Department of Energy
Office of Civilian Radioactive Waste Management
Yucca Mountain Site Characterization Office
P.O. Box 30307
North Las Vegas, NV 89036-0307

QA: N/A

FEB 2 1 2001

C. William Reamer, Chief
High-Level Waste and Performance
Assessment Branch
Branch Division of Waste Management
Office of Nuclear Material Safety
and Safeguards
U.S. Nuclear Regulatory Commission
Two White Flint North
Rockville, MD 20852

U.S. DEPARTMENT OF ENERGY (DOE) TOPICAL REPORT ON DISPOSAL CRITICALITY ANALYSIS METHODOLOGY, REVISION 01

References: (1) Ltr, Reamer to Brocoum, dtd 6/26/00
(2) Ltr, Brocoum to Reamer, dtd 11/19/99

Enclosure 1 is DOE's *Disposal Criticality Analysis Methodology Topical Report,* YMP-TR-004Q, Revision 01, for review by the U.S. Nuclear Regulatory Commission (NRC). Revision 01 of the Topical Report is a continuation of the Topical Report/Safety Evaluation Report process on disposal criticality, and responds to the NRC Safety Evaluation Report (SER), Reference 1, on Revision 0 of the Topical Report.

All of the open items from the SER, with the exception of the item regarding burnup measurement (item # 1), have been addressed in Revision 01 of the Topical Report. Therefore, DOE believes the revised Topical Report supports resolution of the remainder of the items. Some of these items are not intended to be resolved completely in the Topical Report, but are planned to be resolved in future documents, primarily through model validation reports. For each of these items, requisite text is included in the applicable Topical Report sections describing the general approach and where the details will be documented. The issue of burnup measurement/verification will be addressed in a preclosure report, the schedule for which will be provided to the NRC later in this fiscal year. Revision 01 of the Topical Report has been reorganized and reformatted. To aid in the NRC staff's review, two additional enclosures to this letter are provided that correlate the SER open items (enclosure 2), and NRC Requests for Additional Information, Reference 2 (enclosure 3), with the Topical Report sections where they are addressed.

As was discussed with the NRC staff in the Criticality Key Technical Issues meeting on October 23-24, 2000, the technical sequence planned by DOE for disposal criticality is the methodology topical report, the methodology model validation reports, and then the application analyses based on the methodology. A listing and current schedule for the validation reports was provided during the Criticality Key Technical Issues meeting. Final evaluations of the application of the methodology to specific waste forms and waste package designs, for which DOE has sufficient information, will be completed by License Application. DOE intends to continue to discuss these key areas with the NRC staff to keep you informed of progress.

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DOE looks forward to the NRC staff's review of the Topical Report, as well as to future interactions on the subject of postclosure criticality. If you have any questions, please call Paige R.Z. Russell at (702) 794-1315, or Timothy Gunter at (702) 794-1343.

for Stephan Brocoum
Assistant Manager, Office of
Licensing and Regulatory Compliance

OL&RC:TCG-0664

Enclosures:
1. Disposal Criticality Analysis Methodology Topical Report, Revision 01
2. Crosswalk for SER Open Items in Revision 01 of the Topical Report
3. Crosswalk for RAI Action Items for Inclusion in Topical Report, Revision 01

cc w/encls:
Meraj Rahimi, NRC, Rockville, MD
N. K. Stablein, NRC, Rockville, MD
S. L. Wastler, NRC, Rockville, MD
C. J. Glenn, NRC, Las Vegas, NV
S. H. Hanauer, DOE/HQ (RW-2) FORS
W. H. Lake, DOE/HQ (RW-44) FORS
A. B. Brownstein, DOE/HQ (RW-52) FORS
N. H. Slater, DOE/HQ (RW-52) FORS
C. E. Einberg, DOE/HQ (RW-52) FORS
W. D. Barnard, NWTRB, Arlington, VA
Richard Major, ACNW, Rockville, MD
B. J. Garrick, ACNW, Rockville, MD
Budhi Sagar, CNWRA, San Antonio, TX
W. C. Patrick, CNWRA, San Antonio, TX
Steve Kraft, NEI, Washington, DC
J. H. Kessler, EPRI, Palo Alto, CA
R. R. Loux, State of Nevada, Carson City, NV
John Meder, State of Nevada, Carson City, NV
D. A. Bechtel, Clark County, Las Vegas, NV
Alan Kalt, Churchill County, Fallon, NV
Harriet Ealey, Esmeralda County, Goldfield, NV
Leonard Fiorenzi, Eureka County, Eureka, NV
Andrew Remus, Inyo County, Independence, CA
Michael King, Inyo County, Edmonds, WA
Mickey Yarbro, Lander County, Battle Mountain, NV

