from the basket by the breaking and falling processes to cause criticality. Such movement of material would have to occur before much of the waste form itself had also fallen to the bottom of the waste package and would reduce reactivity by displacing water.

4. Mostly degraded fissionable material at the bottom of the waste package with the potential moderator provided by water trapped in clay. Precursor configuration classes

that could lead to sudden insertion would have some remainder of the fuel supported above the clay, by some partly degraded basket or canister.

5. The degraded fissionable material distributed throughout the package. Precursor configuration classes would have the fissionable material in a less homogeneous distribution that could be spread more uniformly by a shaking.

6. The fuel is degraded, but the supporting basket is largely nondegraded. Since the most reactive form of this configuration has the waste form more uniformly distributed than its initial configuration, the precursor of a critical configuration class will be similar to the initial configuration class (which could, presumably, become more uniform following shaking from the seismic event).

3.3.4 Effect of Volcanic Events

Volcanic events have the possibility of affecting the criticality potential of waste form configurations due to loss of containment and increased mobility. A hypothetical volcanic event impacting a drift in the repository is considered to destroy the engineered barrier system including fuel rod cladding, allowing possible rearrangement and/or migration of the exposed waste form. The portion of the methodology approach for identifying potential critical configurations following a volcanic event will generally consist of the following steps:

1. Evaluate the potential patterns for rearrangement and transport, by magma, of the fissionable material.

2. Evaluate the potential for accumulation of fissionable material from the magma flow, including identification of the required geometries and their probability.

3. Characterize any configurations identified by this process that fall outside of those already included in the configuration classes of Section 3.3. Such characterizations will include ranges of important parameters (e.g., amount of silica and/or water moderation).

The criticality potential of these configurations will then be evaluated in accordance with the process discussed in Section 3.5.

The application of step 1 to the complete destruction scenario is expected to show two types of potentially critical configurations. The first type has the fissionable material from several waste packages piled against each other as they block the drift opening (which is also a conservative application of step 2). This family of configurations will be evaluated according to the probability of occurrence of a flow pattern that will simultaneously move enough fissionable material together and enough neutron absorber out of the way. This configuration is quite distinct from any presented as part of the configuration classes, and will be evaluated separately.

Further refinement of this step 1 application suggests that the volcanic event that completely destroys the waste package is also likely to generate a high degree of fragmentation of the waste form. This can, in turn, lead to the relatively rapid release of fissionable material when water returns after the volcanic event is over.

3.4 POTENTIALLY CRITICAL CONFIGURATIONS

Degradation analysis models provide the data for specifying the Range of Parameters that characterize the degraded configurations (Figure 3-1, Geochemical characteristics). These data may be used to develop parameters for models that are implemented in the configuration generator model discussed in Section 3.6. The configuration generator model is, in general, the primary process tool for determining the probability of occurrence of configuration classes and the probability of criticality for potentially critical configuration classes. The configuration generator model utilizes a risk-informed, performance-based methodology for calculating the probability of criticality of the configuration classes. This model incorporates the probability distribution functions for all independent variables required for specific critical configurations. An event tree and fault tree approach based on the scenarios described in Section 3.3 identifies and tracks the sequences to reach each end-state configuration. The configuration boundaries within a class are determined by decisions specifying the event tree sequence leading to any particular configuration. By evaluating the probability model, a discrete probability will be obtained for a potentially critical configuration class during the postclosure time period.

This section describes the portion of the methodology approach for quantifying the parameter ranges of the potentially critical internal configurations as these parameter ranges determine the inputs to the criticality model. Note that, in general, the geochemical analyses are done over a wide parameter range but iteration between these evaluations and the configuration generator may be required (e.g., Step 5 in Section 3.4.1.1) to establish the appropriate Range of Parameters for configuration classes. It is recognized that the actual values of configuration parameters will be sensitive to uncertainties in the parameters of the degradation and accumulation parameters (e.g., corrosion rates, thermodynamic constants for precipitation reactions, fluid mixing). The effects of such uncertainties will be assessed for both internal and external configurations, to ensure that all potentially critical configuration classes are identified and evaluated. This portion of the methodology consists primarily of analysis of degradation processes and estimation of the neutronically significant degradation products that remain in the waste package.

3.4.1 Configurations with the Potential for Internal Criticality

The following subsections describe the models used in implementing the methodology approach and the validation of these models.

3.4.1.1 Methodology Approach for Internal Configurations

There are 10 essential steps to specify the geochemical process (briefly discussed below). These steps are used in analyses and will be applied further in the refined analyses to be documented in support of licensing activities.

1. Identify specific corrosion rates for each internal component, which will be representative of the range of degradation rates for those components and the configuration classes defined previously. The applications submitted in support of licensing activities will utilize qualified corrosion rate data from the Civilian Radioactive Waste Management System database on the subject. This database is expected to reflect consideration of the latest experimental and test data on degradation rates.

2. Identify specific water flow rates, which will be representative of the range of drip rates of water onto a waste package under a fracture that has water dripping from it. This information is available from the performance assessment unsaturated zone flow model.

3. Identify the range of dripping water chemistry parameters, which will cover the range of seepage rates as specified by the appropriate project documents.

4. Use the above information to estimate the location of potentially reacting materials, to determine whether they are actually reacting. This estimation is repeated as the degradation process continues so that the continuing interaction of physical and chemical processes is captured.

5. Perform geochemical calculations for the representative parameter range for each configuration class.

6. Examine results for concentrations of fissionable materials, and neutron absorbers in solution and in solids, and for insoluble corrosion products of other components internal to the waste package. The concentrations in solution are ultimately removed from the waste package and serve as the source term for external criticality. There will be no reactivity credit taken for neutron absorber in solution.

7. Examine results for formation of clay (either from glass matrix waste forms or from the silica and alumina in the flowing water).

8. Quantify the range of hydration of degradation products possible if the package could not be flooded.

9. Quantify the amounts of nondegraded material and solid degradation products present for each configuration class.

10. Evaluate the potential for adsorption of soluble fissionable material or neutron absorber material on corrosion products.

In order to ensure the consideration of all possible configurations at each stage of the degradation scenario, the following physical processes are evaluated at appropriate intervals in the progress of the geochemical processes:

1. Evaluate possible locations for solids (including mechanisms for how to get there) and identify specific configurations for criticality evaluation at each stage of degradation, and the parameters and their ranges to vary for each configuration.

2. Review the corrosion and mineral literature to determine the physical nature of the corrosion product such as density and physical stability of the minerals that form.

3. Evaluate the thermal and structural behavior, particularly the effects of structural failure of various internal components on the location of the corrosion products and the integrity of the waste form (if not in degradation product form).

4. Consider the effects of external events such as waste package orientation, rockfall, or seismic activity on the integrity of the nondegraded internal components and waste form, and on the location of the corrosion products.

3.4.1.2 Internal Configuration Modeling

The models used for characterizing internal configurations fall into two categories. Corrosion models specify the degradation rates for the waste package barrier materials and for the waste package internal components, including the waste form. Geochemistry models determine what happens to the degradation products; those elements that go into solution will eventually be removed from the waste package; those elements precipitating as minerals will remain in the waste package and be part of the internal configuration until they are re-dissolved and flushed from the waste package.

3.4.1.2.1 Corrosion Models

Degradation analysis for a particular component of the waste package begins with identification of the applicable range of corrosion rates for that component. Individual corrosion models are developed based on data from the materials testing program and from published results of other testing programs for each of the materials that make up the waste package barriers, internal components, and contained waste forms. Probability distributions for corrosion rates will be abstracted from such corrosion rate data for use in the configuration generator model. For the waste package barriers, the corrosion models for the individual barrier components are used as an input to the TSPA waste package degradation model. The output of the TSPA waste package degradation model is a distribution of breach times at various locations on the waste package (top, bottom, and sides) for a given set of environmental conditions (temperature history, relative humidity history, exposure to drips, etc.). Disposal criticality analyses will primarily utilize the "nominal case" output distributions from the latest approved version of the TSPA model to determine time frames over which criticality analyses of various configurations should be performed, and as input to the probabilistic analyses. Validation of the TSPA waste package degradation model, and the individual material corrosion models that support it, will be performed as part of the supporting TSPA documentation, and thus will not be addressed as part of the disposal criticality analysis for a particular variant of the package design.

Geochemistry analyses (discussed in the following section) of internal waste package component and waste form degradation begin at the point of waste package breach. The range of waste form degradation rates considered in the geochemistry analyses that specify the configurations to be used in the criticality evaluations will be consistent with the waste form corrosion models utilized for the TSPA. As with the barrier material models, these models will be validated as part of the supporting TSPA documentation, and thus will not be addressed as part of the disposal criticality analysis for a particular variant of the package design. The range of degradation rates considered for the non-SNF components in the waste package will also be based on corrosion models developed from material test data. Information and data validating these models will be provided as part of the disposal criticality analysis supporting licensing activities for any material corrosion model, which is not already considered as part of the TSPA documentation. Whenever these TSPA models are applied to the criticality issue, the selection of parameter values within the range of uncertainties will be conservative with respect to the occurrence of criticality.

3.4.1.2.2 Internal Geochemistry Models

The internal waste package geochemical model is based on equilibrium reaction sequence geochemistry methods with the additional capability of operating in a "solid-centered flow-through mode," which models aqueous solutions entering and exiting a breached waste package at constant and equal rates. Additional capabilities of the model include a provision to incorporate the radioactive decay of certain isotopes. The geochemistry model uses a thermodynamic database developed and verified particularly for these types of applications in the Yucca Mountain repository (Steinborn et al. 2003).

The internal waste package geochemical model addresses material degradation and transport out of the waste package. The main inputs to analyses using the model are (1) volume, mass, surface area, and degradation rate of each component within the waste package, and (2) incoming water composition and flow rate. Degradation rates of the SNF and non-SNF components are varied so that the three internal pooling waste package degradation scenario groups (Figure 3-2a, IP-1 through IP-3) are addressed. A range of flow rates and a variety of water compositions are also considered. Other modeling decisions are (1) determine sequence of degradation, such as a two-stage run in which some components are degraded first, followed by the remainder of the components, (2) determine minerals expected to form in the waste package, and (3) identify a thermodynamic database to correctly model geochemistry.

Outputs from such analyses include concentrations of solutes and amounts and chemical composition of solid precipitates in the waste package. As a source term to the external accumulation model, an additional output is the concentration of the solution exiting the waste package and the quantity of entrained solids or colloids, if applicable. Of particular importance are the concentrations and solid amounts of fissionable materials and neutron absorbers.

3.4.1.3 Validation of Degradation Methodology Approach and Models for Internal Criticality

The internal waste package geochemical model is a combination of simpler sub-models for the corrosion behavior of high-level radioactive waste glass, spent fuel, and steels. The corrosion sub-models depend, in turn, on accurate thermodynamic data to describe the stability of the corrosion products, and on reasonable kinetic data for the corrosion mechanisms. Confidence in the internal waste package geochemical model can be increased by validation of the corrosion sub-models of the individual components. Validation consists partly of showing that the methodology used in the sub-models, when applied to controlled experiments or well-studied analogues, correctly predicts the sequence of corrosion products, or the concentrations of solutes in the coexisting aqueous phases and partly on the validation of the software in the model. The validation process is documented in the model reports and applicable documents developed in support of licensing activities.

3.4.2 Configurations with the Potential for External Criticality

This section describes the portion of the methodology approach for quantifying the parameter ranges of the potentially critical external configurations that determine the inputs to the criticality model. The following subsections also describe the models used in implementing the methodology approach and the validation of these models.

3.4.2.1 Methodology Approach

The external criticality methodology approach consists primarily of analysis of processes for the accumulation of fissionable material from the effluent flow from waste packages. The models for this portion of the methodology will be similar to those for internal criticality, but will use broader uncertainty ranges for those parameters most important to the accumulation of a critical mass. The specific parameters and their uncertainty ranges will be described in the appropriate validation reports. In this manner, the identification of all potentially critical external configurations will be ensured.

All of the external criticality evaluations are performed using input parameters consistent with the description of the repository engineering and geologic environment, as specified in the current project baseline documents. Such parameters include, but are not necessarily limited to:

1. Materials used in the drift liner and invert (drift floor) and their degradation properties (physical and chemical).

2. Fracture density and distribution of aperture sizes.

3. Location and characteristics of possible reducing zones.

The first step in the identification of external configurations with the potential for criticality is the determination of the source term (fissionable material in the solution flowing out of the waste package, or its remnant) as a function of time. This is accomplished through a geochemical analysis of the material degradation and release from waste packages as described in Section 3.4.1.2.2. The essential subsequent steps are:

1. Determination of the flow rate and pattern, which is a strong function of the fracture pattern beneath the waste package.

2. Determination of adsorption on fracture walls or in the matrix of highly porous rock or zeolite deposits, as appropriate.

3. Determination of mineral precipitates from reactions of the waste package plume with the host rock fracture walls or pore water. The calculation must account for both fissionable and other materials because they compete for the limited fracture void space.

4. Determination of alternate sequences, or spreading, when the primary fractures are filled.

5. Determination of reaction products, from the plume encountering a reducing zone, if appropriate, using appropriate geochemical models. This step would include

consideration of the following limiting factors: (1) void space available in the reducing zone for product precipitation, and (2) low flow rate of waste package plume.

For those configurations found to have criticality potential (according to the portion of the methodology approach given in Section 3.5), an estimate of the probability of occurrence will also be made. The probability estimate is based on the distribution of environmental and material degradation parameters, according to the methods discussed in Section 3.6.

3.4.2.2 External Geochemistry Model

The geochemical model applicable to the region external to a waste package is a material transport and accumulation model. The model predicts accumulation of fissionable materials in fractures and lithophysae in the rock beneath a degrading waste package. Inputs to the model include (1) source term from internal waste package geochemical calculations, (2) types, volumes and dissolution rates of minerals in tuff, (3) list of minerals expected to form based on preliminary calculations, (4) fracture characteristics, such as fracture porosity, fracture saturation, and fracture aperture, and (5) local infiltration rate, which will determine the amount of water mixing with the waste package effluent.

The model is used to simulate the transport and interaction of the source term with the resident water and fractured tuff below the repository. In these simulations, the primary mechanism for accumulation is mixing of the high pH, actinide-laden source term with resident water; thus lowering the pH values sufficiently for fissionable minerals to become insoluble and precipitate. The high pH solutions are caused by degrading high-level radioactive waste glass. The outputs from the model are processed to produce the accumulated mass, density of accumulation, and the geometry of the accumulation zone. The density of accumulation and the geometry of the accumulation zone are calculated using a characterization of the fracture system based on field measurements made in the repository. For these high pH conditions, dilution and mixing generate high accumulations and the model does not include other potential mechanisms such as flow through a reducing zone or sorption as they would not significantly alter the external source accumulation.

3.4.2.3 Validation of the Methodology Approach and Models for External Criticality

The validation of the accumulation part of the methodology rests primarily on the validation of the software in the model. The approach used for validation compares predicted accumulation values with experimental measurements, use of field measurements of geologic features at the repository, and evaluation of mineral precipitation mechanisms. The validation process will be documented in the model reports and applicable documents developed in support of licensing activities.

3.5 CRITICALITY EVALUATION OF CONFIGURATIONS

Criticality evaluations are performed for the defined configurations in each class over the Range of Parameters and parameter values that are established based on the methodology approach described in Section 3.4. Configurations both inside and outside of the waste package that may have the potential for criticality are considered. The methodology, modeling, and validation approaches that are used for criticality evaluations are described in this section.

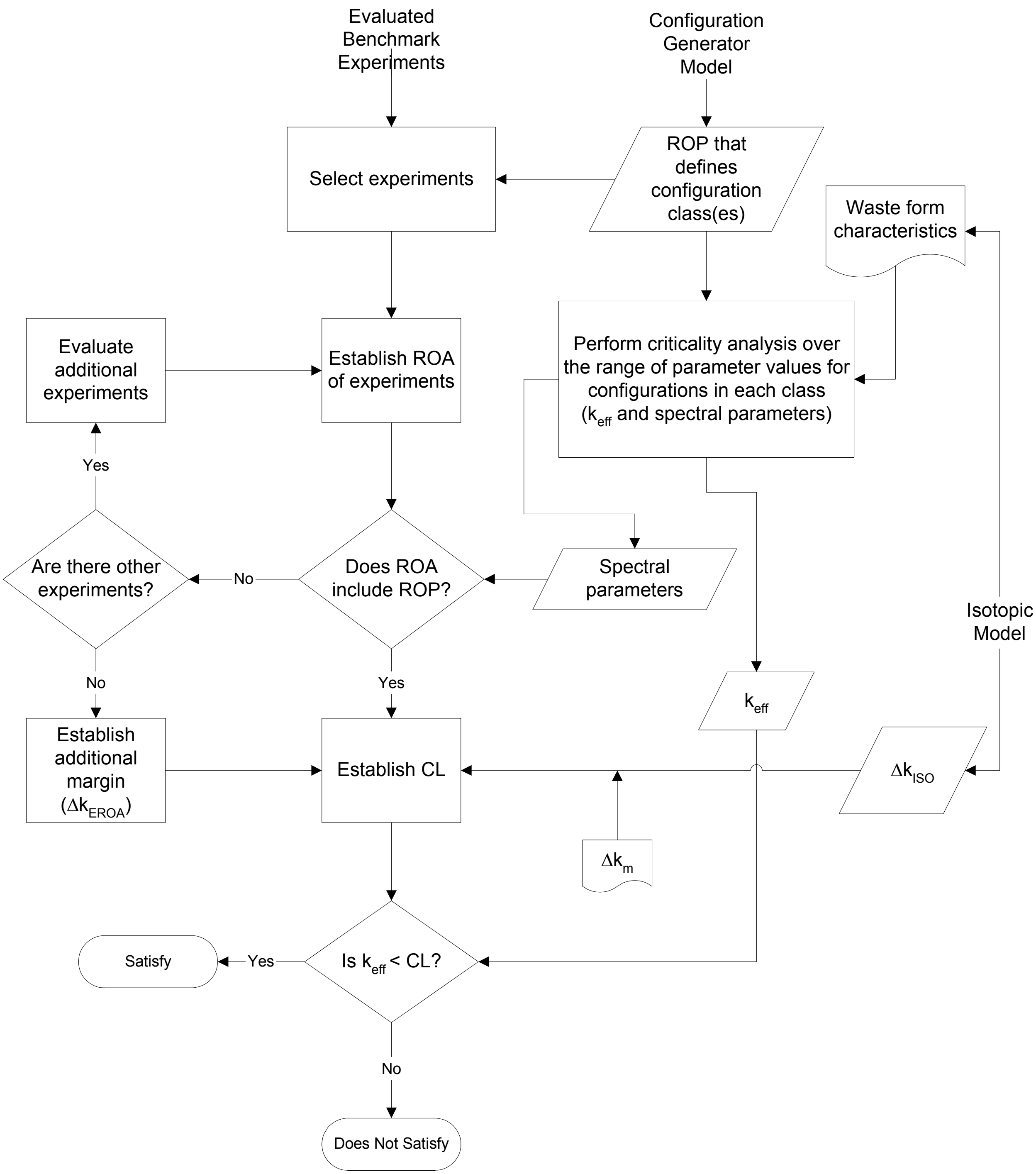
3.5.1 Methodology Approach

An overview of the criticality analysis methodology approach is presented in Figure 3-4 and discussed in the following two subsections. These subsections address the material composition from the degradation analyses, and the k_{eff} evaluation. Figure 3-4 provides an expansion of the criticality evaluation component of the disposal criticality analysis methodology approach that was presented in Figure 3-1. Note that the Δk_m parameter is always zero for postclosure analyses (see Equation 3-1) and that the terminator blocks "Satisfy" and "Does Not Satisfy" connect into Figure 3-1, Box (2).

3.5.1.1 Material Composition

Material composition and geometry of this material (i.e., waste form configuration) determine the potential for criticality. For a commercial SNF assembly, the initial material composition of the SNF (i.e., when placed in a repository) is governed primarily by the initial enrichment, the operating history of the assembly in a nuclear reactor, and the cooling time since the assembly was removed from the reactor. One component of the methodology addresses the effects of reactor operating history and cooling time on the initial material composition of commercial SNF. For other waste forms, no credit is taken for previous operating history, but conservative estimates of fissionable isotopic concentrations based on fabrication design values are used. However, for those waste forms where fissionable isotope production or burnable absorber depletion is a concern, it is assumed that maximum buildup of fissionable isotopes occurs and that no burnable absorber is present. During the long disposal time period, the material composition and geometry will change from their initial condition as a result of isotopic decay and material degradation processes. Thus, the potential for criticality will change during the disposal time period because of this change in material composition and geometry.

For commercial SNF, the reduced reactivity associated with the net depletion of fissile isotopes and the creation of neutron-absorbing isotopes during the period since nuclear fuel was first inserted into a commercial reactor can reduce the criticality potential of SNF configurations. This period includes the time that the fuel was in a reactor and exposed to a high neutron flux (in a power production mode), the downtime between irradiation cycles, and the cooling time since it was removed from the reactor. Taking credit for the reduced reactivity associated with this change in fuel material composition is known as burnup credit. Burnup is a measure of the amount of exposure for a nuclear fuel assembly in a power production mode, usually expressed in units of gigawatt days per metric ton of uranium (GWd/MTU) initially loaded into the assembly. Thus, 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, the initial enrichment of fissile material in the fuel, and the availability of individual isotopes based on degradation analyses.



Note: ROA Range of Applicability
ROP Range of Parameters
CL Critical Limit

Figure 3-4. Criticality Model Overview

The range of parameters and parameter values that define configurations in each class represents the material composition and geometry. As shown in Figure 3-4, the parameters and parameter values used in the criticality evaluations are obtained from the analysis of degradation scenarios using the configuration generator methodology (Section 3.6) that identifies configuration classes inside and outside the waste packages. This information includes output from geochemical degradation (Section 3.4) and isotopic models (Section 3.5.2.1), as well as the waste form(s) characteristics for the configuration classes. The isotopic inventories for commercial SNF are established using the isotopic modeling approach discussed in Section 3.5.2.1 and are provided as input to the geochemical degradation analyses for determining the waste form characteristics. For waste forms other than commercial SNF, the fuel isotopic inventories provided as input for the degradation analysis are based on fabrication design values, with appropriate allowances made for isotopic decay and fissionable isotope production (where applicable).

The degradation analysis establishes the availability of individual isotopes (from the fuel composition) in the degraded material composition comprising the various configurations evaluated for criticality. The removal of burnup credit isotopes by geochemical processes is considered in subsequent criticality evaluations.