cc w/encls: (continued)
Jason Pitts, Lincoln County, Caliente, NV
Judy Shankle, Mineral County, Hawthorne, NV
Jerry McKnight, Nye County, Tonopah, NV
Josie Larson, White Pine County, Ely, NV
R. I. Holden, National Congress of American Indians, Washington, DC
Allen Ambler, Nevada Indian Environmental Coalition, Fallon, NV
J. R. Curtiss, Winston & Strawn, Washington, DC
F. S. Echols, Winston & Strawn, Washington, DC
C. A. Kouts, DOE/YMSCO (RW-2) FORS

cc w/o encls:
D. J. Brooks, NRC, Rockville, MD
K. C. Chang, NRC, Rockville, MD 0
L. H. Barrett, DOE/HQ (RW-1) FORS
R. A. Milner, DOE/HQ (RW-2) FORS
K. M. Cline, MTS, Las Vegas, NV
D. A. Salmon, MTS, Las Vegas, NV
J. G. Linhart, BNC/NSNFP, Las Vegas, NV
J. H. Smyder, BNC/NSNFP, Las Vegas, NV
M. C. Bryan, SEA, Las Vegas, NV
D. A. Thomas, FCF, Las Vegas, NV
J. R. Dyer, DOE/YMSCO, Las Vegas, NV
D. G. Horton, DOE/YMSCO, Las Vegas, NV
Stephan Brocoum, DOE/YMSCO, Las Vegas, NV
D. R. Williams, DOE/YMSCO, Las Vegas, NV
S. P. Mellington, DOE/YMSCO, Las Vegas, NV
J. M. Replogle, DOE/YMSCO, Las Vegas, NV
A. V. Gil, DOE/YMSCO, Las Vegas, NV
T. C. Gunter, DOE/YMSCO, Las Vegas, NV
P. R.Z. Russell, DOE/YMSCO, Las Vegas, NV
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Yucca Mountain Site Characterization Project

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TOPICAL REPORT

YMP/TR-004Q

Revision 01

September 2000

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

Enclosure 1

QA: QA

Yucca Mountain Site Characterization Project

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TOPICAL REPORT

YMP/TR-004Q

Revision 01

September 2000

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

Preparation:

S.P. Mellington, Manager
Office of Project Execution

Date 11/13/00

Approval:

J. R. Dyer, Project Manager
Yucca Mountain Site Characterization Project

Date 11/14/00

R. W. Clark, ~~Acting~~ Director
Office of Quality Assurance
RWC 11/14/00

Date 11/14/00

Author:

D.A. Thomas
Waste Package Department

Date 09/29/2000

Checker:

D.P. Henderson
Waste Package Department

Date 9/29/00

Responsible Manager:

H.A. Benton, Manager
Waste Package Department

Date 9/29/00

CHANGE HISTORY

REV. NO.	ICN NO.		DESCRIPTION OF CHANGE
00	00	11/30/98	Initial issue
01	00	11/16/00	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.

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ABSTRACT

This topical report describes the risk-informed, performance-based methodology to be used for performing postclosure criticality analyses for waste forms in the potential 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 methodology, presents design criteria, and describes the general criticality scenarios. The report also presents the details of the methodology, modeling approach, and validation approach for determining critical configurations, evaluating criticality, estimating probabilities, estimating criticality consequences, and estimating criticality risk.

The methodology provides a systematic approach for evaluating a combined system of a waste form, waste package, engineered barrier, and repository for limiting the potential for criticality through the entire postclosure period of the repository.

The design parameters and environmental assumptions 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. If the U.S. Nuclear Regulatory Commission accepts the methodology as described in this report, the methodology will be fully validated for repository design applications to which it will be applied in the License Application and its references.

The U.S. Nuclear Regulatory Commission staff is being asked to review this topical report and accept the methodology. The U. S. Department of Energy will use the accepted methodology in the License Application for the potential Yucca Mountain monitored geologic repository to demonstrate the acceptability of proposed systems for limiting the potential for postclosure criticality.

Insofar as any sample results from analyses presented in this report are based on specific features of the repository design or performance, which may be subject to change, they 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 or sample results are expected to change significantly.

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CONTENTS (Continued)

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1. INTRODUCTION

The U.S. Congress charged the U.S. Department of Energy (DOE) with managing the geologic disposal of high-level radioactive waste (HLW) 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 a self-sustaining nuclear chain reaction (criticality) is highly unlikely. This report describes a methodology for evaluating criticality potential for HLW and SNF[1], referred to collectively as the waste form, after the repository is sealed and permanently closed (postclosure phase). The methodology described will also be followed in validating the criticality-related models planned for use in the License Application for the potential monitored geologic repository at Yucca Mountain, Nevada.

In addition to this chapter, which presents the background, objective, scope, and quality assurance controls, the report is divided into four other chapters. Chapter 2.0 discusses applicable U.S. Nuclear Regulatory Commission (NRC) regulations and addresses DOE's concerns with existing regulations, along with the regulatory framework within which the topical report is developed. NRC guidance documents and industry standards used in developing the methodology are also discussed.

Chapter 3.0 describes the criticality analysis methodology. This description includes the building of hypothetical scenarios that lead to degraded configurations, defining parameters for each configuration, and evaluating criticality potential for the range and specific values of parameters. The portion of the methodology for estimating the probability of critical configurations and their consequences 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 criticality risk, which is measured by the expected increment in dose rate at the accessible environment due to all potential criticalities. The methodology, modeling approach, and approach for validating the analysis models are discussed for each analysis component of the criticality analysis methodology.

Chapter 4.0 summarizes the methodology presented and provides conclusions regarding the purpose, potential uses, and limitations of its use. Chapter 5.0 lists 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 consequences of, postclosure criticality in the repository. The risk-informed, performance-based methodology presented is consistent with the proposed Code of Federal Regulations (CFR) Title 10, Part 63 (64 FR 8640). The proposed 10 CFR 63 specifies the overall performance objectives of the potential repository at Yucca Mountain prior to closure and during postclosure. The overall performance of the repository is specified for postclosure (10 CFR 63.113) in terms of expected annual dose to the average member of the critical group. There are no specific design criteria for postclosure criticality control in the proposed 10 CFR 63. This regulation is a risk-informed, performance-based regulation, which treats criticality as one

[1] The methodology presented in this report will be applied to the different waste forms; commercial SNF (including boiling water reactor, pressurized water reactor, and mixed oxide); DOE SNF (including degraded naval SNF); immobilized plutonium; and vitrified HLW. The methodology used to address intact naval SNF has been described in a separate addendum (Mowbray 1999).

of the processes or events that must be considered for the overall system performance assessment.

Limiting the potential for, and consequences of, criticality during the postclosure phase of the geologic repository relies on multiple barriers, both natural and engineered. The natural barrier system consists of the climate around, and the rock formations of, the repository, and includes the geologic, mechanical, chemical, and hydrological properties of the site. As defined within 10 CFR 63, the engineered barrier system (EBS) comprises 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, and other absorbent materials immediately surrounding an individual package. The underground facility consists of the underground structure, backfill materials, if any, and openings that penetrate the underground structure (e.g., ramps, shafts, and boreholes, including their seals). The EBS 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 approach of using the natural features and characteristics of the site in combination with the engineered components of the repository design to limit criticality potential supports the defense-in-depth concept; should one system fail, another exists to provide adequate protection. The repository design will incorporate multiple barriers that are both redundant and diverse to minimize the potential for conditions conducive to criticality. Separate barriers that act to protect the fissile material from water (moderator) contact provide an example of redundant barriers. A waste package design with an outer corrosion-resistant barrier and SNF with fuel cladding would provide this function. The combination of a barrier that impedes or limits the amount of water in a waste package and a barrier that contains neutron-absorbing materials provides a set of diverse barriers. For example, borated stainless steel plates inside the waste package absorb neutrons, while the waste package shells prevent water from entering the waste package.

The objective of analyzing the potential for criticality is to project the effectiveness of measures that are implemented before repository closure to minimize criticality potential over thousands of years. The effectiveness of these measures will vary as a function of both time after the waste has been emplaced and of the potential degradation of the waste packages as the repository environment changes.

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 long-term processes. These events take place over hundreds, thousands, and tens-of-thousands of years. Based on the most recent TSPA analysis (CRWMS M&O 2000g), the minimum time required to cause a failure in the waste canister is greater than 10,000 years.

The methodology described in this report addresses the design features of the EBS and how they are affected by various processes (e.g., groundwater flow and corrosion) in the repository. The principal components of the EBS are the waste packages. The waste packages will be 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. For criticality to occur, therefore, 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 analysis. 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 potential repository at Yucca Mountain.

As previously stated, the risk-informed, performance-based methodology presented in this topical report is consistent with the proposed site-specific regulation for Yucca Mountain (10 CFR 63). This topical report is being submitted on the assumption that the proposed regulations, or something similar, will be issued. The existing regulations, and proposed changes to the regulations, are discussed in further detail in Chapter 2.0 of this report.