3.5.1.2 k_{eff} Evaluation

As shown in Figure 3-4, k_{eff} evaluations are performed over the range of parameters and parameter values for configurations in each class as determined by the configuration generator model. The parameters and parameter values for these configurations are obtained from the degradation analyses described in Section 3.4 and include configurations inside and outside the waste packages. For the k_{eff} evaluations, an allowable limit (or critical limit) is placed on the calculated value of k_{eff} for the configuration analyzed. This critical limit, which is the value of k_{eff} at which a configuration is considered potentially critical, accounts for the criticality analysis method bias and uncertainty. The range of parameters and parameter values applied to the k_{eff} evaluations are checked against the range of parameters and parameter values that were used in establishing the critical limit. This is represented in Figure 3-4 by the box containing the Range of Applicability test. The modeling approach for the k_{eff} evaluations is discussed in Section 3.5.2.2. The process for establishing and validating the critical limit values (and hence the criticality potential criterion) is discussed in Section 3.5.3.2. A description of the process for defining the range of applicability of the critical limit values based on the experimental database used in establishing the critical limit values is presented in Section 3.5.3.2.2. As shown in Figure 3-4, when the Range of Applicability does not cover the full Range of Parameters, either additional experiments are required to extend the range or a k_{eff} penalty is applied in establishing the critical limit. In either case, a critical limit is established that is applicable to the range of parameter values that is used in the k_{eff} evaluation. The procedure for extending the range of applicability of the critical limit is described in Section 3.5.3.2.3.

These k_{eff} evaluations are made using bounding values for certain key parameters and the range of values for other parameters. The purpose of these evaluations is to identify configurations where criticality may be a concern. For example, a configuration class of intact commercial SNF in a waste package may be evaluated that has an initial enrichment of 5 weight-percent (wt%) ^{235}U fuel. If the k_{eff} values for the range of parameter values within this configuration class satisfy the criticality potential criterion for burnup values above a specific burnup, there would be no need to evaluate similar configurations with 4 wt% ^{235}U fuel and the same or greater burnup.

When the Range of Applicability criterion is satisfied and an applicable critical limit is identified, the calculated k_{eff} value for each configuration evaluated is compared with the applicable critical limit. If the calculated k_{eff} is less than the critical limit for all configurations within a waste package/waste form set, the configuration class is acceptable for disposal. Configuration classes that have calculated k_{eff} values that are greater than or equal to the critical limit have potential for criticality, and further evaluations are required to estimate the probability of criticality. If the k_{eff} values from all configuration classes within a waste package/waste form group satisfy the criticality potential criterion, then that waste form is acceptable for disposal, as illustrated in Figure 3-1. For those waste forms that fail to satisfy the criticality potential criterion, the region of parameter space where the critical limit is exceeded is established. The maximum probability of criticality is then estimated [Figure 3-1, Box (3)] based upon the cumulative distribution functions developed for configuration parameters.

As noted in Section 3.5.1.1, the material composition and geometry determines the potential for criticality of a waste form configuration. The material composition and geometry of waste forms may change from their initial configuration inside a waste package during the long disposal time period. Potential configurations that may occur are established, in part, by the degradation analyses. The degradation analyses, along with isotopic decay calculations, establish the range of parameters and parameter values that define potential configurations of fissionable and other materials. The disposal criticality analysis methodology evaluates the criticality potential of many possible configurations that may occur over the long disposal period. These configurations may occur either inside or outside of the waste packages and may involve material from more than one waste package. As shown in Figure 3-1, an estimate of the likelihood (probability) of the criticality is made for configuration classes showing potential for criticality. The methodology approach for estimating the probability of occurrence of potential critical configuration classes is described in Section 3.6.

3.5.2 Modeling Approach

The approach for the neutronic models used in assessing the criticality potential of waste forms during the postclosure period of the monitored geologic repository are described in the following subsections. First, the approach for modeling isotopic concentrations from the waste form is described. Secondly, the approach for criticality modeling (k_{eff} calculation) of configurations of SNF and high-level radioactive waste is presented.

3.5.2.1 Isotopic Modeling

The approach for modeling isotopic concentrations from the waste forms is described by a three-step process. First, the initial isotopic concentrations of the waste form at the time of emplacement in the repository are established. Second, the changes in isotopic concentrations that result from isotopic decay are calculated. Finally, the changes in isotopic concentrations based on degradation analyses are determined. The latter two processes are particularly important for the long periods considered for geologic disposal.

For most waste form types, the design values for fissionable isotopic concentrations or the technical specification limits for fissile isotope concentrations will be used in establishing the initial isotopic content of the waste form. When fissile isotope production during reactor operations leads to a higher reactivity, adjustments will be made to the design values to account for the increase in fissile isotopic content. The isotopic concentrations will then be adjusted to account for isotopic decay during the time period leading up to the criticality evaluation. The degradation modeling approach described in Section 3.4 is then used to establish the isotopic concentrations from the waste form that are available in the configurations analyzed for criticality. This modeling approach for these waste forms must be confirmed to be conservative with respect to criticality for a range of potential scenarios (e.g., scenarios where significant plutonium has been generated, and a scenario where the plutonium and uranium may be separated).

The isotopic model determines the concentrations of these isotopes that are present in the SNF and subsequently used in the criticality evaluations. The following discussion of the modeling approach for establishing isotopic concentrations in SNF is for commercial SNF.

3.5.2.1.1 Principal Isotopes for Commercial SNF Burnup Credit

The criticality analysis model that will be applied in designing waste packages for commercial SNF uses a subset of the isotopes present in the commercial SNF. The process for establishing the isotopes to be included is based on the nuclear, physical, and chemical properties. The nuclear properties considered are cross-sections and half-lives (as applicable) of the isotopes; the physical properties are concentration (amount present in the SNF) and state (solid, liquid, or gas); and the chemical properties are the volatility and solubility of the isotopes. Time effects (during disposal) and relative importance of isotopes for criticality (combination of cross-sections and concentrations) are considered in this selection process. None of the isotopes with significant positive reactivity effects (fissionable isotopes) are removed from consideration, only non-fissionable absorbers. Thus, the selection process is conservative.

This process results in selecting 14 actinides and 15 fission products (referred to as "Principal Isotopes" and listed in Table 3-1) as the SNF isotopes to be used for burnup credit. The actinide ^{233}U, included in this table, is not present in current generation commercial SNF. However, for long disposal time periods (beyond the period of regulatory concern), ^{233}U buildup is sufficient to be a potential criticality concern. Preliminary analyses supporting the selection of these isotopes are presented in *Principal Isotope Selection Report* (CRWMS M&O 1998a). The conservatism in the use of the principal isotopes for criticality analyses with spent nuclear fuel is illustrated in *Summary Report of Commercial Reactor Critical Analyses Performed for the Disposal Criticality Analysis Methodology* (CRWMS M&O 1998b, pp. 40 to 42).

Table 3-1. Principal Isotopes for Commercial SNF 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	

Principal isotopes, presented in Table 3-1, may be used for disposal criticality analysis provided that the bias in k_{eff} associated with predicting the isotopic concentrations is established in the validation reports, as described in Section 3.5.3.1.

3.5.2.1.2 Initial Isotopic Concentrations of Commercial SNF

The commercial reactor SNF isotopic model is applicable to two waste forms: pressurized water reactor (PWR) and boiling water reactor (BWR) SNF. This model is used to calculate the change in isotopic inventory that results when the fuel is irradiated in a reactor. The change in isotopic inventory with irradiation (burnup) results in a change in the reactivity of the fuel. The fresh fuel that is initially loaded into the reactor (nominally in the form of ceramic UO_2 pellets) is enriched with the ^{235}U isotope. The initial enrichments for the current inventory of commercial SNF ranges from values slightly less than 2 wt% ^{235}U to values approaching 5 wt% ^{235}U. Most of the remaining uranium is the isotope ^{238}U, with trace amounts of other uranium isotopes present. The fissile isotopic content of the fuel changes with burnup. The ^{235}U concentration decreases, while ^{239}Pu and other fissionable actinides are produced. Additionally, actinide neutron absorbers and fission-product neutron absorbers are produced. The isotopic concentration of burnable absorbers present in the fuel assembly will also decrease with irradiation.

Establishing accurate initial isotopic concentrations at discharge for commercial SNF assemblies requires detailed knowledge of the fuel assembly design and the operating history of the fuel assembly in the commercial reactor. Operating history parameters include power density, fuel temperature, moderator temperature and density, soluble and burnable absorber concentrations, and control rod or control blade insertion history. Detailed knowledge of the operating history parameters for the entire irradiation cycle is desirable to produce accurate isotopic concentrations for the SNF. The fuel assembly design and the operating history of the fuel assembly affect the neutron spectrum that the fuel in the fuel assembly experiences. This, in turn, affects the depletion and buildup of the various isotopes in the SNF. Therefore, it is desirable to model both the geometry and the operating history of the fuel assembly as accurately as possible (e.g., with an exact representation).

It is not practicable to perform this level of detailed modeling of commercial SNF. Detailed fuel assembly design data and detailed operating history data can be obtained for model validation. The modeling approach for the isotopic model applies the transition matrix method along with a nuclear data library to solve the transmutation and radioactive decay equations that describe the isotopic changes as fuel is irradiated in a reactor. Approximations are made in the model to adequately account for three-dimensional neutron spectrum effects in establishing the initial isotopic concentrations of commercial SNF assemblies at discharge. The validation approach for the isotopic model and the establishment of an isotopic bias for k_{eff} are discussed in Section 3.5.3.1.

3.5.2.1.3 Source of Burnup Values for Commercial Fuel Assemblies

The burnup of a nuclear fuel assembly is a key input parameter in determining its isotopic concentrations. As noted in Section 3.5.1.1, burnup is a measure of the amount of exposure for a nuclear fuel assembly in a reactor core power production mode, usually expressed in units of GWd/MTU initially loaded into the fresh assembly. Since burnup is a time-dependent integral of exposure, it is difficult to measure this quantity outside of a reactor. Burnup values are determined from calibrated calculations that are continually verified through in-core measurements throughout the assembly's irradiation history.

Fuel assembly burnup values are used for reactor core reload licensing evaluations, spent fuel pool evaluations, on-site dry cask storage evaluations, and as the basis for the nuclear material accountability reports (NRC 741/742 Forms) filed with the NRC as required by 10 CFR Part 74. The verified burnup values are recorded for each commercial nuclear fuel assembly in reactor records kept by each utility and can be used as the basis for CSNF assembly burnup values for disposal criticality analyses. Standard contract agreements between DOE and the utilities, as well as NRC regulations, ensure that these verified burnup values will be available for every standard commercial fuel assembly intended for disposal.

DOE acknowledges that there is uncertainty in the burnup values from reactor records. As noted in *Determination of the Accuracy of Utility Spent-Fuel Burnup Records* (EPRI 1999, Abstract), the uncertainty associated with current plant measured burnup values (for a single Westinghouse PWR) is less than 2%. It is expected, although not yet demonstrated, that this is fairly consistent among the other vendors and for most utilities. The uncertainty in SNF assembly burnup values for future fuel discharges is expected to be at least as small as this value. For older fuel assemblies and plants, the uncertainty is expected to be somewhat greater. Thus, there are reasonable assurances that the power and burnup measurements made in operating reactors are reasonably accurate. Additional investigations, similar to the EPRI study, will be undertaken for both BWR and PWR reactor types to demonstrate this expectation of reasonable values in the uncertainty associated with reactor records.

The uncertainty associated with the burnup values from reactor records will be addressed in applications of the methodology. One option (i.e., subtracting the uncertainty from each assembly's assigned burnup value) is consistent with Recommendation 5 of *Interim Staff Guidance - 8, Revision 2. Burnup Credit in the Criticality Safety Analyses of PWR Spent Fuel in Transport and Storage Casks* (NRC 2002), which states in part:

> The assembly burnup value to be used for loading acceptance (termed the assigned burnup loading value) should be the confirmed reactor record value as adjusted by reducing the record value by a combination of the uncertainties in the record value and the measurements.

A second option, adjustment of loading curves, is preferable for disposal criticality analysis as it results in fewer data manipulations, and presents less opportunity for introducing calculational errors. For this latter option, a loading curve adjusted for burnup value uncertainty, is generated once and the assigned burnup values of all received assemblies are compared directly against this loading curve.

Also associated with loading fuel into a waste package in accordance with loading curves is the chance of a misload. Waste package misloads are to be evaluated as a preclosure event in the repository surface facility with potential impacts on postclosure performance. A misload of a waste package could occur due to surface-facility operational errors as well as utility shipping errors. It is proposed that effects of a single assembly misload event per waste package will be accounted for during the development of the waste package loading curves and will be evaluated as part of the analyses using the configuration generator model (Section 3.6).

An additional concern associated with burnup values is how to account for the axial profile burnup effect. This effect arises because the axial power and thus the fuel burnup vary along the length of fuel rods; in most cases diminishing near the ends of the rods. Recommendation 3 of *Interim Staff Guidance - 8, Revision 2. Burnup Credit in the Criticality Safety Analyses of PWR Spent Fuel in Transport and Storage Casks* (NRC 2002) states in part:

> "Of particular concern should be: a.) the need to account for and effectively model the axial … variation of the burnup within a spent fuel assembly…".

Axial profile effects will be accounted for by using conservative isotopic concentrations and/or conservative profiles in evaluating the criticality potential of waste package configuration classes.

3.5.2.1.4 Postclosure Isotopic Concentrations Considering Isotopic Decay

The approach used in the methodology to calculate isotopic concentrations over long time periods includes (1) an estimate of the uncertainty in k_{eff} values due to uncertainties in the isotopic decay parameters and (2) the use of bounding parameters in reactivity evaluations to ensure that the calculated values over time are conservative. This section discusses the modeling approach for addressing reactivity uncertainties due to isotopic decay uncertainties in the postclosure period and the next section discusses the use of bounding parameters for assuring conservative reactivity calculations.

An overview of the modeling approach for isotopic decay is presented in Figure 3-5. As shown in this figure, the evaluation starts with the initial isotopic concentrations at discharge. For commercial SNF, the modeling approach described in the previous subsection is used in establishing the initial isotopic concentrations. For other waste forms, design values for fissionable isotopic concentrations or the technical specification limits for fissile isotope concentrations are used in establishing the initial isotopic content. If more reactive isotopic inventories occur for these other waste forms that are based on reactor operations, the more reactive concentrations will be used for the initial isotopic content.

The initial concentrations and the decay time of interest are used in isotopic decay calculations to establish postclosure isotopic concentrations. As noted in Figure 3-5, a nominal criticality calculation is performed using the base isotopic concentrations from the decay calculations and a base reactivity established. The effects of uncertainties in the half-life and branching fractions on postclosure isotopic concentrations are evaluated by a statistical method (using Monte Carlo). This method for propagating uncertainties with a Monte Carlo analysis is based on performing many isotopic decay calculations while allowing the half-life and branching fractions for each isotope to vary randomly over their uncertainty ranges. The isotopic concentrations from each set of decay calculations (i.e., including all isotopes) are used in a criticality calculation and the reactivity reflecting the uncertainty is established. As noted in Figure 3-5, this process is repeated until sufficient trials are completed to achieve the desired confidence level. This approach is used to model the entire system of isotopic decay with all of the parent-daughter relationships and the effects of the uncertainties are quantified in this analysis in terms of the resulting isotopic distribution and its effect on reactivity. All isotopes that affect reactivity (i.e., isotopes in the library of the code used to calculate reactivity) are included in the calculation.

For commercial SNF, uncertainties in k_{eff} resulting from uncertainties in the half-life and branching fractions are established for a range of enrichments, burnups, and decay times. The uncertainties for other waste forms will be established for a range of initial fissionable isotope concentrations and decay times. The process also checks for systematic errors introduced by the method. If systematic errors are found, these are added to the uncertainty as a method bias. Evaluations will be performed for all waste forms and a bounding k_{eff} margin established for the postclosure decay uncertainty for each waste form.

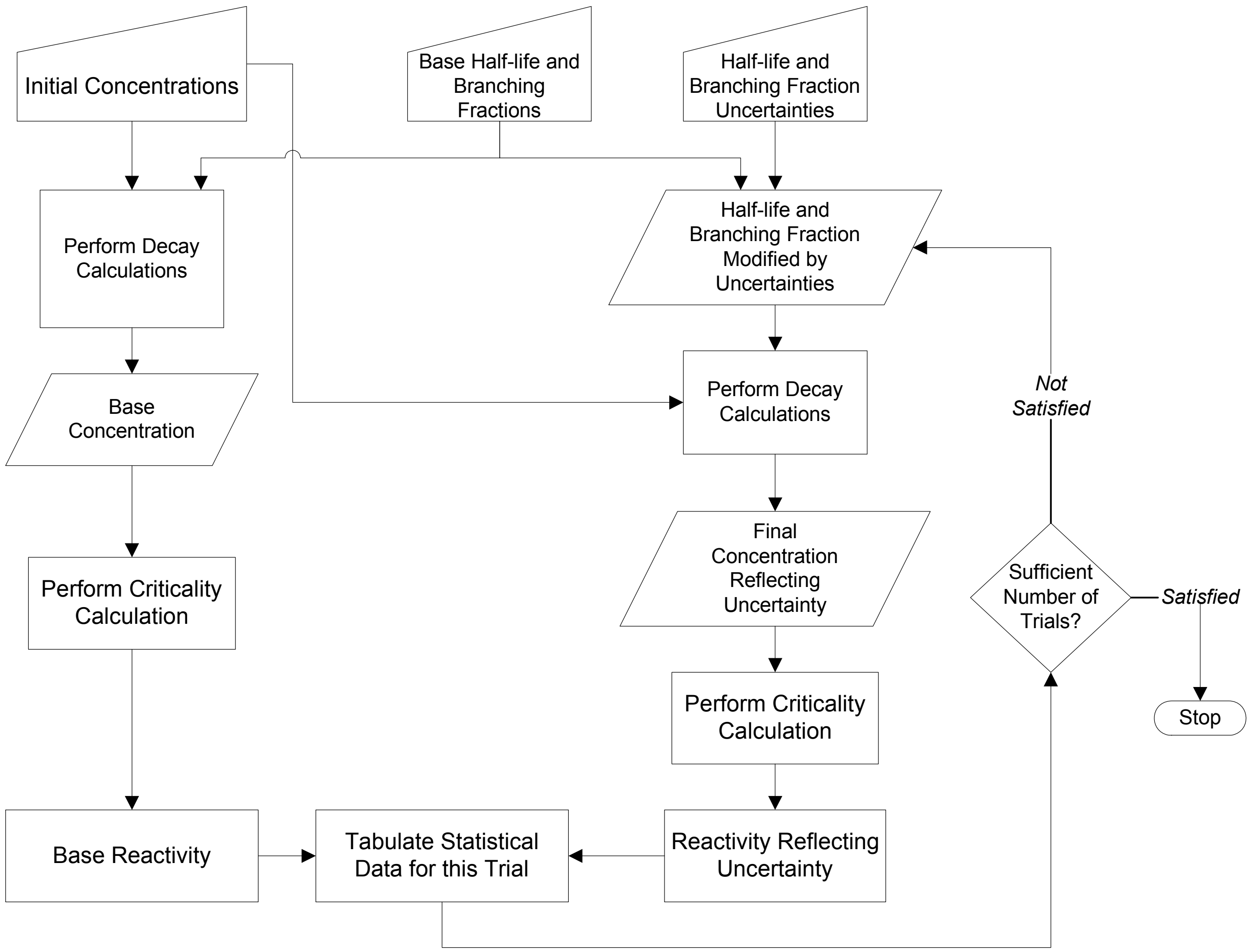


Figure 3-5. Modeling Approach for Postclosure Isotopic Decay

3.5.2.1.5 Isotopic Concentrations of Degraded Configurations

The application of the principal isotopes for commercial SNF or the fissionable isotopes for other waste forms in criticality evaluations is dependent upon their availability in the particular configuration that is analyzed. The isotopic model (including isotopic decay) and the degradation model establish the concentration of specific isotopes in any potentially critical configuration. When a waste form undergoes degradation because of reactions with water, the chemical makeup of the waste form is changed. The geochemical analysis model establishes the effect of the chemical degradation on the concentrations of specific isotopes.

For commercial SNF, the geochemical analysis establishes the fraction of each of the principal isotopes remaining in degraded configurations. This includes configurations ranging from commercial SNF with pinholes and cracks in the cladding to fully degraded configurations. Thus, the effects of radionuclide migration from fuel assemblies through pinholes and cracks in the cladding are considered.

The isotopic model establishes the initial concentration at discharge for each of the principal isotopes. The isotopic model is used for conservatively calculating isotopic concentrations for commercial spent nuclear fuel waste forms. Bounding parameters are chosen to ensure that the calculated reactivity of spent nuclear fuel is conservative. Radiochemical assay data or commercial reactor critical data are used to test the bounding parameter set to ensure that they produce conservative reactivity results for the enrichment and burnup ranges. Therefore, the uncertainty in the isotopic model is subsumed through the test of the bounding depletion parameter set for conservatism. Thus, the uncertainties associated with the capability of the isotopic model to predict isotopic concentrations for each principal isotope are incorporated in the geochemical analysis that establishes the isotopic concentrations of potentially critical configurations.

3.5.2.2 Criticality Modeling

The modeling approach for establishing k_{eff} values for waste form configurations is described in this subsection. The k_{eff} evaluations are performed over the range of parameters and parameter values obtained from the degradation analyses described in Section 3.4. These parameters include the isotopic concentrations that are established by the isotopic model. As discussed in Section 3.5.2.1.4, the geochemical analysis establishes the fraction of the initial isotopic concentrations remaining in the configurations analyzed. For postclosure, the degradation analyses will establish configurations for criticality evaluations that are inside and outside the waste packages, as well as configurations containing material from more than one waste package.

The criticality evaluations for postclosure configurations will be performed using a Monte Carlo method for solving the neutron transport equation. The Monte Carlo method is based on following a number of individual neutrons through their transport, including interactions such as scattering, fission and absorption, and leakage. The cross sections for the various neutron interactions dictate the reaction required for the criticality calculation at each interaction site. 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 loss by escape, parasitic capture, or absorption leading to fission. The average behavior of a sample set of neutrons is used to estimate the average behavior of the system with regard to the number of neutrons in successive generations (i.e., k_{eff}).

The Monte Carlo method allows explicit geometrical modeling of material configurations. Using appropriate material cross-section data in the criticality calculation is essential to obtaining credible results. The accuracy of the Monte Carlo method for criticality calculations is limited only by the accuracy of the material cross-section data, a correct explicit modeling of the geometry, and the duration of the computation. The accuracy of the method and cross-section data is established by evaluating critical experiments. Nuclear cross-section data are available from several source evaluations (data libraries). The choice of specific cross-section data will be evaluated during criticality model validation and documented in the analyses that will support licensing activities.