1.2 OBJECTIVE

The objective of this topical report is to present the planned risk-informed, performance-based disposal criticality analysis methodology to the NRC and to seek acceptance that the principles of the methodology and the planned process for validating individual models within the methodology are sound.

For certain fuel types (e.g., intact naval fuel), any processes, criteria, codes or methods different from the ones presented in this report will be described in separate addenda (Mowbray 1999). These addenda will employ the principles of the methodology described in this report as a foundation. Departures from the specifics of the methodology presented in this report will be described in the addenda.

This topical report seeks the NRC's acceptance of the following aspects of the methodology for performing criticality analyses for the geologic disposal of the waste forms.

A. The following design 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 consequences of, criticality:

   1. The *Critical Limit (CL)* criterion discussed in Subsection 3.2.1: The calculated effective neutron multiplication factor (k_{eff}) for subcritical systems (configurations) for postclosure will be less than the CL. The CL is the value of k_{eff} at which the system is considered potentially critical as characterized by statistical tolerance limits.

2. The *Design Probability* criterion discussed in Subsection 3.2.2: The average criticality frequency will be less than 10^{-4} per year for the entire repository for the first 10,000 years, for all combinations of waste packages and waste forms. This criterion is intended to ensure that the expected number of criticalities is less than one during the regulatory life of the repository (10,000 years). It is used to define a waste package criticality control design requirement in support of defense-in-depth with respect to the Repository Criticality Performance Objective in item 3.

3. The Repository *Performance Objectives* criterion discussed in Subsection 3.2.3: The ability to satisfy dose rate performance objectives will not be compromised by the radionuclide increment due to criticality events (if any).

B. The Master Scenario List (CRWMS M&O 1997d, pp. 13-45) presented in Section 3.3, and summarized in Figures 3-2a, 3-2b, 3-3a, and 3-3b, comprehensively identifies degradation scenarios based on features, events, and processes (FEPs) associated with the potential repository at Yucca Mountain that may significantly affect the potential for, and the consequences of, criticality.

C. The portion of 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. Specifically, the 14 methodology steps specified for internal configurations in Subsection 3.4.1.1 and the five methodology steps specified for external configurations in Subsection 3.4.2.1 are acceptable as comprehensive.

D. The portion of the methodology for performing criticality evaluations of postclosure configurations and using critical limits discussed in Section 3.5 is acceptable in general for disposal criticality analysis.

E. The methodology for estimating the probability of postclosure critical configurations and using multivariate regressions, or table lookup and interpolation discussed in Section 3.6 is acceptable in general for disposal criticality analysis.

F. The portion of the methodology for estimating consequence of postclosure criticality events discussed in Section 3.7 is acceptable in general for disposal criticality analysis.

G. The validation approach for the isotopic, criticality, and regression models are acceptable in general for model validation. Specifically:

1. The isotopic model validation process described in Subsection 3.5.3.1 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 CL values for postclosure repository conditions will be demonstrated in validation reports, which will be referenced in the License Application. NRC acceptance of isotopic bias values for k_{eff} and their applicability for postclosure repository conditions will be sought in the License Application.

2. The criticality model validation process described in Subsection 3.5.3.2 is acceptable in general for model validation. Specifically, the process presented for calculating the

CL values and the process presented for establishing the range of applicability of the CL values define the validation process for the criticality model. This validation process will be followed to calculate CL values for specific waste forms and waste packages as a function of degradation conditions. The applicability of the CL values for postclosure repository conditions will be demonstrated in validation reports, which will be referenced in the License Application. NRC acceptance of CL values and their applicability for postclosure repository conditions will be sought in the License Application.

3. The validation process for the regression analysis model for k_{eff} described in Subsection 3.5.3.3 is acceptable in general for model validation. The applicability of k_{eff} values obtained from the regression model for postclosure repository conditions will be demonstrated in validation reports, which will be referenced in the License Application. NRC acceptance of k_{eff} values obtained from the regression model and their applicability for postclosure repository conditions will be sought in the License Application.

H. The validation process for the degradation analysis portion of the methodology presented in Subsections 3.4.1.3 and 3.4.3.1 for calculating the concentrations of components in solution inside the waste package and waste-package component degradation products is acceptable in general for model validation. Specifically:

1. Validation of the models for geochemical degradation of waste package components (leading to potentially critical configurations within the waste package) is by benchmark comparisons with a set of experiments covering both fixed volume and flow-through conditions.

2. Validation of the models for external accumulation of fissionable material (leading to potentially critical configurations external to the waste package) is by benchmark comparison with precipitation of minerals in laboratory experiments having chemical conditions representative of the repository.

I. The validation process for the probability calculation and configuration generator models described in Subsection 3.6.4 is acceptable in general for model validation. Specifically, the computer code that implements the Monte Carlo probability calculation portion of the methodology is validated by comparison with the hand calculation of combinations of probabilities of individual events taken from distributions similar to those used for the Monte Carlo selection process.

J. The validation process for the criticality consequence models presented in Subsection 3.7.3 is acceptable in general for model validation. Specifically:

1. The range of parameters, permitting selection of the most conservative, demonstrates the acceptability of the criticality consequence models for internal and external criticality and for transient as well as steady-state criticality.

2. Verification of the individual models implementing the basic physical processes by hand calculation, where appropriate.

K. The proposed requirements presented in Subsection 3.5.3.1.2 for modeling burnup of commercial SNF for design applications are sufficient, if met, 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 validation reports, which will be referenced in the License Application. NRC acceptance of the confirmation of the conservatism in the application model for postclosure repository conditions will be sought in the License Application.

L. The principal isotopes selected to model burnup in intact commercial SNF, presented in Table 3-3 in Subsection 3.5.2.1.1, are acceptable for disposal criticality analysis provided that:

1. The bias in k_{eff} associated with predicting the isotopic concentrations is established in the validation reports as described in Subsection 3.5.3.1.

2. Deviations from the predicted concentrations because of radionuclide migration from intact fuel assemblies through pinholes and cracks in the cladding are addressed in the geochemical analysis.

The k_{eff} values from criticality evaluations of intact commercial SNF with pinholes and cracks 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. The applicability of the principal isotopes for intact commercial SNF will be demonstrated in validation reports, which will be referenced in the License Application.

M. The process for selecting isotopes from the list of principal isotopes for degraded commercial SNF presented in Subsection 3.5.2.1.4 is also 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 validation reports, which will be referenced in the License Application. NRC acceptance of the application of the selected isotopes to postclosure repository conditions will be sought in the License Application.

With the exception of the determination of isotopic inventories, the methodology described above will be used for all waste forms, other than intact naval fuel, for which there may be a number of exceptions. The methodology used to address intact naval SNF has been described in a separate addendum (Mowbray 1999).

1.3 SCOPE

This report presents the process and analytical tools for predicting the potential for, and the consequence of, criticality during the postclosure period of the geologic repository. The process and tools make up the methodology for identifying potentially critical configurations (including probability of occurrence), establishing the direct consequence of any potential criticality, and evaluating the risk of any potential criticalities (in terms of risk of dose to the critical group). The methodology provides a means to evaluate potential postclosure criticality events for the range of conditions of the waste form (intact, degraded, and degradation products), for postulated conditions of the engineered systems (waste package and other

engineered barriers), and for the range of possible locations (in-package, near-field, and far-field). The methodology will be applied to the different waste forms: commercial SNF (including boiling water reactor, pressurized water reactor, and mixed oxide SNF); DOE SNF (including naval SNF[2]); immobilized plutonium; and vitrified HLW glass.

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 design criteria imposed by the methodology to ensure appropriate criticality controls are implemented in the waste package design. A standard set of degradation scenarios that may lead to configurations of fissionable material (FM) with the potential for criticality is presented in Section 3.3. A detailed description of the criticality analysis methodology is presented in Sections 3.4 through 3.8.

The analytical tools are the models of the methodology. These include degradation analysis models, neutronic analysis models, probability calculation models (including the configuration generator code), models to project the consequence of criticality, and TSPA models used for estimating dose increment 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 validation reports, which will be referenced in the License Application. Because of its classified nature, models unique to naval SNF are described in a separate submittal (Mowbray 1999).

1.4 QUALITY ASSURANCE

The development of the topical report has been subject to the DOE Office of Civilian Radioactive Waste Management (OCRWM) *Quality Assurance Requirements and Description* (QARD) (DOE 2000) controls. The report was prepared in accordance with the OCRWM Administrative Procedures and a development plan (CRWMS M&O 2000d). The methodology described in this report is related to the evaluation of the Monitored Geologic Repository (MGR) waste package and engineered barrier segment. The waste package and engineered barrier segment have been identified as items important to radiological safety and waste isolation in a number of classification analyses (e.g., CRWMS M&O 1999h).

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

The work that is to be performed to support the License Application using this methodology will be performed in accordance with the then current versions of the QARD and NRC regulations. All information used for the License Application will be developed in accordance with the QARD and NRC regulations, or will be from acceptable sources.