The criticality model applies the Monte Carlo method along with material cross-section data in calculating the k_{eff} values for potential configurations of fissionable and other materials identified by the degradation analyses. For the criticality evaluations, criticality is defined by the critical limit, which is the value of k_{eff} at which a configuration is considered potentially critical. The critical limit includes the criticality analysis method bias and uncertainty, which is consistent with ANSI/ANS-8.17-1984 with the exception noted in Section 2.3.2. Critical limit values are established by evaluating critical experiments that are representative of the range of in-package and out-of-package configurations identified by the degradation analyses. Section 3.5.3.2 provides a detailed discussion of the development of critical limit values and the applicability of these critical limit values to potentially critical configurations in the repository.

3.5.3 Validation Approach

The validation approach for the neutronic models used in assessing the criticality potential of waste forms during postclosure of the repository are described in the following two subsections. First, the validation approach for the isotopic model is described and, secondly, the validation approach for the criticality model is given.

3.5.3.1 Isotopic Validation

Isotopic model validation is performed for commercial SNF where burnup credit is part of the methodology. Design values for fissionable isotopic concentrations or the technical specification limits for fissionable isotope concentrations will be used in establishing the initial isotopic content for other waste form types. If more reactive isotopic inventories occur based on reactor operations, the more reactive concentrations will be used for the initial isotopic content. The validation approach for commercial SNF is described in this section. The approach for establishing the bias and uncertainty in the isotopic model is described in Section 3.5.3.1.1. The applicability of this bias and uncertainty for postclosure repository conditions will be demonstrated in analyses that will support licensing activities.

Additional requirements imposed for modeling burnup of commercial SNF for waste package design applications are presented in Section 3.5.3.1.2. These requirements are not part of the isotopic model validation process, but describe acceptance criteria for confirming that the isotopic model used for the design application of burnup credit is conservative. Confirmation of the conservatism in the application model will be demonstrated in analyses supporting the repository licensing process.

3.5.3.1.1 Establishing Bias and Uncertainty in Isotopic Model

The isotopic model used for burnup credit for commercial SNF is based on the principal isotopes presented in Section 3.5.2.1.1. These isotopes include 14 actinides and 15 fission products. One of the actinides, ^{233}U, is not present in current generation reactors, but this isotope will buildup to sufficient quantities over long disposal time periods (tens of thousands of years) to present a criticality concern. Thus, explicit model validation for this isotope is not included, because it is not present in current generation SNF. The uncertainty in the ^{233}U isotopic concentration can be inferred from the uncertainty in the decay of the precursors in conjunction with the uncertainty in the precursor (^{237}Np) concentration. The method presented in Section 3.5.2.1.3 will be used to establish this uncertainty. The isotopic model validation will consider the remaining principal isotopes.

The validation approach for the isotopic model uses commercial reactor critical and radiochemical assay data from both PWRs and BWRs. The commercial reactor critical and radiochemical assay data can be used to establish the bias and uncertainty in k_{eff} values predicted by the isotopic model. The bias and uncertainty in k_{eff} values will be incorporated in critical limit values established for commercial SNF as described in Section 3.5.3.2.5.

The bias and uncertainty of the commercial reactor critical and radiochemical assay data k_{eff} values are evaluated using a method based upon one of the lower bound tolerance limit determinations presented in Sections 3.5.3.2.8 and 3.5.3.2.9. The overall reactivity bias for the commercial reactor critical data is quantified by calculating Δk_{eff} between the measured (always 1.0) and calculated k_{eff} for each commercial reactor critical case. For the radiochemical assay data, the bias and uncertainty in Δk_{eff} values is established by comparing reactivity calculations performed using measured isotopic concentrations from assay samples with calculations performed using calculated isotopic concentrations for the assay samples obtained from the depletion code. The standard deviation of the data points is calculated, as the pooled standard deviation of the k_{eff} calculations and the standard deviation of the average k_{eff}. A confidence limit (typically 95 percent) is used in calculating the lower bound for the tolerance limit.

Calculations for the data set establish the reactivity effects due to irradiation of the fuel in a commercial reactor. The length of the irradiation time affects the reactivity of the fuel because of changes in uranium isotopic concentrations and the buildup of higher actinides and fission products. These changes in isotopic concentrations will, in general, increase with increasing irradiation time. The bias in Δk_{eff} values is established based on the depletion code's capability to predict the changes in the isotopic concentrations with increasing irradiation time (burnup) in the commercial reactor.

The isotopic model must be capable of predicting conservative reactivities for a variety of commercial spent fuel assemblies without recourse to detailed knowledge of the fuel and reactor characteristics. This can be accomplished by selecting bounding depletion parameters for use in determining Principal Isotope burnup credit loading curves for commercial spent nuclear fuel waste packages. For the analyses of commercial spent nuclear fuel, burnup history parameters such as power densities, moderator temperatures and densities, fuel temperatures, burnable absorber histories, control rod/blade histories, and soluble boron concentrations (for PWRs) affect the neutron spectrum that the fuel experiences. This, in turn, will affect the isotopic concentrations of the fuel. Thus, appropriate values for these parameters must be selected when establishing bounding depletion parameters.

The validation approach is to calculate the reactivity for a nominal fuel assembly with nominal depletion parameters and calculate the reactivity of an equivalent fuel assembly with the bounding depletion parameters. The calculated reactivity with the bounding parameters should be conservative (i.e., larger than the calculated reactivity for the nominal parameters). Further, the difference between these reactivities should be larger than the sum of the bias and uncertainty determined from the commercial reactor critical or radiochemical assay data set in order to ensure conservatism of the isotopic model. If this latter criterion is not met, a revised set of bounding parameters must be selected.

The analyses of the assay samples will use burnup history parameters that are based on three-dimensional neutron diffusion-depletion analyses. Some of the three-dimensional analyses will be based on core-follow calculations where the fuel assembly that contains the assay sample is followed through its entire irradiation history in the core. This level of detailed core-follow data is not available for some of the assay samples. However, the operating history data that is available will be used to reconstruct burnup history parameters based on representative three-dimensional diffusion-depletion calculations. Sensitivity analyses will then be performed to provide an estimate of the uncertainty introduced by the use of reconstructed burnup history parameters.

In cases where a one-dimensional neutron transport-depletion model is used, it will contain additional uncertainty because of the limited capability to represent individual fuel assembly heterogeneities. Limitations in the capability of the one-dimensional model will be addressed through the use of a two-dimensional neutron transport-depletion model. Sensitivity analyses will be performed to estimate the uncertainty associated with the approximations made in the one-dimensional model. The uncertainties established from the approximations in the burnup history parameters and the approximations in the one-dimensional model will be compared to the uncertainty established from analysis of the radiochemical assay data with the two-dimensional neutron transport-depletion model. These uncertainties will be summarized in the isotopic model report.

3.5.3.1.2 Requirements for Confirmation of Conservatism in Application Model

For design applications, two aspects of the isotopic model for commercial SNF must be addressed. First, values for the initial isotopic concentrations must be conservative with respect to their contribution towards criticality. Second, changes to the initial isotopic concentration values as a function of time for postclosure must also be conservative with respect to their contribution towards criticality. Proposed requirements that address these two aspects are presented in this section. Confirmation of the conservatism in the bounding isotopic model used for burnup credit for commercial SNF will be demonstrated in analyses that will support licensing activities.

The first two requirements will ensure that the initial isotopic concentrations are conservative with respect to criticality. The third requirement will ensure that changes to the initial isotopic concentration values as a function of time will also be conservative with respect to criticality. These requirements are stated as follows:

A. Reactor operating histories and conditions must be selected together with burnup profiles such that the isotopic concentrations used to represent commercial SNF assemblies in waste package design shall produce values for k_{eff} that are conservative in comparison to any other expected combination of reactor history, conditions, or profiles.

B. Bounding reactor parameters will be used to predict isotopic concentrations that, when used in criticality evaluations must produce values for k_{eff} that are conservative when compared to similar criticality evaluations using either measured radiochemical assay data or best-estimate isotopic concentrations.

C. The values for the isotopic concentrations representing commercial SNF must produce conservative values for k_{eff} for all postclosure time periods for which criticality analyses are performed.

The first requirement addresses how reactor operating histories and conditions affect the isotope concentrations in commercial SNF assemblies discharged from reactors. The representation of the burnup profiles is also considered in calculations of the isotopic concentrations. The quantities and distributions of the isotopic concentrations are governed by the operating history of the reactor, including accompanying local neutron spectral effects. Local neutron spectral effects are modeled for the burnup calculations by including local power densities, moderator densities, and fuel temperatures, as well as soluble boron, burnable poisons, and control rod histories. Bounding burnup profiles will be identified from an axial burnup profile database. The isotopic concentrations for these fuel assemblies are normally based on the detailed modeling of the reactor operating histories and local conditions within the fuel assemblies during reactor operations. For waste package design, the detailed modeling of reactor operating histories is not practical. Bounding values must also be chosen for the parameters that represent reactor operating histories and conditions. The bounding burnup profiles, along with the bounding parameter values to represent reactor operating histories and conditions will be used to verify that the methodology application for waste package design is conservative with respect to criticality.

The second requirement addresses the problem of using integral experiments (commercial reactor criticals) exclusively for confirming the conservatism in the isotopic model and imposes the additional use of radiochemical assay data for commercial SNF. Radiochemical assay data are generally measured for a small sample of a fuel rod. The measured assay data will be used as input for a criticality calculation. The isotopic model then will be used to generate isotopic concentrations for input to a criticality calculation at the same condition (enrichment, burnup, and decay time) as the assay data. Both calculations will consider those isotopes that were measured, plus moderator and cladding material. Following this procedure, the bounding isotopic model that will be used for design applications must be shown to be conservative with respect to k_{eff} based on analysis of the entire range of radiochemical assay data.

The third requirement addresses changes to the initial isotopic concentration values, as a function of time, for postclosure. As described in Section 3.5.2.1.3, uncertainties in the half-life and branching fractions used in determining postclosure isotopic concentrations are propagated with a statistical method (using Monte Carlo). Using the approach described in Section 3.5.2.1.3, uncertainties in k_{eff} resulting from uncertainties in the half-life and branching fractions are established as a function of enrichment, burnup, and decay time. Satisfying Requirement C will require repeatedly applying the method for treating uncertainties in isotopic decay to a range of sets of initial isotopic concentrations to determine the largest values for uncertainty in k_{eff}.

These requirements are provided to ensure that the assumptions used in modeling fuel depletion (and decay during the disposal time period) for design applications are conservative with respect to criticality. None of these requirements addresses changes in the isotopic concentrations resulting from geochemical processes. Changes in the isotopic concentrations from geochemical processes are addressed by the geochemical model, with the uncertainty in the resulting concentrations being represented in the probability distributions for the configurations analyzed for criticality.

3.5.3.2 Criticality Validation

This section presents a systematic approach for validation of the methodology used to calculate the criticality of a waste package. It is organized as follows: (1) selection of benchmark experiments, (2) establishment of the range of applicability of the benchmark experiments, (3) experiment data types, (4) development of critical limits associated with the computer codes and nuclear data used to calculate criticality, and (5) the criticality potential criteria.

Figure 3-4 showed the approach presented, starting with benchmark experiments and input from analyses using the configuration generator model (Section 3.6) for internal and external waste package configurations. This is the same general approach to validation of calculational methods for criticality given by Dyer and Parks (1997, pp. 15 to 19) and Lichtenwalter et al. (1997, pp. 139 to 182).

In this approach, criticality experiments are selected from a group of experiments that include laboratory critical experiments and commercial reactor criticals. The selected experiments will be used to determine a bias and uncertainty associated with computer code analysis of the experiments. The range of certain physical characteristics of these experiments will establish their Range of Applicability.

Similarly, a set of waste package configurations that are to be analyzed will be selected from the list of Master Scenarios (Section 3.3). The range of parameters chosen for the waste package configuration should be within the parameters chosen for the range of applicability of the experiments. If the Range of Applicability includes the Range of Parameters, the next step will be to establish a critical limit.

If the Range of Applicability does not include the entire Range of Parameters, there are two choices: (1) add other experiments such that the Range of Applicability does include the Range of Parameters or (2) determine a penalty for extending the range of application of the existing set of experiments. Finally, the critical limit will be applied for determining the criticality potential of a configuration class, as described in Section 3.5.3.2.10.

3.5.3.2.1 Selection of Experiments

The calculation method used to establish the criticality potential for a configuration class needs to be validated against measured data that have been shown to be applicable to the configuration under consideration. This section provides background for selecting suitable experiments to use for the validation process.

In the past, criticality experiments were designed to mock-up specific fissionable materials, reactor configurations, fabrication processes, storage casks or transportation systems. These experiments generally consisted of the same, or nearly the same, configurations and materials as the waste package. Many of the experiments were characterized according to elemental constituents, densities, and various parametric ratios. Various ratios of metal-mass-to-water-mass or hydrogen-mass to fissionable-isotope-mass were used. Other parameters included, (a) fuel lattice pitch, and (b) parameters that described material concentrations, geometry, or ratios of moderator to fissionable-isotope physical characteristics (Lichtenwalter et al. 1997, p. 179). With the use of more sophisticated techniques, which could characterize the neutron spectrum, major neutron reactions like fission or absorption were used. Some of these parameters were used as global parameters for correlating experiments to evaluations of systems of similar fissionable species, enrichments, degree of heterogeneity, or homogeneity, and to chemical form. In addition, various neutron energy-weighted parameters, such as thermal neutron absorption versus total neutron absorption and average neutron energy group (where multi-group calculations were used) weighted by fissions were used for the characterization of systems and their associated computational biases. The use of these parameters became a means for determining biases and trends in biases as a function of these parameters. They also became the defining characteristics, or one of several defining characteristics that establish the range (or area) of applicability of the experiments themselves. These parameters and others will be investigated in the same general approach given by Lichtenwalter et al. (1997, pp. 139 to 182) and Dyer and Parks (1997, pp. 15 to 19).

The benchmark experiments will be selected from a set of experiments, which consists of laboratory critical experiments, PWR commercial reactor criticals, and BWR commercial reactor criticals for each applicable scenario/waste class from the list of Master Scenarios (Section 3.3). The selection process will consider such aspects as material type, geometry, and neutron spectrum.

3.5.3.2.2 Range of Applicability

In ANSI/ANS-8.1-1998 (p. 1), the term “area of applicability” means “the limiting ranges of material compositions, geometric arrangements, neutron energy spectra and other relevant parameters (such as heterogeneity, leakage, interaction, absorption, etc.) within which the bias of a calculational method is established.” The term “area of applicability” and Range of Applicability are used interchangeably here.

Bias is a measure of the systematic differences between the results of a calculational method and experimental data. Uncertainty is a measure of the random error associated with the difference between the calculated and measured result. When evaluating biases and uncertainties and choosing parameters (or areas) for which a bias would exhibit a trend, there are three fundamental areas (Lichtenwalter et al. 1997, p. 179) that should be considered:

1. Materials of the waste package and the waste form, especially the fissionable materials
2. The geometry of the waste package and waste forms
3. The inherent neutron energy spectrum affecting the fissionable materials.

There are substantial variations within each of these categories that require further considerations. These are discussed in Lichtenwalter et al. (1997, p. 180). Quantifying the various categories of parameters is complicated and generally requires approaches that use benchmark experiments that are characterized by a limited set of physical and computed neutron parameters that are then compared with the neutronic parameters of a waste package. In this case, the application is a particular waste package in various forms of degradation as defined by the list of Master Scenarios (Section 3.3).

In the general practice of characterizing biases and trends in biases, one would first look at those fundamental parameters that might create a bias. That is, what are the main parameters that could be in error and have the most significant effect on the accuracy of the calculation? Important areas for evaluating criticality are the geometry of the configuration, the concentration of important materials (reflecting materials, moderating materials, fissionable materials, and significant neutron absorbing materials), and the nuclear cross sections that characterize the nuclear reaction rates that will occur in a system containing fissionable and absorbing materials. Quite often, it is not simple to characterize the trends in a bias for some of the fundamental parameters chosen. In most cases, other parameters, called proxy parameters, will exhibit statistically definable trends. Generally, these proxy parameters reflect the effects of a combination of fundamental parameters; therefore, a proxy parameter is one that acts in the place of one or more fundamental parameters.

It is desirable that the range of the fundamental parameters of the benchmark critical experiments (Range of Applicability) and the range of the fundamental parameters of the system (Range of Parameters) evaluated be identical. This is not practical usually, and for those parameters that do not show a bias, it is acceptable to use critical benchmark experiments that cover most, but not all, of the Range of Parameters of the system under evaluation. In these situations, expert judgement may be used to determine if there is a reasonable assurance that the two are sufficiently close.

3.5.3.2.3 Extension of the Range of Applicability

In the case of a geologic repository where the criticality evaluation must cover a period of thousands of years, it is not possible to reproduce with experimental data the numerous geometric and material configurations that could occur. It is sufficient to provide assurance that the selected critical experiments provide a reasonable validation of the calculational methods used. Where data are not available, it is prudent to use appropriate bounding models or assign additional penalties. In these cases, there may be an extension of the Range of Applicability to cover the Range of Parameters of the system.

The means used to extend the Range of Applicability will depend on a number of factors. These include, but are not necessarily limited to: (1) the nature of the critical experiments used to determine the range of applicability and trends with biases, (2) the particular waste form involved, and (3) the availability of other proven computer codes or methods used to evaluate the situation.

ANSI/ANS-8.1-1998 (p. 18) Appendix C, Section C4 will be used for the extension of the Range of Applicability:

> The area (or areas) of applicability of a calculational method may be extended beyond the range of experimental conditions over which the bias is established by making use of correlated trends in the bias. Where the extension is large, the method should be:

A. subjected to a study of the bias and potentially compensating biases associated with individual changes in materials, geometries or neutron spectra. This will allow changes, which can affect the extension to be independently validated. In practice, this can be accomplished in a stepwise approach; that is, benchmarking for the validation should be chosen (where possible) such that the selected experiments differ from previous experiments by the addition of one new parameter so the effect of only the new parameter, on the bias can be observed.

B. supplemented by alternative calculational methods to provide an independent estimate of the bias (or biases) in the extended area (or areas) of applicability.

If a Range of Applicability is extended, where there is a trend in the data, without the use of additional experiments, additional penalty will be added to the criteria used to determine if a system has potential for criticality. The same techniques described above for extending the Range of Applicability when there are trends may be used to determine the additional penalty: (1) expert judgement (an evaluation by someone skilled, by training and experience, in criticality analysis), (2) sensitivity analysis, (3) statistical evaluation of the importance of these parameters, or (4) comparison with other credible methods (code-to-code comparisons).

For situations where a bias (trend) is not established, there are two options for extending the Range of Applicability. If the extension of the Range of Applicability is small and the understanding of the performance of the criticality code for these parameter ranges is also understood, it would be appropriate to use the established lower bound tolerance limit and an appropriate penalty to calculate the critical limit. If the extension is not small, then more data, covering the range of applicability, will be necessary. When more data are obtained, the process illustrated in Figure 3-4 must be applied to the new data set. This applies when the range of applicability for fundamental parameters (material concentrations, geometry, or nuclear cross-sections) does not cover the range of parameters of the waste package configuration and no trend is exhibited.

3.5.3.2.4 Experiment Types

Two types of experimental data will be used in validating the criticality model. These are laboratory critical experiments and commercial reactor criticals. Various parameters will be trended with the k_{eff} values from the laboratory critical experiments and the commercial reactor criticals. These trends will be used to establish biases and uncertainties of the criticality model.

The commercial reactor criticals represent intact commercial SNF in known critical configurations. Although the commercial reactor critical evaluations provide integral criticality benchmarks for SNF in a reactor, they do not provide separate benchmarks for concentrations of individual isotopes. The commercial reactor criticals are used as criticality benchmarks for SNF in an intact form.

Laboratory critical experiments selected to cover the appropriate ROPs will be used to benchmark the criticality model for a range of fissionable materials, enrichments of fissile isotopes, moderator materials, and absorber materials. These experiments will be used to calculate bias and uncertainties for degraded waste forms, including degraded SNF. The laboratory critical experiments will also be used for intact waste forms that are not SNF.

3.5.3.2.5 Determination of the Critical Limit

An essential element of validating the methods and models used for calculating effective neutron multiplication factors, k_{eff}, for a waste package is the determination of critical limit. The critical limit is derived from the bias and uncertainties associated with the criticality code, nuclear data (including appropriate benchmarks), and modeling process. The criticality code and modeling process will be referred to as the criticality code for the discussions in the following sections.

The critical limit for a configuration class is a limiting value of k_{eff} at which a configuration is considered potentially critical. The critical limit is characterized by statistical tolerance limits that account for biases and uncertainties associated with the criticality code trending process, and any uncertainties due to extrapolation outside the range of experimental data, or limitations in the geometrical or material representations used in the computational method.

In equation notation, the CL is represented as (based on Section 5 of ANSI/ANS-8.17-1984):

$$CL(x) = f(x) - \Delta k_{EROA} - \Delta k_{ISO} - \Delta k_m \qquad \text{(Eq. 3-1)}$$

where

- x = a neutronic parameter used for trending
- $f(x)$ = the lower bound tolerance limit function accounting for biases and uncertainties that cause the calculation results to deviate from the true value of k_{eff} for a critical experiment, as reflected over an appropriate set of critical experiments
- Δk_{EROA} = penalty for extending the Range of Applicability
- Δk_{ISO} = penalty for isotopic composition bias and uncertainty
- Δk_m = an arbitrary margin ensuring subcriticality for preclosure and turning the CL function into an upper subcritical limit function (it is not applicable for use in postclosure analyses because there is no risk associated with a subcritical event).

A critical limit is associated with a specific type of waste package and its state (intact or various stages of degradation described by the list of Master Scenarios (Section 3.3). The critical limit is characterized by a representative set of benchmark criticality experiments. This set of criticality experiments also prescribes the basic Range of Applicability of the results. A critical limit function may be expressed as a regression-based function of neutronic and/or physical variable(s). In application, a critical limit function could also be a single value, reflecting a conservative result over the range of applicability for the waste form characterized.

The steps that need to be completed in establishing a critical limit are as follows: (1) selection of benchmark experiments; (2) establishment of the Range of Applicability of the benchmark experiments (identification of physical and spectral parameters that characterize the benchmark experiments); (3) establishment of a lower bound tolerance limit; and (4) establishment of additional uncertainties due to extrapolations or limitations in geometrical or material representations.