The OCRWM Administrative Procedures require that any document that contains references that have not been verified, as completed and correctly entered into the Records Processing Center, be tracked with an unresolved reference number. Three of the references used in this topical report revision are being developed concurrently with the topical report. Since the references are being developed concurrently, they will not be complete and entered into the Record Processing Center by the time the topical is approved for issuance. Therefore, the

[2] Discussions of naval fuel in this report refer primarily to degraded, or the dissolution products from degraded naval fuel. Principals and concepts of the methodology are also applicable to intact naval fuel; however, details of the criticality analysis methodology have been discussed in a classified addendum (Mowbray 1999).

references can not be verified and are being tracked with unresolved reference numbers. The OCRWM Administrative Procedures also require a specific paragraph be added to documents that have references with unresolved reference numbers. The references in question give additional background information that does not need to be confirmed and does not affect any conclusion stated in the topical. In addition, the references will have been approved and verified by the time this report is released for regulatory review. Therefore, the specific paragraph is not applicable to the topical, but is included as required per the administrative procedure. The following is the required paragraph:

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

2. REGULATORY PERSPECTIVE

The purpose of this topical report is to present, for the review and acceptance of the U.S. Nuclear Regulatory Commission (NRC), a new methodology for analyzing the potential for criticality during the postclosure phase of the repository at Yucca Mountain. Chapter 2.0 discusses applicable NRC regulations and expected changes to the regulations, along with the regulatory framework within which the topical report is developed. Application of the methodology will provide input to total system performance assessments that will determine if the repository will meet its overall performance objectives in the NRC's proposed new regulations for Yucca Mountain (64 FR 8640) to be issued at 10 CFR Part 63.

The topical report is being submitted in accordance with the *Topical Report Review Plan* (Holonich 1994) issued by the NRC's Division of High-Level Waste Management. Consistent with the purpose of a topical report as described in that plan, the *Disposal Criticality Analysis Methodology Topical Report* focuses on the postclosure disposal criticality methodology under evaluation during the pre-licensing consultation phase, as applied specifically to the Yucca Mountain site. If accepted by the NRC staff, the topical report will be referenced in the License Application for the Yucca Mountain repository should the site be found suitable for development of a repository.

This topical report describes a probabilistic postclosure criticality analysis methodology that is intended to support risk-informed demonstration that public health and safety are protected against postclosure criticality in the repository. The methodology is believed to be fully compliant with proposed 10 CFR Part 63. However, should the methodology not clearly support compliance with the new regulations as eventually issued, the U.S. Department of Energy (DOE) will identify an appropriate course of action for postclosure criticality analysis. The choice of approach to postclosure criticality analysis, the existing disposal criticality regulations, and potential changes to those regulations are discussed in Sections 2.1 and 2.2.

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 evaluation of postclosure criticality.

This topical report was submitted to the NRC as Revision 0 (YMP 1998) in January 1999. The NRC staff reviewed the document and issued to the DOE a Request for Additional Information (Reamer 1999) that contained questions and comments on a number of aspects of the methodology as described in the topical report. The DOE responded in writing to the Request for Additional Information (Brocoum 1999). The DOE's response provided clarifications and corrections as appropriate to address the NRC's questions and comments.

Since submittal of the Revision 0 topical report, it has become evident that some DOE work needed to support full NRC acceptance of the methodology will not be immediately available. Also, some discussions in the topical report pertain to application of the methodology rather than to the methodology itself. These aspects will be addressed in future documents that will support the License Application, rather than in the topical report.

For these reasons, and to fully address the NRC's Request for Additional Information, the DOE indicated in its response that the topical report would be revised in 2000. Revision 1 to this report is the revision discussed in the response, and it is intended to address all planned revisions to the topical report discussed therein.

The NRC staff reviewed the DOE's response and issued a draft Safety Evaluation Report (SER) (Reamer 2000a). The draft SER stated that the staff accepted certain aspects of the methodology (in some cases subject to verification of DOE plans described in its response to the Request for Additional Information). Other aspects of the methodology for which the NRC staff believes the DOE has not provided sufficient justification or detailed information were carried in the draft SER as open items. These open items will need to be addressed satisfactorily before the NRC can fully accept the methodology.

The NRC and DOE staffs held a technical exchange in March 2000 to discuss the draft SER. Subsequent to the meeting, the DOE provided comments on the draft SER (Brocoum 2000). The NRC then issued the final SER (Reamer 2000b). Like the draft SER, the final SER accepts certain aspects of the methodology while leaving other aspects the subject of open items.

2.1 REGULATORY FRAMEWORK

The existing regulation pertinent to Yucca Mountain is 10 CFR Part 60. However, the NRC plans to make this regulation inapplicable to a repository at Yucca Mountain when it issues a new Yucca Mountain site-specific regulation as 10 CFR Part 63 (64 FR 8640). Since the proposed Part 63 regulation has become available for public view and comment, NRC and DOE interactions have focused exclusively on the proposed Part 63 and not on Part 60. Therefore, this document focuses on compliance with proposed Part 63.

The proposed regulations to be issued in 10 CFR Part 63 would eliminate subsystem performance objectives and most specific design criteria found in Part 60. There would be no design criterion for postclosure criticality. Instead, the proposed regulations focus on performance assessment, the "bottom-line" measure of repository postclosure performance. To ensure the DOE develops and supports a defensible and rigorous performance assessment, proposed § 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 expected annual dose would be significantly changed by their omission.

Postclosure criticality is an alteration process for the waste form, which is by definition in proposed 10 CFR Part 63 part of the waste package and therefore 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).

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

> 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 of very low probability of occurrence (less than one chance in 10,000 over 10,000 years) can be excluded from the analysis.

It is expected that the methodology described in this topical report can and will be used to demonstrate that the probability of criticality is very low during the period of regulatory concern. Further, it is expected that the methodology will demonstrate that the effects of one or more criticalities on repository performance would be negligible even if such events were to occur. Therefore, it is expected that postclosure criticality will be screened out of the base case for the performance assessment as allowed by proposed 10 CFR Part 63.

The methodology discussed in this topical report is based on risk-informed, performance-based analysis. This methodology is believed to be fully consistent with proposed 10 CFR Part 63.

The proposed EPA standard and the proposed NRC regulations are not fully consistent with each other and have been the subject of much interagency discussion, and therefore the exact form of the new standards and regulations (particularly the dose limits) is not definitively known. However, because the topical report presents a methodology, the exact values of the dose limits are not considered relevant to the acceptability of the topical report. In the unlikely event the new regulations, as eventually promulgated, require the methodology to be revised, the topical report will also be revised.

2.2 USE OF THE CRITICALITY METHODOLOGY IN DEMONSTRATING COMPLIANCE

This section discusses the approach taken in this topical report to support demonstration that postclosure disposal criticality regulations based on a risk-informed approach to limit criticality potential will be met. 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 existing applicable NRC regulation (10 CFR 60.131(h)) is deterministic in nature.

It is possible to specify measures that can be deterministically demonstrated to prevent criticality. However, their implementation becomes increasingly impractical for more highly enriched waste forms (with the expected exception of intact navy spent fuel, a uniquely robust waste form) and for longer time periods of concern. Furthermore, it is very difficult, for the extremely long time periods being discussed, to define a credibility standard, or threshold probability, acceptable to all parties in a licensing proceeding. Accepted standards exist in reactor and spent fuel storage licensing, but the period of regulatory concern is many orders of magnitude smaller than that likely to be applicable to a geologic repository. For example, an event with a very low probability of occurring in any individual's lifetime could have a relatively high probability of occurring over the much longer period of concern for a geologic repository. This type of contrast can lead to differing positions regarding a reasonable basis for a credibility threshold, and there is no known precedent for establishing a credibility threshold in this type of situation.

The approach to addressing postclosure criticality described in this topical report is intended to provide a rigorous method of demonstrating 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 the NRC's proposed 10 CFR Part 63. As discussed in the subsections that follow, the approach combines probabilistic analysis with defense-in-depth against postclosure criticality.

2.2.1 Probabilistic Analysis

The analysis methodology presented in this topical report does not attempt to support the demonstration that postclosure criticality either will not occur or is incredible (that is, has a probability below some threshold of concern). Instead, the methodology focuses on evaluation of the risk of criticality. In this document, risk is defined as the product of the probability and consequence for each particular criticality process or event under consideration. This focus on risk is consistent with the recommendations of the National Academy of Sciences to meet risk-based performance objectives to protect the health and safety of the public and with the NRC staff's draft site-specific regulations for Yucca Mountain. Use of risk-informed, performance-based analysis in regulatory matters is consistent with the NRC policy statement 60 FR 42622, and with correspondence among the NRC commissioners on risk-informed, performance-based regulation (Memorandum from NRC Chairperson S. Jackson to Commissioners Dicus, Diaz, and McGaffigan, subject Discussion on Risk-Informed, Performance-Based Regulation, February 20, 1998) (Jackson 1998).

The analysis methodology is a combination of (1) the evaluation of the risk of criticality for the range of possible waste package/waste form configurations, and (2) the comparison of these risks to identify candidates for additional criticality control measures. Risk posed by criticality will be determined by analyzing criticality as a potential detractor to the repository's overall performance using the methodology described in this report. The probabilities and consequences of potential criticality events will then form a part of the repository performance assessment.