Modeling and inputs for computing the effective neutron multiplication factor for a critical experiment with a criticality code often induce bias in the resulting k_{eff} value. These k_{eff} values deviate from the expected result (k_{eff} = 1) from benchmark sets of critical experiments. The experimental value of k_{eff} for some benchmarks may not be unity, however it is assumed to be unity for purposes of calculating errors. This assumption is permitted per ANSI/ANS-8.1-1998, Section 4.3.1.

Sections 3.5.3.2.6 through 3.5.3.2.9 address the statistical methods to account for differences in the results from exercising the criticality code in the calculation of k_{eff} and the expected value of k_{eff}.

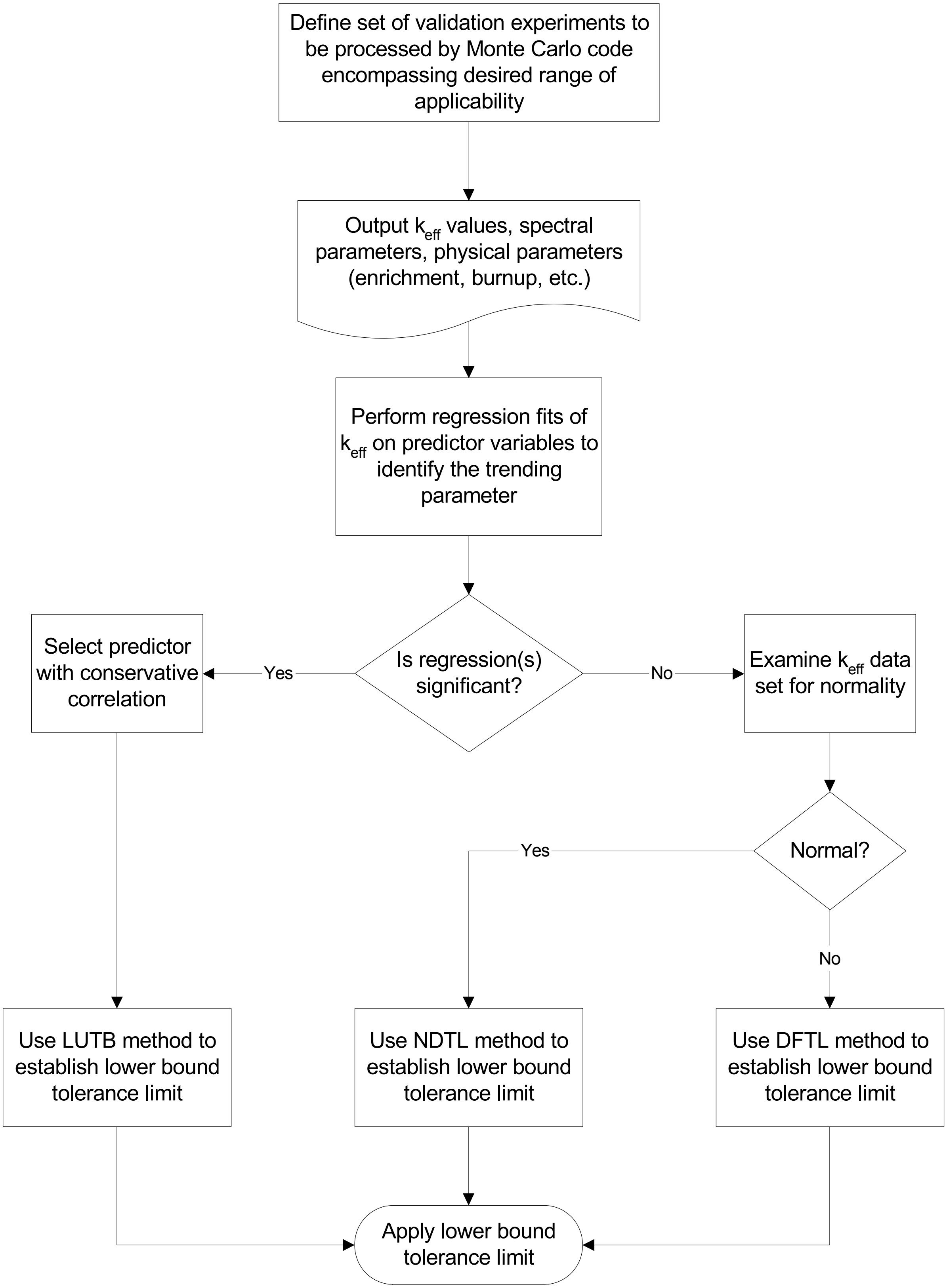
3.5.3.2.6 Development of Lower Bound Tolerance Limit Functions

The application of statistical methods to biases and uncertainties of k_{eff} values is determined by trending criticality code results for a set of benchmark critical experiments that will be the basis of establishing lower bound tolerance limits for a waste form. This process involves obtaining data on various neutronic parameters that are associated with the set of critical experiments used to model the code-calculated values for k_{eff}. These data, with the calculated values of k_{eff}, are the basis of the calculation of the lower bound tolerance limit function.

The determination of lower bound tolerance limit functions for a waste form is data dependent, and the set of benchmark critical experiments must be carefully selected to cover the range of parameters expected in the repository. Quantity, diversity, and quality of data are important considerations to assure appropriate Range of Applicability coverage for a waste form.

The lower bound tolerance limit function for a waste form results from the process shown in Figure 3-6. The data set and the resulting k_{eff} values produced by the criticality code must be confirmed as appropriate and valid for the waste form. This is fundamental to the development of the lower bound tolerance limit function. The objective of this process is to produce lower bound tolerance limit's that are statistically meaningful and practical in application.

The purpose of the lower bound tolerance limit function is to translate the benchmarked k_{eff} values from the criticality code to a design parameter for a waste form/waste package combination. This design parameter is used in criteria for determining criticality potential. To meet this purpose, it is necessary to account for criticality code calculation differences from the true value of the effective neutron multiplication factor of 1.0. This latter value is an assumption, as explained above. The lower bound tolerance limit definition addresses biases and uncertainties that cause the calculation results to deviate from the true value of k_{eff} for a critical experiment, as reflected over an appropriate set of critical experiments.



Note: LUTB Lower Uniform Tolerance Band
NDTL Normal Distribution Tolerance Limit
DFTL Distribution Free Tolerance Limit

Figure 3-6. Process for Calculating Lower Bound Tolerance Limits

Figure 3-6 displays two general statistical methods for establishing lower bound tolerance limit functions. These two methods are: (1) regression-based methods reflecting criticality code results over a set of critical experiments that can be trended, and (2) random sample based methods that apply when trending is not an appropriate explanation of criticality code calculations. The regression approach addresses the calculated values of k_{eff} as a trend of spectral and/or physical parameters. That is, regression methods are applied to the set of k_{eff} values to identify trending with such parameters. The trends show the results of systematic errors or bias inherent in the calculational method used to estimate criticality. In some cases, a data set may be valid, but might not cover the full range of parameters used to characterize the waste form. The area (or areas) of applicability of a calculational method may be extended beyond the range of the experimental conditions of the data set over which the bias is established by making use of correlated trends in the bias. This is covered in Section 3.5.3.2.3.

If no trend is identified, a single value may be established for a lower bound tolerance limit that provides the desired statistical properties associated with the definition of this quantity. The data are treated as a random sample of data (criticality code values of k_{eff}) from the waste form population of interest and straightforward statistical techniques are applied to develop the lower bound tolerance limit. For purposes of differentiation, this technique will be described as "non-trending." The normal distribution tolerance limit method and the distribution free tolerance limit method, described below, are "non-trending" methods.

The regression or "trending" methods (Section 3.5.3.2.7) use statistical tolerance values based on linear regression techniques to establish a lower bound tolerance limit function. Trending in this context is linear regression of k_{eff} on the predictor variable(s). Statistical significance of trending is determined by the test of the hypothesis that the regression model mean square error is zero. Here the predictor variable(s) may be a parameter such as burnup, or a parameter that indicates the distribution of neutrons within the system, such as the average energy of a neutron that causes either fission or absorption. Where multiple candidates are found for trending purposes, each regression model will be applied and the conservative model will be used to determine the value of the lower bound tolerance limit. The lower uniform tolerance band method, described below, trends a single parameter against k_{eff}. Multiple regression methods that trend multiple parameters against k_{eff} may also be used to establish the lower bound tolerance limit function. In either single or multiple situations, the regression trend that produces the lowest lower bound tolerance limit is defined to be the more conservative regression.

In non-trending situations, standard statistical tolerance limit methods, which characterize a proportion of a population with a confidence coefficient, are used to establish the single-valued lower bound tolerance limit function that applies for the range of applicability of the set of critical experiments. There are two standard tolerance limit methods described, each specific to the result of examination of the hypothesis of normality of k_{eff} values of the benchmark set of critical experiments. Section 3.5.3.2.8 addresses situations in which the distribution of the k_{eff} values for the set of benchmark critical experiments can be treated as coming from a normal probability distribution. This technique is the normal distribution tolerance limit. Section 3.5.3.2.9 describes the distribution free tolerance limit method. The distribution free tolerance limit method applies when trending is not appropriate and the data for the benchmark critical experiments do not pass the test for normality. In this situation, there is no assumption about the form of the underlying probability model. Assumptions, however, are necessary about the randomness of the process and the data as representing a random sample from the population of interest.

In all calculations of lower bound tolerance limit functions, the concept described as the "no positive bias" (Lichtenwalter et al. 1997, p. 160) rule must be accommodated. This rule excludes benefits for raising the lower bound tolerance limit for cases in which the best estimate of the bias trend would result in a lower bound tolerance limit greater than 1.0. The treatment of this element is discussed below in the context of each method used to establish the basic lower bound tolerance limit function.

The lower bound tolerance limit function is defined as:

$$f(x) = k_C(x) - \Delta k_C(x) \qquad \text{(Eq. 3-2)}$$

where

- x = parameter vector used for trending
- k_C (x) = the value obtained from a regression of the calculated k_{eff} of benchmark critical experiments or the mean value of k_{eff} for the data set if there is no trend
- Δk_C (x) = the uncertainty of k_C based on the statistical scatter of the k_{eff} values of the benchmark critical experiments, accounting for the confidence limit, the proportion of the population covered, and the size of the data set.

The statistical description of the scatter quantifies the variation of the data set about the expected value and the contribution of the variability of the calculation of the k_{eff} values for the benchmark critical experiments.

Based on a given set of critical experiments, the lower bound tolerance limit is estimated as a function (f[x]) of a parameter(s). Because both Δk_C (x) and k_C (x) can vary with this parameter, the lower bound tolerance limit function is typically expressed as a function of this parameter vector, within an appropriate range of applicability derived from the parameter bounds, and other characteristics that define the set of critical experiments.

The calculational bias, β, is defined as:

$$\beta = k_C - 1 \qquad \text{(Eq. 3-3)}$$

and thus the uncertainty in the bias is identical to the uncertainty in k_C (i.e., $\Delta k_C = \Delta\beta$). This makes the bias negative if k_C is less than 1 and positive if k_C is > 1.

To prevent taking credit for a positive bias, the lower bound tolerance limit is further reduced by a positive bias adjustment. The positive bias adjustment sets k_C = 1.0 when k_C exceeds 1.0.

The following sections discuss the various methods for estimating a lower bound tolerance limit function. Section 3.5.3.2.7 presents the regression method for trending k_{eff} versus a parameter vector. Sections 3.5.3.2.8 and 3.5.3.2.9 detail the other two methods to be used if statistically significant trends cannot be identified via regression methods for a set of benchmark experiments.

3.5.3.2.7 Regression Methods

The method preferred for assessing criticality code calculation trending biases and associated uncertainties is to use statistical tolerance limits based on a regression-modeled trend on a single predictor variable. This preference for a single trending variable allows simpler interpretation and application of a lower bound tolerance limit function of some neutronic or physical parameter. The statistical tolerance limit method, discussed in *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages (*Lichtenwalter et al. 1997, pp. 157 to 162) as Method 2, is applicable only for a single predictor variable.

A method similar to the regression-based statistical tolerance limit described as Method 2 in *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages (*Lichtenwalter et al. 1997, pp. 157 to 162) is found in "Simultaneous Tolerance Intervals in Regression" (Lieberman and Miller 1963, p. 165). The latter method can be used for single or multiple predictor variables and requires only readily available probability functions.

The objective is to use regression methods that are appropriate for the data generated by the criticality code for the relevant set of critical experiments. The purpose is to define the lower bound tolerance limit function as a statistically meaningful result that yields a conservative lower bound tolerance limit over the range of applicability associated with the predictor(s).

A process that identifies the significant predictor variable(s) described above begins with multiple regression techniques on a field of candidate trending variables the same or similar to those described in Section 3.5.3.2.1. The multiple regression models can be used as a filter to identify predictor variables that should be examined in detail.

Collinearity is the existence of near-linear relationships (strong correlation) between predictor variables in multiple regression analyses. Where a strong correlation exists between two or more predictor variables, each of these variables provides essentially the same contribution to the prediction result. Predictor variables that have statistically significant coefficients in multiple regression may not have a statistically significant coefficient in a simple linear regression model. That occurs when one variable is highly correlated with another predictor variable, but not with the dependent variable. Such a variable would not be an asset for trending the bias of a criticality code. The variable with which it is highly correlated and which exhibits statistical significance in the simple linear regression model would be considered for further evaluation relative to other possible predictor variables.

Those predictor variables that result in statistically significant linear regression models would be investigated to establish a conservative lower bound tolerance limit function. From these results, the conservative value may be selected as the lower bound tolerance limit. If use of a single predictor variable is not practical, then multiple predictor variable regressions will be evaluated using the methods in Lieberman and Miller (1963, p. 165).

For situations in which there is a single predictor variable in the trending regression, the method for estimating a lower bound tolerance limit function uses a tolerance band approach referred to as a single-sided, uniform width, closed interval, approach by Lichtenwalter et al. (1997, pp. 160 to 162). This will be referred to as the lower uniform tolerance band method. This approach produces a lower tolerance band that is a constant difference from the regression estimate of the effective neutron multiplication factor, accounting for non-positive bias considerations. Further, this approach deals with estimates of criticality for a population of waste material, which is the approach used here for a repository. This is the preferred method for estimating a conservative lower bound tolerance limit provided a significant trend is identified with a single predictor variable.

The purpose of this method is to estimate a uniform width tolerance band over a specified closed interval for a linear least-squares regression fit. The neutronic or physical parameter chosen to trend the lower bound tolerance limit is the one that 1) exhibits a meaningful correlation, 2) has a meaningful interpretation, and 3) results in a conservative lower bound tolerance limit function. A detailed description of the basic lower uniform tolerance band method is given by Lichtenwalter et al. (1997, pp. 160 to 162), Bowden and Graybill (1966, pp. 182 to 198), and Johnson (1968, pp. 207 to 209).

Provisions are made to keep the lower bound tolerance limit constant once the trended k_{eff} of the benchmark data exceeds 1.0. This " no positive bias" concept is maintained for conservatism in all proposed methods for estimating a lower bound tolerance limit.

There is a specified confidence that, at least, a specified percentage of the systems that are above the lower bound tolerance limit are not critical systems. Consequently, there is also this same confidence that a small portion of the systems with a k_{eff} less than the lower bound tolerance limit function value are critical systems.

3.5.3.2.8 Normal Distribution Tolerance Limit

The normal distribution tolerance limit method is one of two techniques for estimating a lower bound tolerance limit for the repository in a non-trending situation. In this case, the capability of the criticality code to calculate k_{eff} values varies in a random fashion that is not correlated with a particular neutronic or physical parameter(s). The normal distribution tolerance limit method assesses the capability of the criticality code to predict k_{eff} values as a single figure of merit encompassing all the evaluations for the set of benchmark criticality experiments.

The normal distribution tolerance limit method is used for conditions in which the values of k_{eff} are sufficient in number and scope to determine reasonable justification of normality of the k_{eff} values for the critical experiments. When data do not justify normality as an underlying probability model, it is common and practical to apply mathematical transformation techniques to the data, and test these transformed values for normality. If the transformed data can be considered normally distributed, then statistical tolerance limits may be computed on this data set, and an inverse transformation of this result back to k_{eff} becomes the basis of the normal distribution tolerance limit.

Given that the k_{eff} values produced by the criticality code for the benchmark experiments are shown to be normally distributed, the lower bound tolerance limit can be calculated as

$$\textit{lower bound tolerance limit} = k_{ave} - k(\gamma, P, n) \times S_P \qquad \text{(Eq. 3-4)}$$

where

k_{ave} = the average of the k_{eff} values, unless k_{ave} is greater than unity (1.0), in which instance the appropriate value for kave should be 1.0 to disallow positive uncertainty

$k(\gamma, P, n)$ = a multiplier (Natrella 1963, pp. 1-14 and 1-15) in which γ is the confidence level, P is the proportion of the population covered, and n is the sample size

S_P = the square root of the sum of the inherent variance of the critical experiment data set plus the average of the criticality code variances for the critical experiment data set (Lichtenwalter et al. 1997, p. 159).

In the event that data transformation is necessary to justify normality, the contribution of the criticality code uncertainty cannot be included in the quantity S_P resulting from a normalizing transformation. For this instance, the quantity

$$k(\gamma, P, n) \times S_{Ccave} \qquad \text{(Eq. 3-5)}$$

where S_{Ccave}, the square root of the average of the criticality code variances, will be used to reduce the value determined via inverse transformation. This would be a conservative result.

3.5.3.2.9 Distribution Free Tolerance Limit

The distribution free tolerance limit method applies when trending is not appropriate and the data for the benchmark critical experiments do not pass the test for normality. This approach establishes the lower bound tolerance limit through the use of distribution-free statistical tolerance limit methods. The term non-parametric methods is also used to describe this approach, but for consistency and to emphasize that the underlying nature of the distribution from which the random sample is obtained is unimportant, the term distribution-free is used in this report.

The requirement for applying distribution-free methods to establish a statistical tolerance limit is that the data be from a random sample from a continuous distribution. The methods are described in *Experimental Statistics* (Natrella 1963, pp. 1-14, 1-15, 2-15) and *Introduction to Mathematical Statistics (*Hogg and Craig 1966, pp. 182 to 185).

Applying this method is straightforward when the resulting indices for the sample size, confidence level, and the portion of the population to be covered are included in published tables (Natrella 1963, Tables A-31, A-32). In this case, one uses the table for the appropriate values for confidence, population coverage, and sample size and obtains an index value, which is applied to the ranked (sorted) values of the k_{eff} results. For instance, if the sample size is 100 and a 95/95 percent lower tolerance limit is desired, the index is two. This means that the second smallest observation serves as the 95/95 percent lower one-sided tolerance limit. Specific computations would be required for cases not included in published tables (e.g., 95/99.5 percent).

For this method, the number of observations must be sufficient to accommodate the desired confidence level and portion of the population to be covered. For instance, if normality is not justified, and the number of observations is fewer than 59, one cannot make a 95 percent confidence statement about 95 percent of the population being above the smallest observed value. Such a limit would be close to, but not quite, a 95/95 percent lower tolerance limit because at least one of the statement descriptors would not be strictly met.

The "no positive bias" concept can be met by substituting 1.0 minus three standard deviations ($3 \times \sigma$) for all values of k_{eff} that are greater than 1.0, where σ is the variation of k_{eff} taken from the criticality code calculation. If, for instance, the set of k_{eff} values to be validated consisted of N "experiments," then applying this method involves sorting the k_{eff} values in ascending order such that,

$$k_{eff1} < k_{eff2} < k_{eff3} < \ldots < k_{effN} \quad \text{(Eq. 3-6)}$$

and the values of k_{eff} greater than 1.0 are modified as defined above, and all N k_{eff} are then sorted in ascending order. The next step is to establish the value of the subscript index that will provide the desired confidence level that the desired portion of the population is covered. If the subscript is I, then

$$\textit{lower bound tolerance limit} = k_{eff\,I} \quad \text{(Eq. 3-7)}$$

is the lower bound tolerance limit with the characteristics of confidence and population coverage available for the data set of interest.

3.5.3.2.10 Criticality Potential Criterion

The criticality potential criterion is determined by the final comparison of the k_{eff} for a configuration class with the applicable critical limit. This will determine which configuration classes have a potential for criticality. In equation notation, the criticality potential criterion for a waste package system is as follows:

$$k_s + \Delta k_s < CL \quad \text{(Eq. 3-8)}$$

where

k_s = calculated k_{eff} for the system

Δk_s = an allowance for:

(a) statistical or convergence uncertainties, or both in the computation of k_s

(b) material and fabrication tolerances, and

(c) uncertainties due to the geometric or material representations used in the computational method

[Note: allowance for items (b) and (c) can be obviated by using bounding representations]

CL = the value of k_{eff} at which a configuration is considered potentially critical, accounting for the criticality analysis method bias and uncertainty, and any additional uncertainties (i.e., Δk_{EROA} and/or Δk_{ISO}).

3.6 ESTIMATING PROBABILITY OF CRITICAL CONFIGURATIONS

This section describes the general methodology approach for estimating the probability of occurrence of configurations with fissionable material in the repository and the probability of criticality for configurations with potential for criticality. The probability calculation has two objectives. The first objective is to support an estimate of the risk of criticality in terms of the overall increase in radionuclide inventory available for transport and the effect of this increase on the dose at the accessible environment. The second objective is to provide a criterion for estimating the effectiveness of the variety of measures used to control or limit postclosure criticality.

3.6.1 Criticality Probability Methodology Approach

Potential critical configurations are states of a degraded waste package/waste form defined by a set of parameters characterizing the quantity and physical arrangement of the material that have a significant effect on criticality. There are various uncertainties associated with these parameters depending on the combination of FEPs that result in degraded configurations. These uncertainties need to be accounted for in the criticality evaluation. In order to handle parameter uncertainty, analyses will use a risk-informed, performance-based approach to evaluate the range and physical arrangement of all parameters associated with waste package/waste form configurations. This methodology is developed in a configuration generator model that forms a risk-informed, performance-based analysis tool.

The purpose of the configuration generator model is to provide a process to identify configuration classes that have the potential for criticality and then evaluate the probability of criticality for any configuration classes that exceed the critical limit for the waste form. The configuration generator model provides a systematic process to address the standard criticality scenarios (Section 3.3), having the potential to increase the reactivity of the in-package system, and the parameters associated with identified potentially critical waste package configurations (see Figure 3-1). The approach utilizes event tree/fault tree sequences to define end states of degradation scenarios. The probability of the end states is derived from PDFs for degradation parameters.

The configuration generator methodology can be summarized as performing the following functions:

- Identify possible sequences required for the development of configuration classes and their various end states
- Evaluate the probability of occurrence for the configuration classes
- Provide configuration classes and their associated parameter ranges to the criticality model to identify configuration classes with potential for criticality
- Evaluate the probability of criticality for configuration classes that have potential for criticality
- Evaluate the total probability of criticality for the monitored geologic repository.

The first step in estimating the probability of occurrence of degraded configurations is to develop sequences to possible end-states from the standard scenarios (Section 3.3). These sequences are the result of repository environmental circumstances and waste package/waste form evolution.

Probabilities are associated with branches in the sequences that contribute to estimating the probability of occurrence of the end-states. The individual waste forms will generally have a range of characteristics (e.g., burnup and enrichment, which vary significantly over the family of commercial SNF) that also have associated probabilities that contribute to estimates of the probability of criticality for a given configuration.

For the probabilistic analysis part, the configuration generator model uses an event tree approach to express the degradation processes and sequences that lead to the different configurations. The construction of the event tree captures all of the configurations included in the list of Master Scenarios (Figures 3-2a and 3-2b). The Master Scenario List shown in Figures 3-2a, 3-2b, 3-3a, and 3-3b represents three general degradation configurations in the repository having criticality potential. These configurations are based on locations inside the waste package (IP), outside the waste package in the near field (NF), and outside the waste package in the far field (FF). These three different locations are broken down into specific configuration classes (i.e., six IP configuration classes, five NF configuration classes, and three FF configuration classes).

Event tree sequences start with a listing of the different waste forms for a configuration class anticipated for the repository that provides a bookkeeping mechanism. However, for analysis purposes, specific waste forms will be used in order to tailor the degradation parameters for both the waste form and waste package. The event tree then lists in sequential order the degradation processes required to reach each of the end-states of the event tree for the particular class. The top events in the event tree sequences are the specific processes required for degradation. The branching under the top events (degradation processes) provides a traceable sequence to each configuration class. The different configuration classes are identified as end states in the event tree.

The degradation processes listed as top events are developed into fault tree logic submodels. The majority of the fault trees contain single inputs; however, some processes (i.e., drip shield failure) contain multiple inputs. The fault tree inputs need to consider many variables, the most important of which is the time dependency. The whole degradation process and the achievement of the configurations are based on time, starting at the closure of the repository.

The second major part of the configuration generator model addresses the calculation of the criticality potential for a given configuration and ties the criticality analysis together with the probability analysis. The configuration generator model identifies the different configurations based on the Master Scenario List following the sequences through the event tree to reach the different waste form and waste package configurations. Once the configurations have been identified, the probability of the configurations are evaluated and compared to the screening criteria (Section 3.1) and if not satisfied, the potential for criticality needs to be evaluated (Figure 3-1). A detailed criticality evaluation is performed for these configurations and if the calculated k_{eff} is greater than the critical limit, then a probability analysis of the critical configuration is performed.

In order to perform the probabilistic analysis, probability density functions (PDF) for the parameters associated with the potential critical configurations are required. These PDFs are derived from the information concerning the drift environment, waste form variables, and waste package variables and is obtained from various sources such as the TSPA model or developed from abstractions.

Both the criticality potential and the probability of criticality calculations are dependent entities that use the PDFs as input. A detailed analysis is performed for all configurations that have a k_{eff} greater than the critical limit. A probability analysis is then performed only if the waste package and waste form combination for a specific configuration has a k_{eff} greater than the critical limit as required (Section 3.1). The probability analysis will use the Range of Parameters determined from the criticality analysis.

The potential for criticality of a waste form configuration in the waste package is determined by the material composition and the physical arrangement (or geometry) of this material composition. For a waste package containing CSNF, for example, the initial configuration is the waste package as loaded with commercial light-water-reactor fuel assemblies. The fuel assemblies in this initial configuration are intact or contain detected pinhole leaks; thus, the fuel rods within the fuel assembly have the same geometry as during their operation in the commercial reactor. This initial configuration in the waste package is subcritical since the waste package is designed to ensure that condition. Thus, potential criticalities can only occur for degraded configurations.

3.6.1.1 Configuration Generator Model Event Tree

The configuration generator model event tree represents the degradation processes and sequences that lead to the different configuration classes included in the Master Scenario List shown in Figures 3-2a and 3-2b (Section 3.3). The event tree is developed in a comprehensive manner in order to capture all of the processes and sequences that lead to one of the configuration classes associated with the IP scenarios, the NF scenarios, or the FF scenarios. These related configuration classes are constructed in the configuration generator model event tree software that is appropriate for performing probabilistic risk assessment evaluations. The configuration generator model event tree is used to evaluate all of the degraded configurations to identify those having potential for criticality, thus requiring further analysis. The top events on the event tree are the specific processes required for degradation. Branching under the top events (degradation processes) provide a traceable sequence to each end-state. The different configuration classes are a collection of particular end states in the configuration generator model event tree.

3.6.1.2 Fault Tree Model

The processes listed as top events are managed by fault trees that may contain multiple inputs depending on the process being evaluated. The fault trees have their logic broken into different gates that represent the probability of the particular process occurring at each time step that represents the time in years after closure of the repository. These time steps can be adjusted for particular analyses. By breaking the fault tree up into these specific time steps, only the probability of the process at that particular time step is included in the final result. The fault trees are developed in this manner to account for the different time dependent probabilities of the processes.

Fault trees that contain multiple inputs are those required to represent both time dependent and time independent probabilities. An example of this type of fault tree is the one representing the drip shield failure mechanisms. The drip shield has two major failure mechanisms, the first is due to static failures (i.e., time independent) and the second is due to general corrosion, which is time dependent. Static failures are those that can happen randomly at any time during emplacement or during the life of the drip shield. An example, for instance, is drip shield emplacement failure. These static failures contain a single failure probability that does not change over time. General corrosion of the drip shield progresses with time and affects the number of patches on the drip shield and the fraction of failed drip shields at any particular time. The number of drip shield failures due to general corrosion thus changes over time and is accounted for by structuring the fault tree with these time dependent inputs.

3.6.1.3 Parameter Probability Distributions

There are two general types of parameter probability distributions. There are those that characterize the time for completion of a scenario process, and are represented by a probability density function for the time of occurrence of the completion event (e.g., time of occurrence of waste package breach). There are also parameter distributions that characterize the value of configuration-related parameters, and are represented by the cumulative distribution function of the parameter in question (e.g., the thickness of absorber plate remaining in the waste package).

The distributions developed for scenario-related parameters involve the physical and chemical analyses identified in Sections 3.3.1 and 3.3.2. These models are the ones developed for use in the TSPA, and the justification of the models is accepted as part of the performance assessment process. The following is a list of the major probability distribution models and parameter uncertainties:

1. Performance Assessment (PA) Nominal Case distribution of breach times for waste packages developed using TSPA methodology (e.g., the waste package degradation model). Essential inputs to waste package degradation model come from output form various PA models, (e.g., climate model and seepage model). Such information on the spatial distribution of waste package penetrations on a single package may also be useful to develop distributions of other important configuration parameters, such as how long the waste packages can hold water. The waste package breach time is an important parameter because the internal degradation processes are all driven by aqueous corrosion.

2. Distribution of times for the complete degradation of the waste form or non-SNF components in the waste package. The distribution is based on the uncertainty in degradation rates, which, in turn, stems from the uncertainty in the environmental parameters causing the degradation (particularly the flow of water) and the uncertainty in the underlying degradation processes. Since criticality can occur without complete degradation of these waste package components, it is generally more useful to consider the distribution of degradation parameters, which is best analyzed as a configuration-related distribution, as described below.

For the configuration-related parameters, the concern is with the range of possible parameter values that can arise, and with the subrange(s) that can lead to a critical configuration class. Generally, criticality is determined by several configuration parameters acting together so the criticality potential of a configuration class can be determined only after all the parameters have been specified. The following is a partial list of such parameters:

1. Waste form isotopics (based on burnup, enrichment, and time since discharge for commercial SNF).

2. Parameters characterizing the amount of waste form remaining intact.

3. Parameters characterizing the amount and geometry of fissionable material released by the degradation of the waste form and remaining in the waste package.

4. Parameters characterizing the amount of neutron-absorber material remaining in the partially degraded or collapsed structural intact components.

5. Parameters characterizing the amount and geometry of neutron absorber released by the degradation of its carrier and remaining in the waste package.

6. The amount of moderator (principally water, but also including the evaluation of silica where appropriate, particularly for external configurations). For potential fast criticalities, the amount of moderator needed would be low.

7. The amount and distribution of moderator displacing material (e.g., iron oxide).

8. The amount of neutron reflector material surrounding the fissionable material.

This determination of critical configurations is based on the premise that the waste forms are loaded into the proper waste package. Misloads within the same waste form can be accommodated within the parameter ranges. For commercial SNF, there may be several different designs or means of limiting the criticality potential to correspond to different ranges of burnup and initial enrichment.

3.6.1.4 Validation of the Configuration Generator Model

Because the configuration generator model is a probabilistic model, indirect validation methods are used since experimental data are not available for comparison with model results. However, where applicable, the configuration generator model uses the output from a number of validated model abstractions that do not need further validation. Where validation activities are required, these consist of the following as appropriate:

- Technical review of the probabilistic structure of the configuration generator model and the parameter abstractions.

- Determining the goodness-of-fit for parameter abstractions developed as sub-models in the configuration generator model. The quality test results from several functional fits were evaluated to select the particular distribution for use in the configuration generator model.

3.7 ESTIMATING CRITICALITY CONSEQUENCES

This section describes the portion of the methodology approach for estimating the consequences of potentially critical events internal and external to the waste package[5]. As discussed in Section 3.1, when the total probability of criticality for the repository satisfies the design probability criterion but does not satisfy the 10 CFR Part 63 regulatory probability criterion for exclusion of events from TSPA, a consequence analysis of the contributing waste forms will be performed (Figure 3-1, Box 8). The probability weighted radionuclide source term from the consequence analysis and, as needed, other consequence analysis results of criticality events will be input to the TSPA process, as indicated in Section 3.8.

The objective of the consequence evaluation is to identify and quantify the important parameters associated with criticality events that affect the TSPA risk assessment and provide this information to TSPA. The conservatism in the consequence evaluations will be demonstrated in the analyses. Thus, quantifying the parameters will include demonstrations of sensitivities and/or bounding values.

A description of the criticality consequence methodology approach is given in Section 3.7.1 and a discussion of specific models within the approach in Section 3.7.2. Methods for validation and verification of the specific models are described in Section 3.7.3.

3.7.1 Criticality Consequence Methodology Approach

The general criticality consequence approach used in the methodology involves an evaluation of the physical processes that can occur in configurations having the potential for criticality. The contributing physical processes are generally inter-dependent and determine the types of direct consequences that may emerge from the hypothetical events. The principal consequence of a criticality event with respect to the repository risk assessment is the incremental increase in the radionuclide inventory accessible for transport to the external environment. However, criticality events exhibit other consequence phenomena such as increased temperatures and engineered barrier system degradation that can affect the radionuclide transport mechanisms, and their effects are also considered in the consequence methodology.

The steady state criticality consequences are determined by the configuration power level that is a function of the seepage or percolation rate into the system as well as other configuration parameters that affect the system reactivity. Transient criticality consequences are determined primarily by the reactivity values (Δk), positive and/or negative that control the power production. These latter reactivity values are relative changes from a base configuration that is assumed to be critical.

3.7.1.1 Type of Criticality Event

The consequences of a criticality event depend upon the type of event and the configuration in which the criticality event occurs. Before describing the methodology approach for evaluating

[5] The need to perform criticality consequence calculations for Naval Nuclear Propulsion Project SNF is discussed in "Transmittal of the Naval Nuclear Propulsion Program Addendum to the Yucca Mountain Site Characterization Office 'Disposal Criticality Analysis Methodology Topical Report'" (Mowbray 1999).

possible criticality events that might occur in, or near, the repository at Yucca Mountain, it is useful to summarize those physical aspects of criticality that strongly influence the nature of the consequence. These characteristics are identified and then summarized.

1. Slow versus fast reactivity insertion rates
2. Steady-state versus transient events
3. Under-moderated versus over-moderated configurations.

Slow versus fast reactivity insertion rate–Potential worst-case reactor criticality events could involve reactivity insertion times of somewhat less than 1.0 second. Most geologic processes will provide slow reactivity insertion mechanisms (one week or more), but certain configurations have the potential for more rapid insertion (0.3 to 100 seconds) if initiated by a sudden mechanical disturbance. Examples of phenomena causing possible rapid reactivity insertions are disruptive events that may include, but are not necessarily limited to, seismic events and/or rockfall (CRWMS M&O 1997c, p. 60).

Steady-state versus transient events–A steady-state (or static) criticality event produces energy at a relatively low but fairly constant rate whereas a transient criticality event has the potential of generating a much higher power level than a steady-state event. However, a transient criticality event generates significantly less total energy because of its short duration. Significant kinetic energy releases will not likely occur during transient criticality events since the events that can occur in the repository will be sufficiently slow to preclude such consequences. Some theoretical analyses (Bowman and Venneri 1996; Gratton et al. 1997) have identified situations conducive to large, disruptive consequences, but the required accumulation and geometry of the requisite fissionable mass is expected to be beyond anything physically possible in the repository (Van Konynenburg 1995), which will be demonstrated as part of the support of licensing activities. In order to produce a sufficiently rapid transient criticality releasing an amount of kinetic energy sufficient to cause the movement of material within or outside the waste package, the fissionable mass would have to:

- Be confined either externally or inertially

- Have a reactivity sufficiently above critical that the rate of increase of neutron density and power generated (proportional parameters) is rapid (e.g., has a doubling time of less than 1/1000 second).

The steady-state methodology approach starts with the already identified potentially critical configurations and estimates the power and duration of a steady-state criticality using a zero-dimensional model. The primary consequence resulting from a steady-state criticality is the incremental change in the radionuclide inventory over the duration of the event. A second consequence that can exacerbate the radionuclide mobility for an internal steady-state criticality is an increase in the corrosion rate of the engineered barrier system resulting from increased local temperatures. This could potentially permit an increase in the nuclide mobility from sequence alteration and/or chemical alteration of the environment.

The transient methodology approach uses codes that evaluate both the neutronic evolution and the response of the physical system to any heat or pressure pulse caused by the criticality event. Transient criticality events could experience immediate mechanical consequences from a pressure pulse that could lead to barrier deterioration if the pressure exceeded the barrier yield strength. Preliminary analyses have thus far failed to indicate such severe mechanical consequences (Section 3.7.2.2), but evaluation of such effects will continue as part of the methodology approach. Longer-term consequences will include not only the incremental increase in the radionuclide inventory, but also, for internal waste package events, effects resulting from elevated temperatures such as enhanced corrosion rates. Thus, both short- and long-term consequences from hypothetical transient criticality events can lead to an increase in the radionuclide mobility. The specific approach for evaluating consequences of steady-state and transient criticality events is discussed in Section 3.7.2, Criticality Consequence Modeling Approach.

Under-moderated versus over-moderated configurations–For well moderated configurations that are potentially critical, there is an optimum moderator concentration (which yields the smallest possible critical mass for that moderator material). Physically, this moderator concentration balances the slowing-down properties of the moderator against its neutron-absorbing properties. A configuration is said to be under-moderated if it has less moderator than this optimum concentration, and over-moderated if it has more. An over-moderated configuration has more than enough moderator for slowing down the neutrons, but increased parasitic neutron capture diminishes the net neutron slowing-down density. Therefore, for an over moderated configuration, removing moderator may increase the k_{eff}, because neutron absorption decreases, and at the same time, there is still sufficient moderating capacity to support thermal criticality. A second function of a moderator is as a neutron reflector that may be either internal or external to a waste package, enhancing the neutron population and thereby increasing the k_{eff} of the configuration.

The most efficient moderating material available in the repository is water percolating through the drift tuff, primarily through fractures, and into the waste package (internal criticality). Silica in the rock itself or precipitated from the percolation flow as well as carbon in any form can also serve as somewhat less efficient moderators. However, since they are less effective moderators than water, it is unlikely that a critical mass can be accumulated with these moderators alone, as explained in Section 3.7.2.

3.7.1.2 Evaluating Direct Criticality Event Consequences

Steady-state and transient criticality analyses are used to calculate the increase in radionuclide inventory with the steady-state analysis providing a more conservative (larger compared to a transient analysis) estimate of total radionuclide increase for similar parameter ranges.

The steady-state analysis approach focuses upon the power and duration of a criticality event. The power level is determined by the reactivity feedback (the influence of material inventories and thermodynamic parameters on k_{eff}), the heat removal, and the rate of replenishment of the moderator. The latter is most strongly determined by the environmental parameters, particularly the drift seepage fraction that enters the waste package, for internal criticality, or the percolation rate into the region of accumulation, for external criticality. The next step is to evaluate the total burnup for the power history in order to estimate the incremental increase in the radionuclide inventory caused by the criticality event.

Coupled processes involving temperature, corrosion rates, and nuclide mobility will be considered in evaluating steady-state criticality consequences. It is possible that localized temperature increases might lead to enhanced corrosion rates of the engineered barrier system that might subsequently lead to increased nuclide releases. However, tests have shown that the general corrosion rates of Alloy 22 and Titanium are not very sensitive to temperature in the parameter range expected in the repository (CRWMS M&O 2000a, Section 3.4.1.2). Since the consequence methodology proceeds in an explicit manner, coupled processes must be evaluated through sensitivity analyses.

Identifiable mechanisms leading to possible transient criticality events without water moderation are limited to situations involving highly enriched fissionable material. These situations are all unlikely, requiring large accumulations of fissionable material or special circumstances such as disruptive events. Thus, the transient criticality methodology utilizes hydraulic mechanisms to connect processes and the analyses consider both the neutronic and other physical responses of the system to the temperatures and pressures generated if rapid energy releases occur during criticality events. The first part of the transient analysis evaluates the power, temperature, and pressure pulses from the event. Immediate consequences primarily result from the pressure pulse and may include, for internal criticalities, engineered barrier system deterioration if the pressure exceeds the barrier yield strength contributing to possible enhancement of the radionuclide mobility. Mechanical consequences from external criticalities may increase rock fracturing near the location of the event if sufficient pressures are generated, and thus affect nuclide mobility. Longer-term consequences resulting from elevated temperatures may include, for internal criticality events, effects such as enhanced corrosion rates. However, the duration of elevated temperatures from transient criticality events is of short duration, which will mitigate any effects on the corrosion rates. Both immediate and long-term consequences to the physical system will be evaluated, as appropriate, although any significant mechanical consequences are expected to be unlikely. The next step in the analysis is to compute the total burnup for the power history to estimate the increment in radionuclide inventory caused by the criticality event.

Potential critical configurations in the repository will be in a neutronically compact form that ensures the system reacts in phase (i.e., different sub-regions in a reaction-zone will not have different characteristic time constants). The transient neutronic behavior can be adequately described with zero-dimensional methods using parameters that reflect the net effects of spatial and neutron energy variation. In applications, these variations are determined at each time step by the spatially and temporally dependent models for the thermodynamic and mechanical behavior of the system. Higher order methods (multi-dimensional and/or explicit spectral effects) are available for use in the averaging process for input parameters to the zero-dimensional models (e.g., point reactor kinetics) utilized in the consequence methodology.

3.7.2 Criticality Consequence Modeling

There are two different time dependent behaviors of a criticality to be considered: transient and steady-state. The modeling approach to critical consequence evaluation emphasizes the use of hydraulic mechanisms to couple processes. This approach derives from an absence of alternative moderators (see Section 3.7.1.2 for high enrichment fissionable materials) that would allow an internal criticality event without the contribution from water moderation (e.g., the critical volume with silica moderation might require more than the enclosed waste package volume), and from the greater effectiveness of water moderation for external criticality events. However, any potential critical configurations that incorporate alternate or additional moderators will be evaluated. The specific models used by the methodology for each time domain will be refined for activities in support of the licensing process. Examples of possible criticality configurations involving multiple moderators are internal waste package clay environments and external environments, each containing both water and silica.

The steady-state model applies when the approach to criticality is sufficiently slow to permit the negative feedback mechanisms to hold the k_{eff} close to unity, so that there is no rapid energy release. While the most efficient critical configurations include water moderation, potential configurations with moderators other than water are considered in estimating criticality probabilities and any subsequent consequence analysis. The other possible moderators present in the repository are carbon and silica. Primary sources of carbon are carbonate precipitates and microbial communities (DOE 1998, Section 3.3). Carbon in any form can serve as a neutron moderator, but the likelihood of its presence in the repository in sufficient quantities to act as a moderator is negligible. Silica is a component of the tuff around the repository (77 wt% SiO_2) and in some SNF forms. However, external criticality evaluations (CRWMS M&O 1998c, Section 7 and Table 7.4-8), where silica is the only moderating material, indicate that it is not an effective moderator, requiring fissile mass accumulations of ~100 kg per cubic meter to approach criticality (this estimate is for fissile plutonium in a tuff cube with no water: the mass required for fissile uranium under these conditions is larger than for plutonium). Moderation by silica-water mixtures is more efficient than silica alone, and can lead to reductions in the fissile mass required for criticality (CRWMS M&O 1998c, Table 7.4-8). The steady-state criticality portion of the methodology will additionally consider static heat and mass transfer phenomena. For such a steady-state criticality, the principal concern is with the increased radionuclide content remaining after the duration of the criticality event. However, the effect of an elevated temperature on the integrity of the engineered barriers for the duration of the steady-state criticality will also be evaluated.

The transient model applies to the case in which the approach to criticality (reactivity insertion) is fairly rapid, so that the k_{eff} will overshoot the value of unity leading to an (initially) exponential increase in power that is coupled to thermal and mechanical effects, until the negative feedback mechanisms cause the k_{eff} to drop back below unity. The transient criticality portion of the methodology will incorporate equations of heat, mass, and momentum transfer plus equations of state for the materials involved. The transient criticality model is concerned with the characterization of the energy release in two regimes that are differentiated by the magnitude of the reactivity feedback to possibly produce either a high power pulse with short duration, or the cumulative buildup of radionuclide increments over a periodic pulsing regime. The distinguishing characteristic between these two regimes is the potential for reactivity recovery through moderator replacement. Pulsing can only occur if the expelled moderator can return to the critical volume. The possibilities and consequences for attaining specific configurations that enable either transient regime will be determined by the analyses supporting licensing activities.

Both transient and steady-state models will be developed for the two general locations where a criticality event may occur: (1) internal to the waste package, (2) external in either the near field (i.e., drift) or in the far-field. The region of applicability of these models will be demonstrated prior to their use in activities supporting the repository licensing process.

3.7.2.1 Steady-State Criticality, Internal

The methodology approach to quasi-steady-state internal criticality uses a bounding concept based upon the premise that a critical condition is attained through a slow (on the order of years), possibly cyclic, process such as the inflow of water increasing the neutron thermalization capability of the system. 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 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 (terminate) the criticality process. 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 a criticality event is bounded either by the length of the high moisture part of a climatological cycle, which might be as long as 10,000 years (DOE 1998, Volume 3, p. 3-13), or by the amount of excess reactivity available to sustain the event. The subsequent return of a moist cycle, upwards of 10,000 years after the shutdown, would be unlikely, and would likely be irrelevant for the steady state criticality events because continued degradation of the waste package would have removed the conditions necessary for criticality (e.g., intact waste package bottom that supports water ponding, or optimum spacing between fuel rods). Possible additional factors influencing the criticality duration within the above bound are the available fissile mass, thermally enhanced degradation rates, and loss of soluble neutron absorbers. Implementation of the first factor in the modeling will likely shorten the duration through burnup of fissile material. Enhanced degradation rates will likely shorten the criticality duration through increased loss of fissionable material as well as an increased displacement of moderator material with accumulation of insoluble degradation products. The last factor (i.e., loss of soluble absorbers) if relevant, will tend to extend the duration of the event by reducing non-fission neutron losses in the system. Processes allowing the loss of soluble fission products from spent fuel rods include the transport of radionuclides through cladding perforations. A range of parameter values will be used in the simulations for determining the steady-state power level for a critical configuration resulting in a probability distribution for the incremental radionuclide inventory.

It should be noted that the steady-state model can be applied to a criticality event in which there is no standing water, but only water loosely bound to clay. Although such water can be removed by evaporative heating, wicking moisture into porous clay (i.e., rewetting) requires more time than allowing an equivalent water ingress to a free-volume. Therefore, comparatively low evaporation rates are sustained in wet clay, and the steady power levels and consequent incremental radionuclide production rates are conservatively maximized by ignoring the presence of the clay and considering only water moderation.

The principal direct consequence of a steady-state criticality is an increase in the radionuclide inventory that is primarily dependent on the power level of the criticality and its duration, both of which are strongly determined by the drip rate of water into the package. The incremental radionuclide inventory is readily computed from the isotopic model (Section 3.5.2.1) with a given initial set of isotopes obtained from the same model for a criticality event (or process) of a specified power level and duration. The isotopic concentrations used in the calculations are those that lead to the criticality event. A criticality event, if one occurs, will generate shorter-half-life radionuclides not included in the TSPA calculations because they will have decayed away before the waste form is mobilized. They can also be excluded from criticality event consequence calculations because they will decay away before they can reach the biosphere. However, the neutron flux, which is the principal determinant of the radionuclide increment, is determined primarily by the power level, and is relatively insensitive to the slight difference in fissile concentration that is reflected in the difference between k_{eff} at the critical limit and a $k_{eff} = 1$.

Degradation rates for waste package materials may increase slightly as a consequence of a steady-state criticality due to the potential elevated temperatures in the critical system. Temperature dependent degradation rates will be incorporated into the geochemistry corrosion models used in support of licensing activities to evaluate such consequences. Corrosion rate enhancement due to elevated temperatures may result in an increased radionuclide inventory available for release and transport to the accessible environment by reducing the time to failure. These effects will be considered in the complete evaluation of criticality consequences (Section 3.7.1.2 and 3.7.3.1).

3.7.2.2 Transient Criticality, Internal

The transient internal criticality methodology approach is based upon the premise that a critical condition is attained through some relatively rapid (seconds to hours) shift in the internal waste package geometric arrangement that increases the fissionable mass participating in a reaction to a critical size, decreases neutron absorber efficiency, or alters neutron reflection. Configurations allowing fast criticalities will be considered for SNF and other waste forms, and will be evaluated for transient criticality potential. Most cases of relevance will involve water moderation, and the methodology approach emphasizes situations (supported by preliminary criticality analyses) where significant water retention is required to initiate a criticality event, even where mixtures of different moderator materials are present. An example of such a circumstance is if one or more assemblies shift (or fall) from above the waste package water level to below the water level due to some mechanical disturbance. Such criticality events involving commercial SNF within a waste package are similar to transient criticality events in reactor systems that a number of transient criticality codes have been developed to analyze. Thus, there is reasonable confidence in the capability of such codes to provide conservative results for the transient internal criticality applications within this analysis methodology. The validation methods for the computational models that are essential to the flow analysis most appropriate to a transient criticality in a horizontal waste package are discussed in Section 3.7.3.2.

The transient internal criticality methodology approach includes both slow and relatively rapid reactivity insertion mechanisms such as described in Section 3.7.1.1. The reactivity insertion rate is determined by sudden initiating events affecting the waste package. Such events may include, but are not limited to, seismic shaking, rock fall, or volcanism. The more rapid reactivity insertion mechanisms might typically have a duration of approximately 0.3 seconds (e.g., the time an SNF assembly might take to fall a short distance). The transient criticality code is used to calculate the time dependent evolution in k_{eff} resulting from the reactivity addition coupled with the following negative reactivity feedback mechanisms:

1. Doppler broadening of absorption cross-sections in relevant nuclides

2. Moderator voiding due to thermal expansion and evaporation or boiling at heated surfaces.

The methodology approach is applicable to configurations having a wide variation in fissile content that primarily affects the Doppler reactivity coefficients. However, negative moderator void reactivity coefficients will always be present for under-moderated configurations and ultimately control a transient criticality event. The moderator reactivity is supplied as a tabulated set of critical calculations that include the effects of over- and under-moderated configurations and is determined as the difference between the dynamic tabular values and the critical reference value. The moderator coefficient is a derived quantity implicit in the reactivity as a derivative with respect to density. For over-moderated systems, reactivity increases with decreasing density. For under-moderated systems, reactivity decreases with decreasing density. Although the neutronic time evolution in the methodology is calculated from a zero-dimensional model, the reactivity parameters incorporate spatial effects through integration of the distributed thermal-hydraulic calculations for the configuration.

As the transient power increases, the fission energy heats the fuel material and water moderator, pressurizing the system (to a degree inversely proportional to the total area of waste package openings) and leading ultimately to expulsion of the moderator from the waste package, terminating the criticality. Sensitivity of the consequences to variations of the configuration parameters will be evaluated to aid in quantifying the conservatism in the analysis. The particular parameters to be evaluated will be identified during the critical limit screening process. These may include, but are not necessarily limited to, parameters such as partially collapsed arrangements or the volume of water and iron oxide within the waste package.

There is no single consequence measure for a transient criticality event. Direct consequences can occur in four categories:

1. An incremental increase in the radionuclide inventory that depends on the excursion power history and the isotopic composition of the fuel material at the beginning of the excursion

2. Mechanical consequences resulting from waste package pressurization during rapid or cyclic volatilization of water with power production

3. Mechanical consequences resulting from rapid heating or thermal cycling of the waste package internals, including the possibility of accelerated structural degradation

4. Thermal consequences resulting from the effects of heating or thermal cycling vaporizing water or accelerating chemical reactions.

Thus, all parameters directly related to potential damage (to waste package barriers or SNF cladding) will be considered in the criticality consequence evaluation. Peak overpressures are primarily determined by the reactivity insertion rate and the exit area (defined as the total area of penetrations through the waste package).

The increase in the radionuclide inventory following the criticality event is computed from a point-depletion code for the incremental burnup accrued during the transient criticality, given an initial isotopic inventory at the point in time when the criticality event is assumed to occur. The initial inventory, derived from the geochemical degradation analysis, is also the basis for evaluating the reactivity parameters.

Criticality consequences associated with mechanical effects are evaluated relative to failure criteria for the waste package materials. Mechanical effects from transient criticalities are a direct result of pressure and temperature cycling leading to failures that possibly enhance the radionuclide inventory available for transport. Vessels subjected to repetitive pressure-temperature stresses experience fatigue, with fewer cycles required before failure as the periodic peak stress approaches the yield point. However, cyclic transient criticalities exhibiting pressure increases sufficient to induce cyclic fatigue effects are not anticipated for repository configurations because of the elapsed times necessary for package reflooding (and the reestablishment of conditions conducive to criticality) between the episodic moderator losses (CRWMS M&O 1999b, Section 6). Thus, criticality consequences from mechanical effects will be evaluated in all cases. However, significant effects are expected to be limited to events where pressures exceed the waste package failure criteria derived from stress analyses on the configuration. Consequences associated with the elevated thermal environment will also be evaluated with temperature thresholds for structural failures and phase transitions, but the short duration of that environment is expected to mitigate the consequences.

The additional analyses for support of licensing activities will include an evaluation of possible positive feedback mechanisms, particularly the so-called autocatalytic effect entailing positive reactivity feedback, which can arise in an over-moderated system. It is expected that this effect will occur only in an external configuration, which is discussed in Section 3.7.2.4.

3.7.2.3 Steady-State Criticality, External

The methodology approach to quasi-steady-state external criticality also uses the bounding concept based upon the premise that a critical condition is attained through a slow (on the order of years), possibly cyclic, processes such as the percolation flow of water increasing the neutron thermalization capability of the system and the localized deposition of fissionable material. If a criticality condition is reached, the power level can be expected to rise until the local water loss balances the influx rate. Therefore, the steady-state temperature is that at which the water losses, evaporative or other wise, are just equal to the total (net) water influx. If the temperature were to increase beyond this point, the net decrease in moderator would shut down (terminate) the criticality process. Once the temperature is determined, the power level can be computed as the total of the power lost through conduction, convection, and possibly evaporation. The length of the high moisture part of a climatological cycle conservatively bounds the duration of a criticality event, which might be as long as 10,000 years (DOE 1998, Volume 3, p. 3-13). The subsequent return of a moist cycle would be unlikely to extend the duration of a steady state criticality event for reasons analogous to those presented in Section 3.7.2.1 (e.g., here the k_{eff} of the fissionable material deposit declines with isotopic burnup and loss by mass transport modes enabled by the criticality event). A factor influencing the criticality duration within the above bound is the available fissile mass that will likely shorten the duration of the criticality through burnup of fissile materials.

The analysis to determine the operating temperature and power level for an external steady-state criticality follows the same process described above for internal steady-state criticality, except that the radiation and buoyant heat convection-heat dissipation mechanisms are not available for external criticality. The principal direct consequence of an external steady-state criticality is the same as for an internal criticality, namely, an increase in the radionuclide inventory. The consequence analyses likewise follow the same procedure.

3.7.2.4 Transient Criticality, External

The slowly progressing environmental processes that would determine the composition of a critical mass create the expectation that there are no mechanisms for rapid reactivity insertion in the external environment (to be demonstrated in the analysis supporting licensing activities). Hence the principal potential mechanism for a transient external criticality is an autocatalytic configuration, such as has been postulated for accumulations of fissile material in tuff fractures (Gratton et al. 1997). External configurations having potential for exhibiting autocatalytic behavior are restricted to ones having sufficiently large accumulations of fissile material (e.g., ^{233}U, ^{235}U, and/or ^{239}Pu), coupled with a large water infiltration rate that permits system assembly to occur in an over-moderated configuration. Then, as the infiltration rates decrease during a climatic cycle, or as the power generation from an incipiently critical fissile material accumulation increases the temperature, moderator loss introduces positive reactivity that further increases the power level. Termination of the criticality event occurs when sufficient negative reactivity is generated through continued moderator loss, a sufficient system temperature increase, or system dilation to produce a sub-critical configuration.

There is no single consequence measure for an external transient criticality event. The incremental increase in radionuclide inventory is a factor for transient criticalities, although incremental production is likely to be significantly lower than for steady-state criticalities with comparable configurations. However, mechanical effects from locally elevated pressures and temperatures in the reaction-zone must also be considered for transient criticality events. Thus, all parameters directly related to potential damage to the repository will be considered in the criticality consequence evaluation.

The potential for accumulating sufficiently large masses of fissile material to support autocatalytic criticalities will be evaluated using the geochemistry degradation and transport model. If such accumulations are found to be possible, the evolution/consequences of such a criticality will be evaluated using a combined thermal-hydraulic-neutronic code.

The thermal-hydraulic-neutronic code for analyzing possible external criticality events will be specifically designed for the evaluation of transient external criticalities in an unsaturated repository environment. The coupled thermal-hydraulic-neutronic code is expected to calculate the time dependent evolution of nuclear reactivity and fission power for fissionable material assemblies with heterogeneous compositions and simple geometries. The code will use a point kinetics model to compute the neutron flux amplitude as determined by a time dependent composite reactivity having the following components:

1. Doppler broadening of the material absorption cross-sections in the reaction-zone
2. Water moderator voiding or expulsion from the pore spaces in the reaction-zone
3. Spatially progressive homogenization of fuel and moderator materials by melting
4. Expansion and/or dilation of the reaction-zone.

Data structures used by the code in analyses supporting licensing activities will reflect the actual characteristics of the rock (particularly compressibility) that would regulate any mechanical effects of the criticality. The code used in analyses supporting licensing activities will also include delayed fission-neutron groups in the evaluation of system neutron kinetics and the incorporation of variable thermodynamic and transport properties.

Variations of system temperatures, pressures, and mechanical strain-rates are calculated after the instantaneous power levels are determined. The code also must calculate the time varying kinetic energies possessed by materials in the reaction-zone and the energy transferred to the surrounding host rock for simulations involving non-trivial mechanical effects. Although the neutronic time evolution in the methodology is calculated from a zero-dimensional model, the reactivity parameters incorporate spatial effects through spatial integration of the distributed but coupled thermal-hydraulic and mechanical conditions.

If the geologic chemistry and transport analyses indicate that external fissile material accumulations having autocatalytic capability are possible, the direct consequences of potential criticalities can be grouped into three categories and evaluated as follows:

1. The increase in the radionuclide inventory following the criticality event is computed for the incremental burnup accrued during the transient criticality, given the excursion power history and an initial isotopic inventory at the point in time when the criticality event is assumed to occur.

2. Thermal consequences of the criticality are evaluated by comparison of the calculated tuff temperature increase with the temperature change necessary for significant alteration of the tuff.

3. Mechanical and hydrologic consequences of the criticality are evaluated by comparison of the peak predicted mechanical strains and strain-rates of the rock with those values necessary to modify the hydraulic properties of the tuff near the disturbance.

The criticality consequences, as enumerated, provide input to the nuclide transport component of the risk assessment evaluation (Section 3.8) with respect to the overall nuclide inventory and possible sequence alteration information.

3.7.3 Validation Approach of Criticality Consequence Analysis Process

The validation process will cover the range of environmental conditions expected in the repository, for both internal and external criticality events. If the range of conditions exceeds the expected bounds for the criticality consequence methodology, then the validation range will be extended.

3.7.3.1 Steady-State Criticality Consequence Analysis Process

The equations used to model the simple steady-state heat and mass transfer processes are applicable over the range of parameters considered. The radionuclide increment is directly proportional to the power level and duration of the criticality; it is less strongly dependent on the isotopic concentrations of the SNF immediately prior to the onset of criticality.

As stated in Sections 3.7.2.1 and 3.7.2.3, the principal direct consequence of a steady-state criticality is an increase in the radionuclide inventory resulting from the incremental exposure. Temperature effects on waste package material degradation rates will be validated as part of the geochemistry input parameter validation.

No direct experimental analogs to the scenarios for, or conditions affecting, internal or external steady-state criticality events at the repository exist. Therefore, validation of the codes, calculations, and procedures used in analyses processes with this approach must be made by technical reviews and, as available, comparison of the calculated responses in simulations of representative experiments with those from actual experimental responses. Any representative experiments and incidents chosen for the validation tests will have significant physical process similarities to the internal and external criticality scenarios at the repository.

Validation of the steady-state assessment approaches for internal and external criticalities will demonstrate that the methods can be used in an appropriate manner and aid in quantifying the degree of conservatism in the power and temperature rise estimates. These quantities are the primary contributors to the criticality consequence evaluation of radionuclide inventories and temperature effects on both degradation rates and transport mechanisms.

Radionuclide releases may occur prematurely for fuel pins initially received at the repository with cladding micro-perforations and could be accelerated by the thermodynamic conditions imposed during a criticality. Accelerated radionuclide releases may affect the incremental radionuclide inventories and the criticality duration by the selective relocation of isotopes. These inventories, in turn, contribute to the mobilized source that is a consequence of the steady-state criticalities. The potential for pinhole release affects only a minor fraction of the commercial SNF inventory, as conservative estimates produce the expectation that 0.16 percent of the rods in a waste package may have small perforations at the time of emplacement (CRWMS M&O 2000b, p. 3-33, Figure 3.4-4).

The transport of radionuclides through pinholes in breached fuel pins is expected to be a diffusion limited process that is insensitive to the flow conditions present at the cladding exterior. The small-dimension internal sequences characterizing the interiors of swollen and cracked fuel pellets would limit mass transport to diffusive modes.

3.7.3.2 Transient Criticality Consequence Analysis Process

The consequence portion of the methodology approach for transient criticality is implemented by computer codes incorporating time dependent mathematical descriptions for mass, momentum, and energy transfer processes coupled with the equations of state for the materials involved. For the variety of waste forms and waste packages, there are different implementations of such a code (e.g., model and parameter variations). Additionally, there also are different implementations for internal versus external criticality consequence analyses.

The validation of the transient criticality codes is primarily by comparison of computed time histories with the observations from the transient criticality experiments, as described in the following paragraphs. However, the effects of transient thermodynamic and mechanical variations on the instantaneous neutronic state of a system can also be summarized with reactivity coefficients. This can be conveniently implemented because the transient criticality consequence models employ tabulated reactivity statepoint matrices, which, combined with the transient behaviors of other physical quantities in a transient analysis, allow the calculation of reactivity coefficients (which are generally non-linear functions of state parameters). These reactivity coefficients can be used in a simplified, linear model to generate an independent time history, which can also be compared with the observed experimental data.

For transient criticality consequence analyses internal to an SNF waste package, the transient criticality code serving as the basis for the analysis is an appropriate tool that can be validated in a manner acceptable to the NRC. The validation process has or will demonstrate that the code can be used in an appropriate manner and within its intended range for transient internal waste package criticality events.

The waste package transient criticality analysis differs from the typical reactor plant analyses by having:

1. Initial conditions in the waste package at atmospheric pressure and low temperature
2. Static fluid conditions (zero flow rate)
3. Absence of movable control rods
4. Flow directions not necessarily in the axial direction of the waste forms.

The principal limitation of hydraulic codes that affects the waste package analyses is that the flow systems are primarily one-dimensional. However, techniques such as multiple connections can often be used to extend the flow system to cover limited two-dimensional capability.

If the SNF assemblies are not fully degraded, a transient criticality inside of an SNF waste package would commence with horizontally oriented assemblies and static fluid conditions. The buoyancy gradients created by the initial fission heating would drive a fluid flow transverse to PWR SNF assemblies. Therefore, frictional effects in the PWR waste package analysis are mainly due to flow across the fuel rods in assemblies because there is no barrier to the transverse flow. Frictional coefficients for other waste forms will be evaluated for each configuration analyzed. Loss coefficients for specific analyses will be obtained from experimentally derived correlations for flows in compatible geometries and regimes (Idelchik 1966).

A different type of code is needed for analyzing the direct consequences of transient criticality events external to the waste package where analyses of external configurations exhibiting the autocatalytic effect may be required, should such configurations be identified. As described in Section 3.7.2.4, the code must be able to simulate the dynamics of coupled physical and nuclear processes for systems composed of fissile material, water, and rock. The model implementation must couple the transient fission power, non-equilibrium multi-component thermodynamics, and rock-mechanical effects to the reactivity feedback mechanisms to evaluate the consequences of an external criticality. Considerations for the complex properties and mechanical behaviors of porous tuff, such as unsaturated compressibility and inelastic pore compaction, are also important for inclusion in the consequence models. A comprehensive set of internal nuclear reactivity feedback mechanisms that influence the transient power trajectories will be reviewed for consequence evaluations of transient external criticalities.

The transient criticality consequence analysis process and model validation is based on comparisons to experimental test results. There are no direct natural analogs or experiments with exactly the geometry and parameter ranges expected for repository configurations for either the internal or external hypothetical transient events. Thus, the validation approach will be to use comparisons with representative experiments or incidents covering subsets of the conditions expected in the repository. Taken together, these subsets are expected to cover the range of actual conditions and parameter values expected for critical configurations. If, during criticality consequence analyses, any parameter values exceed their validated range, the validation process will be extended to include additional relevant data or to incorporate greater conservatism. These representative experiments and incidents will be carefully chosen for the validation tests to:

1. Have significant physical process similarities to the transient internal and external criticality scenarios in the repository
2. Bound the range of possible configuration and dynamic characteristics anticipated for either internal or external criticality events in the repository.

Validation of the transient assessment methodologies for internal and external criticalities will demonstrate method and model applicability for such representative transient experiments or incidents. The criticality consequence methodology utilizes a number of different but related phenomena that are not necessarily invoked in any particular single analysis. Thus, validation of the analysis process will utilize a number of cases to span the various phenomena as well as the expected parameter ranges.

3.8 ESTIMATING CRITICALITY RISK

The risk of criticality in the repository is not evaluated explicitly but is an undifferentiated part of the overall risk determined, in part, by the enhanced radionuclide concentrations and the dose in the accessible environment, evaluated as part of the TSPA methodology. The incorporation of criticality risk into the TSPA process is described in the following subsections.

3.8.1 Criticality Risk Methodology Approach

The purpose of this section is to summarize the role of criticality in the performance assessment process for illustrative purposes; acceptance of the performance assessment methodology approach, per se, is not within the scope of this document. An increase in the radionuclide inventory due to criticality events has the potential for increasing the dose at the accessible environment. This section presents the portion of the TSPA methodology approach for estimating the potential dose in the accessible environment due to potential criticality events that cannot be screened from further consideration on a probability basis. The TSPA approach evaluates the dose range in the accessible environment from a time-dependent source term for comparison with regulatory standards specified in 10 CFR Part 63.

The evaluation of radiation doses in the accessible environment, estimated as part of TSPA, will incorporate into the input any enhanced radionuclide inventory generated as a consequence of any potential criticality event. Any significant mechanical effects identified from the consequence analyses (e.g., elevated temperature for the duration of a steady-state criticality, or peak pressure pulse from a transient criticality) will be reflected in the TSPA analysis by modifying the degradation characteristics of the effected barriers.

The doses will be evaluated for the total expected radionuclide inventory (the nominal repository inventory enhanced by the additional probability weighted criticality consequence inventory) using the TSPA radionuclide mobilization and transport methodology. If the dose range from the enhanced radionuclide inventory is calculated to be within the 10 CFR Part 63 performance objectives, no additional TSPA evaluations will be conducted. If the dose range is calculated to exceed the 10 CFR Part 63 performance objectives, mitigating actions will be required (see Figure 3-1).

The approach to evaluating the potential dose (significant consequence) from a criticality applies to both internal and external waste package environments and is as follows. The initial step takes as input the previously determined probability weighted radionuclide source term and any parameter adjustments resulting from thermal-mechanical effects from the criticality consequence analyses. Thermal effects may alter the ambient drift flow conditions (if the event generates significant thermal output) in the near-field vicinity of the criticality. This serves to define the time when water in this region can begin flowing back through the radionuclide inventory augmented by radionuclides produced during the criticality event. Next, the waste form alteration and dissolution models are used to estimate the release rate of radionuclides from the repository. Finally, the criticality-enhanced source term is used in the TSPA model to evaluate the dose history in the accessible environment and other locations as required for testing against the repository performance objectives.

The TSPA model tracks radionuclides as they are leached from the inventory and transported through the unsaturated and the saturated zones (above and below the water table, respectively), and provides the concentration of radionuclides in groundwater at the accessible environment. For any critical events that occur within a failed waste package, or in the near field, the source term is located in the unsaturated zone; for those occurring in the far-field, the source term may be located in the saturated zone. Radioactive decay may either reduce or increase the concentration of a particular radionuclide over the transport sequence (the increase being produced by ingrowth of daughter products).

The performance assessment approach used to evaluate the dose at the accessible environment can track several inventories simultaneously (e.g., commercial SNF and DOE SNF). The approach can also incorporate a distribution of criticality events in time and space to evaluate the long-term effects that various events have on the total dose at the accessible environment.

3.8.2 Total System Performance Models (Risk Evaluations)

This section describes the application of the performance assessment approach to estimate the risk associated with consequences of a criticality in the repository. Any evaluation of the risk associated with potential criticality events done in support of licensing activities will utilize the most appropriate qualified versions of the performance assessment models and codes. Because of the variability and uncertainty in model input parameters, TSPA analyses will incorporate numerous realizations of the processes comprising the scenarios important to repository performance. These realizations will provide a basis for the statistical representation of the effects of the variability and uncertainty.

The major features of the performance assessment methodology approach include:

(1) waste package behavior and radionuclide release models
(2) radionuclide transport models
(3) disruptive events model (which may include criticality)
(4) biosphere dose/risk models.

The information flow between these models is indicated in Figure 3-7.

In summary, it should be noted that criticality may affect the performance assessment evaluations in two of the performance assessment areas: waste package and radionuclide release and disruptive events (providing enhanced source terms).

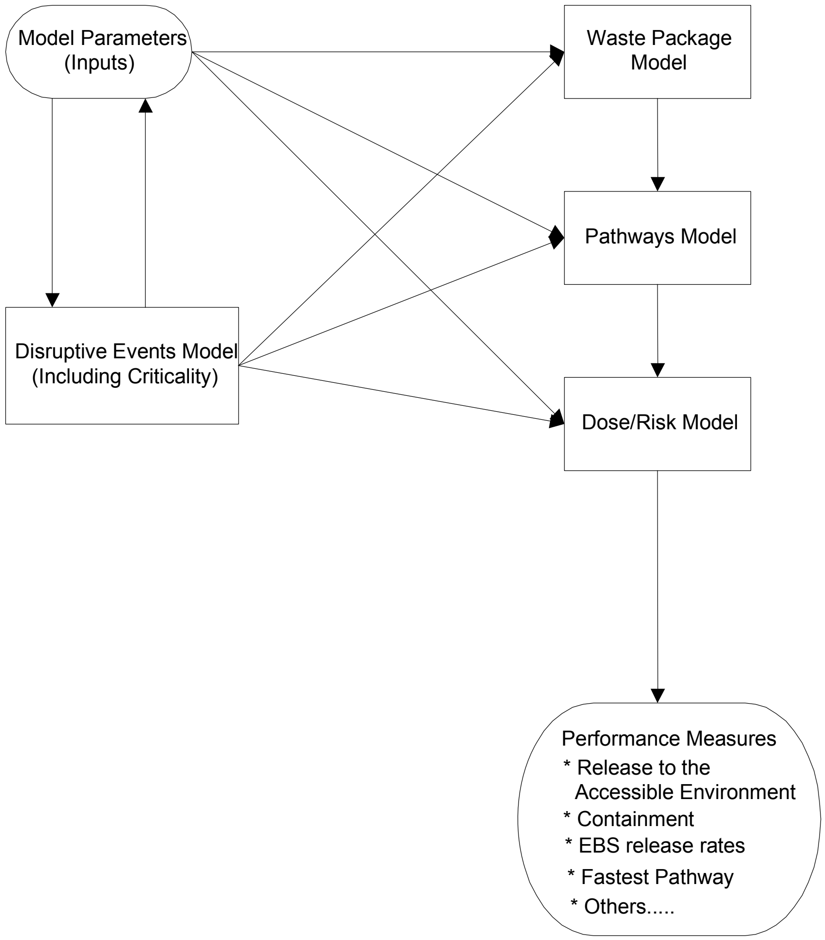


Figure 3-7. Components of Total System Performance Assessment Model

4. SUMMARY AND CONCLUSIONS

The proposed methodology approach for performing criticality analyses for waste forms for long-term disposal in the repository at Yucca Mountain is presented in this report. The methodology approach presented is a risk-informed, performance-based approach, which treats criticality as one of the processes or events that must be considered for the overall performance assessment. The methodology approach, modeling approach, and validation process for the models are described for each analysis component.

The starting point for the methodology is the establishment of the range of waste forms, the waste package/engineered barrier system design, the characteristics of the site, and the degradation characteristics of the waste package materials of construction. Based on this information, the process looks at how the emplaced material may degrade and builds scenarios that result in degraded configurations that are grouped into classes. Parameters that affect criticality are identified for each class, and ranges of values for these parameters are established based on degradation analyses. These parameters may include the amounts of fissionable material, neutron absorber material, corrosion products, and moderator and reflector materials. The probability of occurrence is calculated for the configuration classes and, if the probability screening criterion is exceeded, criticality evaluations are performed for the configuration classes over the range of parameters characterizing the configuration class. Configuration classes that have a k_{eff} exceeding the critical limit for the waste form are further evaluated to estimate the probability of criticality for the configuration. Additional design features for reducing k_{eff} are to be implemented if the overall probability of criticality exceeds the design probability criterion. If such a situation is identified, the defense-in-depth strategy requires either strengthening the waste package criticality control measures or limiting the waste forms that can be loaded.

Consequence analyses are performed when the total probability of criticality in the repository exceeds the 10 CFR Part 63 probability criterion for exclusion of events from TSPA, which is one chance in 10,000 over 10,000 years of an (criticality) event occurring. The consequence analyses establish the impact of potential criticality events on the radionuclide inventory, thermal effect, and mechanical failures in the repository. The perturbation in the radionuclide inventory, the thermal effect, and the effects of mechanical failures established by the criticality consequence analysis are treated as disruptive scenarios within the TSPA conducted for the repository. The results from the criticality consequence analyses for all waste forms and waste packages that provide a significant contribution to the repository probability of criticality are provided as input for the TSPA. The TSPA determines if the risk to the health and safety of the public is acceptable, as defined in the repository performance objectives. If these performance objectives are not satisfied, implementation of additional design features for reducing the contributing factors is required (Section 3.1).

Although guidance documents from the NRC and various applicable industry standards (NUREGS, Regulatory Guides, and American National Standards Institute) have been used in developing the methodology approach presented in this report, none of the guidance documents or industry standards were written to specifically address disposal in the repository. However, 10 CFR Part 63 was developed specifically for the repository at Yucca Mountain, Nevada. The methodology approach presented in this report starts with the guidance documents and industry standards discussed in Chapter 2 and extends their applicability to high-level radioactive waste disposal while following the requirements of 10 CFR Part 63. It is concluded that the methodology approach presented in this report is fully compliant with 10 CFR Part 63.

This topical report discusses the following aspects of the approach used in the methodology for performing criticality analyses for the geologic disposal of the waste forms and seeks acceptance of those parts not previously accepted in *Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0* (Reamer 2000b).

A. The following performance criteria presented in Figure 3-1 (discussed in Sections 3.1 and 3.2) are acceptable for ensuring that design options are properly implemented for minimizing the potential for, and subsequent postulated consequences of, criticality:

   1. The *Probability Screening Criterion* discussed in Section 3.2.1: The probability screening criterion is defined to be well below (a minimum of two orders of magnitude) the 10 CFR 63.114(d) probability criterion for exclusion of events from TSPA that is one chance in 10,000 of an (criticality) event occurring in the repository over 10,000 years. This screening level is set such that, if satisfied, no single configuration class would be a significant contributor to the total probability of criticality for the repository.

   2. The *Criticality Potential Criterion* discussed in Section 3.2.2: The maximum calculated effective neutron multiplication factor (k_{eff}) for subcritical systems (configuration classes) for postclosure will be less than the critical limit. The critical limit is the value of k_{eff} at which the system is considered potentially critical as characterized by all the appropriate biases and associated uncertainties for each internal and external configuration class analyzed for the repository. Configuration classes satisfying this criterion have an insignificant potential for criticality and can be excluded from further consideration. (accepted subject to implementation, [Reamer 2000b, Section 3.2.1])

   3. The *Design Probability Criterion* discussed in Section 3.2.3: The probability of one criticality occurring will be less than one over the entire repository for the first 10,000 years. This probability includes all combinations of waste packages and waste forms. This probability criterion is used to define a waste package criticality control limit in support of defense-in-depth with respect to the repository criticality performance objectives discussed in Section 2.2.2. If the calculated probability of criticality exceeds this design criterion, implementation of criticality mitigating strategies will be required. (self-imposed criterion, no NRC objections to its use [Reamer 2000b, Section 3.2.3])

B. The list of Master Scenarios, presented in Section 3.3 and summarized in Figures 3-2a, 3–2b, 3-3a, and 3-3b, comprehensively identifies degradation scenarios associated with the repository at Yucca Mountain that may significantly affect the potential for, and the subsequent postulated consequences of, criticality. The degradation processes of interest for criticality are related to a combination of FEPs that result in configuration classes that have the potential for criticality requiring further evaluation of this potential. Generic degradation scenarios and potential critical configuration classes have been identified by considering the features of the site and the characteristics of the waste form and other waste package internal components. Potential critical configuration classes are states of a degraded waste package defined by a set of parameters characterizing the quantity and physical arrangement of the materials that have a significant effect on criticality. (Internal Criticality Scenarios accepted subject a proviso on seismic events [Reamer 2000b, Section 3.3.1], External Criticality Scenarios accepted subject to contingencies [Reamer 2000b, Section 3.3.2])

C. The portion of the approach used in the methodology for developing internal and external configurations discussed in Section 3.4 is acceptable in general for developing a comprehensive set of potentially critical postclosure configurations for disposal criticality analysis. Acceptance is sought for the part of the methodology approach, described in Sections 3.4.1.1 and 3.4.2.1, for evaluating the parameter ranges of configuration classes over the range of environmental conditions currently postulated for the repository at Yucca Mountain. Specifically, the 14 steps in the approach specified for internal configurations in Section 3.4.1.1 and the five steps in the approach specified for external configurations in Section 3.4.2.1 are acceptable and sufficiently comprehensive. (degradation approach provisionally accepted for internal configurations, [Reamer 2000b, Section 3.4.1.1], accumulation approach accepted for external configurations [Reamer 2000b, Section 3.4.2.1]).

D. The methodology approach based upon event tree/fault tree sequences for estimating the probability of postclosure critical configuration classes discussed in Section 3.6 is acceptable in general for disposal criticality analysis. The applicability of the method for postclosure conditions in the repository will be demonstrated in model reports that will be developed in support of licensing activities. NRC acceptance of probability values for the occurrence of critical configurations over the period of regulatory concern obtained from the model and their applicability for postulated postclosure conditions will be sought in analyses developed in support of licensing activities.

E. The portion of the approach used in the methodology for estimating consequences of potential postclosure criticality events (as discussed in Section 3.7) is acceptable in general for disposal criticality analysis. Specifically, that technical reviews of the consequence models and, as available, comparisons of specific experimental results with simulation results are sufficient to demonstrate the acceptability of the criticality consequence models for postulated internal and external criticality and for transient as well as for steady-state criticality events.

F. The methodology approach for the isotopic and criticality models is acceptable in general for disposal criticality analysis. Specifically:

1. For commercial SNF, acceptance is sought for use the reduced reactivity (burnup credit) associated with the net depletion of fissile isotopes and the creation of neutron-absorbing isotopes during reactor operations as discussed in Sections 3.5.1 and 3.5.2. Acceptance is sought for the use of the principal isotope selection process for burnup credit in criticality analyses of intact commercial SNF discussed in Section 3.5.2.1.1.

2. The approach to the methodology described in Section 3.5.3.1 for the isotopic model is acceptable for establishing the isotopic bias in k_{eff} to be used for commercial spent nuclear fuel burnup credit. The applicability of this bias in critical limit values for postulated postclosure conditions in the repository will be demonstrated in model reports that will be developed in support of licensing activities. NRC acceptance of isotopic bias and uncertainty values for k_{eff} and their applicability for postclosure conditions will be sought in analyses supporting the licensing activities. (approach for evaluating the uncertainties associated with isotopic decay and branching ratios provisionally accepted for internal and external waste forms [Reamer 2000b, Section 3.5.3.1])

3. The approach to criticality modeling process described in Section 3.5.3.2 is acceptable in general for disposal criticality analysis. Specifically, the process presented for calculating the critical limit values and the process presented for establishing the Range of Applicability of the critical limit values is acceptable. This process will be followed to calculate critical limit values and/or functions for specific waste forms and waste packages as a function of degradation conditions. The applicability of the critical limit values for postulated postclosure conditions in the repository will be demonstrated in model reports that will be developed in support of licensing activities. NRC acceptance of critical limit values and their applicability for postclosure repository conditions will be sought in analyses supporting licensing activities. (k_{eff} evaluation approach provisionally accepted for internal and external waste forms [Reamer 2000b, Section 3.5.2.2])

4. The approaches for estimating the bias and uncertainty in the critical limit calculation and establishing the lower bound tolerance limit functions for a waste form discussed in Section 3.5.3.2 are acceptable. (approach to evaluating the statistical uncertainty portion of Δk_c accepted subject to contingencies [Reamer 2000b, Section 3.5.3.2])

G. The methodology approach for the degradation and release model and the external accumulation model (as presented in Sections 3.4.1.3 and 3.4.2.3) is acceptable in general for disposal criticality analysis. (degradation approach provisionally accepted for internal configurations, [Reamer 2000b, Section 3.4.1.1], accumulation approach accepted for external configurations [Reamer 2000b, Section 3.4.2.1])

H. The proposed requirements presented in Section 3.5.3.1.2 for modeling burnup of commercial SNF for design applications are sufficient to ensure adequate conservatism in the isotopic concentrations used for burnup credit. These requirements describe acceptance criteria for confirmation of this conservatism. The confirmation of the conservatism in the application model used for burnup credit for commercial SNF will be demonstrated in model reports that will be developed in support of licensing activities. NRC acceptance of the confirmation of the conservatism in the application model for postulated postclosure conditions in the repository will be deferred until required for the License Application process.

I. The approach for selecting principal isotopes to model burnup in intact (non-leakage) commercial SNF, resulting in the set presented in Table 3-1 (Section 3.5.2.1.1), is acceptable for disposal criticality analysis provided that the bias in k_{eff} associated with predicting the isotopic concentrations is established in the model reports as described in Section 3.5.3.1. The applicability of the principal isotopes selected for intact commercial SNF will be demonstrated in model reports that will be developed in support of licensing activities.

The k_{eff} values from criticality evaluations of breached commercial SNF will reflect both the isotopic bias in k_{eff} established from radiochemical assay analysis and the changes in the principal isotope concentrations established by the geochemical analysis.

J. The selection process for identifying isotopes from the list of principal isotopes for degraded commercial SNF presented in Section 3.5.2.1.5 is acceptable for disposal criticality analysis. The applicability of isotopes selected from the list of principal isotopes for degraded commercial SNF configurations will be demonstrated in model reports that will be developed in support of licensing activities. NRC acceptance of the use of selected isotopes in postulated postclosure conditions in the repository will be sought in activities supporting the licensing process.

K. Verified burnup values are recorded for each commercial nuclear fuel assembly in reactor records kept by each utility. Consistent with other NRC regulated operations, DOE is seeking acceptance for using reactor records as the primary basis for commercial nuclear fuel assembly burnup values to be used for disposal criticality analyses with on-site measurements required only under special circumstances. Uncertainties in burnup values will be addressed in applications of the criticality methodology. Acceptance is sought that the requirements discussed in Section 3.5.3.1 are sufficient to ensure adequate conservatism in the isotopic model for burnup credit.

The methodology approach outlined above will be used for the following waste forms: commercial SNF, DOE SNF, and vitrified HLW with the exception of the determination of isotopic inventories and burnup credit which is inappropriate for DOE SNF and vitrified HLW.

INTENTIONALLY LEFT BLANK

5. REFERENCES

5.1 DOCUMENTS CITED

Bowden, D.C. and Graybill, F.A. 1966. "Confidence Bands of Uniform and Proportional Width for Linear Models." *Journal of the American Statistical Association*, *61*, (313), 182-198. Washington, D.C.: American Statistical Association. TIC: 238570.

Bowman, C.D. and Venneri, F. 1996. "Underground Supercriticality from Plutonium and Other Fissile Material." *Science and Global Security*, *5*, 279-302. New York, New York: Gordon and Breach Science Publishers. TIC: 238269.

Brocoum, S. 1999. "U.S. Department of Energy (DOE) Response to U.S. Nuclear Regulatory Commission (NRC) Request for Additional Information on the DOE Topical Report on Disposal Criticality Analysis Methodology." Letter from S. Brocoum (DOE/YMSCO) to C.W. Reamer (NRC), November 19, 1999, with enclosures. ACC: MOL.20000119.0208.

Brocoum, S. 2000. "U.S. Department of Energy (DOE) Comments on U.S. Nuclear Regulatory Commission (NRC) Draft Safety Evaluation Report (SER) for Disposal Criticality Analysis Methodology Topical Report, Revision 0." Letter from S. Brocoum (DOE/YMSCO) to C.W. Reamer (NRC), May 17, 2000, with enclosure. ACC: MOL.20000616.0041.

BSC (Bechtel SAIC Company) 2003a. *Technical Work Plan for: Risk and Criticality Department*. TWP-EBS-MD-000014 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20031002.0003.

BSC 2003b. *Q-List.* TDR-MGR-RL-000005 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20030930.0002.

CRWMS M&O (Civilian Radioactive Waste Management System Management and Operating Contractor) 1997a. *Criticality Abstraction/Testing Workshop Results*. B00000000-01717-2200-00187. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980528.0040.

CRWMS M&O 1997b. *Construction of Scenarios for Nuclear Criticality at the Potential Repository at Yucca Mountain, Nevada*. B00000000-01717-2200-00194. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980204.0281.

CRWMS M&O 1997c. *Waste Package Probabilistic Criticality Analysis: Summary Report of Evaluations in 1997*. BBA000000-01717-5705-00015 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980204.0095.

CRWMS M&O 1998a. *Principal Isotope Selection Report*. B00000000-01717-5705-00104 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980827.0187.

CRWMS M&O 1998b. *Summary Report of Commercial Reactor Critical Analyses Performed for the Disposal Criticality Analysis Methodology*. B00000000-01717-5705-00075 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980825.0001.

CRWMS M&O 1998c. *Criticality Analysis of Pu and U Accumulations in a Tuff Fracture Network*. A00000000-01717-0200-00050 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980216.0260.

CRWMS M&O 1999b. *Criticality Consequence Calculation Involving Intact PWR MOX SNF in a Degraded 21 PWR Assembly Waste Package*. CAL-EBS-NU-000008 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990929.0048.

CRWMS M&O 2000a. *Total System Performance Assessment for the Site Recommendation*. TDR-WIS-PA-000001 REV 00 ICN 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20001220.0045.

CRWMS M&O 2000b. *Waste Form Degradation Process Model Report*. TDR-WIS-MD-000001 REV 00 ICN 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000713.0362.

DOE (U.S. Department of Energy) 1998. *Total System Performance Assessment. Volume 3 of Viability Assessment of a Repository at Yucca Mountain*. DOE/RW-0508. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19981007.0030.

DOE 2001. *Civilian Radioactive Waste Management System, Total System Description.* DOE/RW-0500, Rev. 02. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: HOQ.20011127.0016.

DOE 2003. *Quality Assurance Requirements and Description*. DOE/RW-0333P, Rev. 13. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: DOC.20030422.0003.

Dyer, H.R. and Parks, C.V. 1997. *Recommendations for Preparing the Criticality Safety Evaluation of Transportation Packages*. NUREG/CR-5661. Washington, D.C.: U.S. Nuclear Regulatory Commission. TIC: 238893.

EPRI (Electric Power Research Institute) 1999. *Determination of the Accuracy of Utility Spent-Fuel Burnup Records*. EPRI TR-112054. Palo Alto, California: Electric Power Research Institute. TIC: 254706.

Freeze, G.A.; Brodsky, N.S.; and Swift, P.N. 2001. *The Development of Information Catalogued in REV00 of the YMP FEP Database.* TDR-WIS-MD-000003 REV 00 ICN 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20010301.0237.

Gratton, L.J.; Kastenberg, W.E.; and Peterson, P.F. 1997. "Bounding Energy Production Estimates for Autocatalytic Fissile Material Deposits in Geologic Media." *Proceedings of the Topical Meeting on Criticality Safety Challenges in the Next Decade, Chelan, Washington, September 7-11, 1997*. Pages 130-141. La Grange Park, Illinois: American Nuclear Society. TIC: 238680.

Hogg, R.V. and Craig, A.T. 1966. *Introduction to Mathematical Statistics*. 2nd Edition. Pages 182-185. New York, New York: The Macmillan Company. TIC: 238588.

Holonich, J.J. 1994. "Transmittal of the 'Topical Report Review Plan.'" Letter from J.J. Holonich (NRC) to D.E. Shelor (DOE/OCRWM), February 28, 1994, with enclosure. ACC: NNA.19940331.0074.

Idelchik, I.E. 1966. *Handbook of Hydraulic Resistance, Coefficients of Local Resistance and of Friction*. Grunaer, D., ed. AEC-TR-6630. Jerusalem, Israel: Israel Program for Scientific Translations. TIC: 239152.

Jackson, S.A. 1998. "Discussion on Risk-Informed, Performance-Based Regulation." Memorandum from S.A. Jackson (NRC) to Commissioner Dicus, Commissioner Diaz, Commissioner McGaffigan, February 20, 1998, COMSAT-9B-003, with attachment. ACC: MOL.19980626.0154.

Johnson, N.L., ed. 1968. "Query: Tolerance Interval in Regression." *Technometrics*, *10*, (1), 207-209. Rochester, New York: American Society for Quality Control. TIC: 238567.

Lichtenwalter, J.J.; Bowman, S.M.; DeHart, M.D.; and Hopper, C.M. 1997. *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages*. NUREG/CR-6361. Washington, D.C.: U.S. Nuclear Regulatory Commission. TIC: 233099.

Lieberman, G.J. and Miller, R.G., Jr. 1963. "Simultaneous Tolerance Intervals in Regression." *Biometrika*, *50*, (1-2), 155-168. London, England: The Biometrika Office, University College London. TIC: 238568.

Mowbray, G.E. 1999. Transmittal of the Naval Nuclear Propulsion Program Addendum to the Yucca Mountain Site Characterization Office "Disposal Criticality Analysis Methodology Topical Report." Letter from G.E. Mowbray (Department of the Navy) to C.W. Reamer (NRC), October 29, 1999. ACC: MOL.20000316.0531.

Natrella, M.G. 1963. *Experimental Statistics*. National Bureau of Standards Handbook 91. Washington, D.C.: U.S. Department of Commerce, National Bureau of Standards. TIC: 245911.

NRC (U.S. Nuclear Regulatory Commission) 1983. *PRA Procedures Guide, A Guide to the Performance of Probabilistic Risk Assessments for Nuclear Power Plants*. NUREG/CR-2300. Two volumes. Washington, D.C.: U.S. Nuclear Regulatory Commission. TIC: 205084.

NRC 2002. *Interim Staff Guidance - 8, Revision 2. Burnup Credit in the Criticality Safety Analyses of PWR Spent Fuel in Transport and Storage Casks.* ISG-8, Rev. 2. Washington, D.C.: U.S. Nuclear Regulatory Commission. ACC: MOL.20030124.0248.

NRC 2003. *Yucca Mountain Review Plan, Final Report.* NUREG-1804, Rev. 2. Washington, D.C.: U.S. Nuclear Regulatory Commission, Office of Nuclear Material Safety and Safeguards. TIC: 254568.

Reamer, C.W. 1999. "U.S. Nuclear Regulatory Commission Request for Additional Information on the U.S. Department of Energy Topical Report on Disposal Criticality Analysis Methodology." Letter from C.W. Reamer (NRC) to S. Brocoum (DOE/YMSCO), August 18, 1999, with enclosure. ACC: MOL.19991203.0125.

Reamer, C.W. 2000a. "Draft Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0." Letter from C.W. Reamer (NRC) to S. Brocoum (DOE/ YMSCO), March 2, 2000, with enclosure. ACC: MOL.20000413.0695.

Reamer, C.W. 2000b. Safety Evaluation Report for Disposal Criticality Analysis Methodology Topical Report, Revision 0. Letter from C.W. Reamer (NRC) to S.J. Brocoum (DOE/ YMSCO), June 26, 2000, with enclosure. ACC: MOL.20000919.0157.

Reamer, C.W. and Williams, D.R. 2000. Summary Highlights of NRC/DOE Technical Exchange and Management Meeting on Subissues Related to Criticality. Meeting held October 23-24, 2000, Las Vegas, Nevada. Washington, D.C.: U.S. Nuclear Regulatory Commission. ACC: MOL.20001208.0097 through MOL.20001208.0110.

Regulatory Guide 3.71. 1998. *Nuclear Criticality Safety Standards for Fuels and Material Facilities*. Washington, D.C.: U.S. Nuclear Regulatory Commission. Readily available.

Steinborn, T.L.; Wolery, T.J.; Alcorn, S.R.; Arthur, S.E.; Bernot, P.A.; Brady, P.V.; Chen, Y.; Domski, P.S.; Jolley, D.M.; Metcalf, R.C.; and Thomas, E. 2003. *Data Qualification: Update and Revision of the Geochemical Thermodynamic Database, Data0.ymp*. TDR-EBS-MD-000022 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20030331.0003.

Van Konynenburg, R.A., ed. 1995. *Comments on the Draft Paper "Underground Supercriticality from Plutonium and Other Fissile Material," Written by C.D. Bowman and F. Venneri (LANL)*. UCRL-ID-120990 COM. Livermore, California: Lawrence Livermore National Laboratory. TIC: 215460.

YMP (Yucca Mountain Site Characterization Project) 1998. *Disposal Criticality Analysis Methodology Topical Report*. YMP/TR-004Q, Rev. 0. Las Vegas, Nevada: Yucca Mountain Site Characterization Office. ACC: MOL.19990210.0236.

YMP 2000. *Disposal Criticality Analysis Methodology Topical Report*. YMP/TR-004Q, Rev. 01. Las Vegas, Nevada: Yucca Mountain Site Characterization Office. ACC: MOL.20001214.0001.

5.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

10 CFR 63. Energy: Disposal of High-Level Radioactive Wastes in a Geologic Repository at Yucca Mountain, Nevada. Readily available.

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

10 CFR 72. Energy: Licensing Requirements for the Independent Storage of Spent Nuclear Fuel, High-Level Radioactive Waste, and Reactor-Related Greater than Class C Waste. Readily available.

10 CFR 74. Energy: Material Control and Accounting of Special Nuclear Material. Readily available.

10 CFR 960. Energy: General Guidelines for the Recommendation of Sites for Nuclear Waste Repositories. Readily available.

10 CFR 961. Energy: Standard Contract for Disposal of Spent Nuclear Fuel and/or High-Level Radioactive Waste. Readily available.

40 CFR 191. Protection of Environment: Environmental Radiation Protection Standards for Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes. Readily available.

60 FR 42622. Use of Probabilistic Risk Assessment Methods in Nuclear Regulatory Activities; Final Policy Statement. Readily available.

ANSI/ANS-8.1-1998. *Nuclear Criticality Safety in Operations with Fissionable Material Outside Reactors*. La Grange Park, Illinois: American Nuclear Society. TIC: 242363.

ANSI/ANS-8.10-1983. *Criteria for Nuclear Criticality Safety Controls in Operations with Shielding and Confinement*. La Grange Park, Illinois: American Nuclear Society. TIC: 205015.

ANSI/ANS-8.15-1981. *Nuclear Criticality Control of Special Actinide Elements*. La Grange Park, Illinois: American Nuclear Society. TIC: 231624.

ANSI/ANS-8.17-1984. *Criticality Safety Criteria for the Handling, Storage, and Transportation of LWR Fuel Outside Reactors*. La Grange Park, Illinois: American Nuclear Society. TIC: 231625.

ANSI/ANS-8.21-1995. *American National Standard for the Use of Fixed Neutron Absorbers in Nuclear Facilities Outside Reactors.* La Grange Park, Illinois: American Nuclear Society. TIC: 247030.

Nuclear Waste Policy Act of 1982. Public Law No. 97-425. 96 Stat. 2201. Readily available.

Nuclear Waste Policy Amendments Act of 1987. Public Law No. 100-203. 101 Stat. 1330. Readily available.

INTENTIONALLY LEFT BLANK

APPENDIX A

ACRONYMS AND SYMBOLS

INTENTIONALLY LEFT BLANK

APPENDIX A

ACRONYMS AND SYMBOLS

Acronyms

BWR	Boiling Water Reactor
DOE	U.S. Department of Energy
FEP	Features, Events, and Processes
FF	Far-field
GWd/MTU	Gigawatt-Days per Metric Ton of Uranium
IP	In-package
J-13	The designation of a well on Yucca Mountain
k_{eff}	Effective neutron multiplication factor
mSv	milli-Seiverts
NF	Near-field
NRC	U.S. Nuclear Regulatory Commission
NUREG	NRC Document Designator
OCRWM	Office of Civilian Radioactive Waste Management
PA	Performance Assessment
PRA	Probabilistic Risk Assessment
PWR	Pressurized Water Reactor
SNF	Spent Nuclear Fuel
TSPA	Total System Performance Assessment
wt%	Weight Percent

Symbols

β	Bias or the reciprocal of the time duration over which there is a significant probability of criticality occurrence
Δ	Change or increment
°C	Degrees Celsius
N	Sample size
Eh	Negative of the common logarithm of the electron chemical activity of electron in solution, multiplied by 2.303RT/F, where R is the universal gas constant, T is the absolute temperature, and F is the Faraday constant
γ	The confidence level
P	The proportion of the population covered
pH	Negative of the common logarithm of the hydrogen ion chemical activity in solution (approximate concentration in moles per liter)
S_P	The square root of the pooled variance

APPENDIX B

GLOSSARY

INTENTIONALLY LEFT BLANK

APPENDIX B

GLOSSARY

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

Abstraction is generally the process of consideration apart from specific instances; for this document, the process of converting a large body of data generated by a low level, detailed computer code into a heuristic algorithm suitable for inclusion in a higher level computer code.

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.

Adsorption is the transfer of solute mass, such as radionuclides, in groundwater to the solid geologic surfaces with which it comes in contact. The term sorption is sometimes used interchangeably with this term.

Aperture is the opening (distance) between fracture walls.

Approach used in the methodology as used in this document refers to a descriptive overview of the principal elements of the methodology and the models with respect to their basic form and function. Details of the respective models are included in the model and validation documentation.

Aquifer is a subsurface, saturated rock unit of sufficient permeability to transmit groundwater and yield useable quantities of water to wells and springs.

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

Barrier means any material, structure, or feature that, for a period to be determined by NRC, prevents or substantially reduces the rate of movement of water or radionuclides from the Yucca Mountain repository to the accessible environment, or prevents the release or substantially reduces the release rate of radionuclides from the waste (10 CFR 63.2).

Burnable poisons are materials found in fuel assemblies that absorb neutrons and are depleted (burned) in the process.

Burnup is the amount of exposure a nuclear fuel assembly receives, 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 is an approach used in criticality evaluations that 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. This credit applies specifically to the ceramic form of commercial spent nuclear fuel.

Canister is the structure surrounding the waste form that facilitates handling, storage, transportation, and/or disposal. A 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 SNF, it may provide structural support for intact SNF, loose rods, nonfuel components, or it may provide confinement of radionuclides.

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

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 metallic outer sheath of a fuel element generally made of stainless steel or a zirconium alloy. It is intended to isolate the fuel element from the external environment. An example is the metal cylinder that surrounds the uranium pellets in commercial and some types of DOE fuels.

Colloids are, as applied to radionuclide migration, large molecules or small particles that have at least one dimension with a size range of 10^{-9} to 10^{-8} that are suspended in a solvent. Colloids that are transported in groundwater can be filtered out of the water in small pore spaces or narrow fractures because of the large size of the colloids.

Configuration is the relative disposition of the parts or elements of a scenario.

Configuration class is a set of similar configurations whose composition and geometry is defined by specific parameters that distinguish one class from another. Within a class, the configuration parameters may vary over a given range.

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 means the confinement of radioactive waste within a designated boundary (10 CFR 63.2).

Corrosion is the process of dissolving or wearing away gradually, especially by chemical action.

Critical limit is a limiting value of k_{eff} at which a configuration is considered potentially critical, as characterized by statistical tolerance limits.

Criticality analysis is a mathematical estimate, usually performed with a computer, of the neutron multiplication factor of a system or configuration that contains material capable of undergoing a self-sustaining chain reaction.

Criticality control is the suite of measures taken to control the occurrence of self-sustaining nuclear chain reactions in fissionable materials, including spent fuel. For postclosure disposal applications, criticality control is ensuring that the probability of a criticality event is so small that the occurrence is unlikely, and the risk that any criticality will violate repository performance objectives is negligible.

Cross section is the extent to which neutrons interact with nuclei. It is the proportionality factor that relates the rate of a specified nuclear reaction to the product of the number of neutrons per second impinging normally onto a unit area of a thin target and the number of target nuclei per unit area.

Defense-in-depth is a term used to describe the property of a system of multiple barriers to mitigate conditions, processes, or events such that failure in any one barrier does not result in failure of the entire system. For repository postclosure, the barriers are also used to mitigate the effects of uncertainty and limitations in performance assessment models.

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 basket no longer exists.

Disposal means the emplacement of radioactive waste in a geologic repository with the intent of leaving it there permanently (10 CFR 63.2), whether or not such emplacement permits the recovery of such waste (10 CFR 961.11), Nuclear Waste Policy Amendments Act of 1987, Section 2[9]).

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)).

Diverse, in reference to defense-in-depth for this report, refers to barriers that provide different functions that support the goal.

Dose receptor is an individual receiving the radiation dose.

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.

Engineered barrier system means the waste packages, including engineered components and systems other than the waste package (e.g., drip shields), and the underground facility (10 CFR 63.2).

Enrichment is the weight-percentage of ^{233}U or ^{235}U in uranium, or ^{239}Pu in plutonium.

Far-field (FF) is the volume outside the emplacement drifts and extends to the accessible environment for purposes of the disposal criticality analysis methodology.

Fissile materials are those materials that will undergo fission with slow neutrons (e.g., ^{235}U, ^{239}Pu).

Fissionable materials are those materials that will undergo fission by neutrons with sufficient energy. Note that all fissile materials are fissionable, but not vice versa. “Fissile” is used in most places in this report instead of “fissionable,” although fissionable may be applicable for some configurations.

Geochemical is the distribution and amounts of the chemical elements in minerals, ores, rocks, soils, water, and the atmosphere, and the circulation of the elements in nature on the basis of their properties.

Geochemistry is the study of the abundance of the elements and atomic species (isotopes) in the earth. Geochemistry, or geochemical study, looks at systems related to chemicals arising from natural rock, soil, soil processes such as microbe activity, and gases, especially as they interact with man-made materials from the repository system. In the broad sense, all parts of geology that involve chemical changes.

Geologic repository means 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 the engineered barrier system and the portion of the geologic setting that provides isolation of the radioactive waste (10 CFR 63.2).

Groundwater is water that is contained in pores or fractures in either the unsaturated or saturated zones below ground level.

High-level radioactive waste or 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; (2) irradiated reactor fuel; and (3) other highly radioactive material that the Commission, consistent with existing law, determines by rule requires permanent isolation (10 CFR 63.2). The repository will only accept solidified high-level radioactive waste. For the purposes of this document, high-level radioactive waste is also vitrified borosilicate glass cast in a stainless steel canister (Nuclear Waste Policy Amendments Act of 1987, Section 2[12]) (10 CFR 72.3) (10 CFR 960.2) (10 CFR 961.11).

Hydration is the process of adding OH ions or H_2O molecules.

Infiltration rate is the velocity of water entering the soil at the ground surface. Infiltration becomes percolation when water has moved below the depth at which it can be removed to the atmosphere by evaporation or evapotranspiration.

In-Package (IP) is the volume interior to the outer shell of a waste package for purposes of the disposal criticality analysis methodology.

Intact fuel. See Spent nuclear fuel.

Invert is the level bottom placed in the drifts.

Isolation means inhibiting the transport of radioactive material to: (1) the reasonably maximally exposed individual so that the radiological exposures will not exceed the requirements of § 63.113(b); and (2) the accessible environment so that releases of radionuclides into the accessible environment will not exceed the requirements of § 63.113(c) (10 CFR 63.2).

J-13 is the designation of a well on Yucca Mountain from which water has been taken from the saturation zone. The water is representative of the groundwater in the vicinity of the repository.

k_{eff} is the effective neutron multiplication factor for a system. It provides a measure of criticality potential for a system (k_{eff} = 1.0 for criticality).

Lithophysae are voids in the rock having concentric shells of finely crystalline alkali feldspar, quartz, and other materials that were formed due to entrapped gas that later escaped.

Methodology as used in this document refers to the systematic procedures and models proposed to evaluate the risk of criticality in the repository. Specific computer programs and mathematical procedures are not part of the methodology, but rather are tools used to execute individual procedures in the methodology.

Mixed oxide SNF is the light-water-reactor SNF that was fabricated using plutonium as the principal fissile element with ^{238}U for most of the matrix.

Moderating material is material that "slows down" or lowers the energy state of neutrons.

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).

Multivariate regression is an equation, developed from statistical analysis of data, relating one dependent variable (k_{eff} for this report) to several independent variables.

Near-field (NF) is the volume inside an emplacement drift, excluding the interior of the waste package, for purposes of the disposal criticality analysis methodology.

Neutronic parameter is a physical variable that either describes the behavior of a neutron in a system or describes a characteristic of a system that effects or is effected by a neutron.

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

Over-moderated is a state of a system in which removing moderating material increases the reactivity of the system, while adding moderator material decreases the reactivity of the system.

Package means the packaging together with its radioactive contents as presented for transport (10 CFR 71.4).

Perched water is a groundwater deposit isolated from the nominal flow (normally above) and not draining because of impermeable layer beneath.

Percolation rate is the velocity of water movement through the interstices and pores under hydrostatic pressure and the influence of gravity.

Performance assessment (PA) 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. For the repository, PA analyses are the analyses that predict the impact of repository events and processes on the repository environment.

Permanent closure means the final backfilling of the underground facility, if appropriate, and the sealing of shafts, ramps, and boreholes (10 CFR 63.2).

Plume, for this document, is the envelope of groundwater sequences from a single source.

Pond is used in the conventional sense to describe some standing water internal to the waste package or in the drift. It is also used in a special sense to represent any localized combination of water solution and solid material that can be subject to analysis by a geochemistry code.

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.

Probability density function is a function that is used to compute the probability that a random variable (representing some physical parameter) falls within an interval specified by the argument of the function and a multiplier specifying the length of interval in units of the argument of the function. The probability in question is the product of the probability density function and the interval multiplier. The probability density function has the units of reciprocal of its argument, and it is computed as the derivative of the cumulative distribution over the range of argument for which the cumulative distribution function is continuous.

Process model is a model that quantifies uncertainties in the model parameters and predicts the likelihood of the scenarios used for the model.

Radioactive waste or **waste** means HLW and radioactive materials other than HLW that are received for emplacement in a geologic repository (10 CFR 63.2).

Reactivity is the relative deviation of the neutron multiplication factor of the system from unity (i.e., reactivity = $(k_{eff} - 1)/k_{eff}$).

Redox front is the boundary between two converging, or mixing, groundwaters each having sufficiently different oxidation states so that upon mixing, an oxidation-reduction reaction takes place. Dependant on the oxidation potential of the mixed water, this may result in the precipitation of either an oxidized or reduced mineral(s). However minerals do not always precipitate; the aqueous speciation may only change to reflect the resulting oxidation potential of the mixed water.

Reducing zones are layers or rocks containing elements at less than their maximum valence, so that they have significant capacity for oxidation.

Repository is any system licensed by the U.S. Nuclear Regulatory 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 (Nuclear Waste Policy Amendments Act of 1987).

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

Saturated zone is the region below the water table where rock pores and fractures are completely saturated with groundwater.

Sorption is the binding, on a microscopic scale, of one substance to another. A term which includes both adsorption and absorption. The sorption of dissolved radionuclides onto aquifer solids or waste package materials by means of close-range chemical or physical forces is an important process modeled in this study. Sorption is a function of the chemistry of the radioisotopes, the fluid in which they are carried, and the mineral material they encounter along the flow sequence.

Spent nuclear fuel (SNF) is fuel which has been withdrawn from a nuclear reactor following irradiation, the constituent elements of which have not been separated by reprocessing. 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 (Nuclear Waste Policy Act of 1982, Section 2(23)) (10 CFR 961.11). The specific types of SNF discussed in the disposal criticality analysis methodology include:

> **Intact (Waste form or fuel)**. Retaining the initial geometry and chemical composition (except for radioactive decay). Intact is any waste form identified and received at the repository as "intact."
>
> **Degraded (Waste form or fuel)**. Material that was initially part of a waste form/fuel that is no longer intact. The spectrum of such material includes detected pinhole leakers, intact SNF degraded after receipt, fragments of partially degraded waste forms/fuel, elements in solution, and elements in minerals that have precipitated (either interior or external to the waste package). Except for the intact fragments, this material is more specifically referred to as degradation products.
>
> **Degradation product**. Material that was part of a waste form, but has become part of a solution or a precipitate.

Steady-state criticality is a criticality event that has a quasi-static, possibly cyclic, history over a lengthy period of time.

Stratigraphy is the branch of geology that deals with the definition and interpretation of the rock strata, the conditions of their formation, character, arrangement, sequence, age, distribution, and especially their correlation by the use of fossils and other means of identification.

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.

Topographic is the physical features of a district or region.

Transient criticality is a criticality event in which the rate of neutron production may either rapidly or slowly increase due to changes in the nuclear characteristics of the system. The transient criticality may terminate due to loss of moderation or energetic rearrangement of the system, resulting in more leakage and/or less production of neutrons.

Trending is calculating a linear regression of k_{eff} on a predictor parameter that exhibits the strongest correlation coefficient with k_{eff}, with a statistically significant slope.

Uncertainty is an absence of precision that prevents exact information. It may be evaluated as the sum of the systematic and random effects. Systematic effects are due to measuring instruments or calculational methods or both. Random effects occur when different observations are obtained when using the same procedures.

Underground facility means the underground structure, backfill materials, if any, and openings that penetrate the underground structure (e.g., ramps, shafts, and boreholes, including their seals (10 CFR 63.2).

Under-moderated is a state of a system in which adding moderating material increases the reactivity of the system, while removing moderating material decreases the reactivity of the system.

Unsaturated zone is the zone of soil or rock below the ground surface and above the water table in which the pore spaces contain water, air, and other gases. Generally, the water saturation is below 100 percent in this zone, although areally limited perched water bodies (having 100 percent water saturation) may exist in the unsaturated zone. Also called the vadose zone.

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

Waste form means the radioactive waste materials and any encapsulating or stabilizing matrix (10 CFR 63.2). A loaded multi-purpose canister is a canistered waste form (YMP 1998).

Waste package means the waste form and any containers, shielding, packing and other absorbent materials immediately surrounding an individual waste container (10 CFR 63.2).

Waste package degradation (WAPDEG) is a computer code developed as part of the total system performance assessment process to predict the degradation of waste packages.

Zeolites are a large group of hydrous aluminosilicate minerals that act as molecular “sieves’ because they can adsorb molecules with which they interact. They are secondary alteration products at the Yucca Mountain site in tuff rocks when the rocks are exposed to groundwater and could act to retard the migration of radionuclides by their sieving action.