It is recognized that defense-in-depth is needed against criticality events even if, as currently expected, the predicted consequences of such events for the repository's performance and for the health and safety of the public would be very small. Therefore, scenarios and conditions that contribute significantly to the overall postclosure criticality risk will be examined, with an intent to incorporate reasonable and feasible measures (add or strengthen diverse or redundant barriers to criticality) to reduce the risk. Determination of feasibility will be based on balancing the benefit of given measures against their cost. Risk-informed, performance-based analysis will be used to determine the effectiveness of the measures.

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 Project's overall approach to defense-in-depth against criticality is discussed in Subsection 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.

Mechanistic but not necessarily probabilistic criticality analysis methodology is expected to be sufficient for intact navy spent fuel, which is a uniquely robust waste form. The methodology

for this analysis is described in an addendum to this topical report that has been submitted to the NRC (Mowbray 1999).

2.2.2 Defense-in-depth Against Postclosure Criticality

Proposed 10 CFR Part 63 discusses "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 criticality analysis methodology in that approach. The approach includes three aspects.

The first aspect of defense-in-depth involves taking advantage of the many natural and engineered features of the site and repository to make the probability and consequences of postclosure criticality as low as feasible. The natural and engineered barriers will collectively make the probability of a postclosure criticality low. For a criticality to occur, multiple changes in conditions (waste package breach, water intrusion and retention, removal of neutron absorbers) must occur. 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 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 reduces the probability of criticality). Examples of diverse barriers are the waste package inner barrier, neutron-absorbing materials in the basket, and the iron (which displaces 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, and the drip shield limits or prevents damage to the waste package from dripping water or rockfall. Numerous other features are either planned or under consideration. The result is expected to be a site and repository with considerable resistance to postclosure criticality either occurring or resulting in a hazard to the public. Because specific site and design features are outside the scope of this topical report, design of the repository and use of the site to provide defense-in-depth are not discussed further in the report.

The second aspect of the defense-in-depth philosophy will be implemented in conjunction with the methodology presented, as discussed earlier in this section. In addition to an assessment of risks associated with potential criticality events, the methodology includes evaluation of the probability of the events and the contributing factors to their potential for occurrence. This analysis will attempt to 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.

The third aspect of the defense-in-depth philosophy is using appropriate conservatism in the analyses, although this conservatism is notably outside the 10 CFR 63 definition. 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. Additional guidance may be used to further refine the methodology.

2.3.1 NUREGS

The information and guidance contained in NUREG/CR-2300, *PRA Procedures Guide* (NRC 1983), have been reviewed for application to the postclosure criticality analysis methodology. 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 presented in this topical report is consistent with the objectives of the three levels of a PRA described in NUREG/CR-2300 (NRC 1983).

As stated in NUREG/CR-2300, Subsection 2.1.3, *Scope and Results of Analysis* (NRC 1983) 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 methodology identifies a sequence of events and/or processes that leads to criticality and determines the probability of each sequence. The development and use of the Master Scenario List (CRWMS M&O 1997d) and associated configuration class, as discussed in Chapter 3.0 of this report, emulates the purpose of a level 1 PRA.

This section of NUREG/CR-2300 (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 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 the level 3 analysis (or in the TSPA, in the case of the methodology presented in this topical report).

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 each criticality sequence on the performance of the repository.

The methodology presented in Chapter 3.0 of this topical report is intended to provide a similar rigor and systematic approach to those 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 the Master Scenario List (CRWMS M&O 1997d), developed and refined with careful consideration of the ways a waste package can be affected by each scenario.

However, though there are similarities in 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 very different. A PRA for a nuclear power plant looks at an initiating event followed by the success or failure of a variety of actively and 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 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. However, the general philosophy for performing a PRA for a nuclear power plant, and the systematic and rigorous approach used, have been incorporated into the methodology described in Chapter 3.0.

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 code system in methodology and in establishing an upper subcritical limit (USL) and CL. This NUREG references American National Standards Institute and American Nuclear Society standard ANSI/ANS-8.17, Criticality Safety Criteria for the Handling, Storage, and Transportation of LWR Fuel Outside Reactors (discussed below) 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 below (ANSI/ANS-8.1, American National Standard for Nuclear Criticality Safety in Operations with Fissionable Materials Outside Reactors).

2.3.2 Industry Standards

Four industry standards have been used in developing the methodology: ANSI/ANS-8.1, ANSI/ANS-8.15, Nuclear Criticality Control of Special Actinide Elements, ANSI/ANS-8.17, and ANSI/ANS-8.10 Criteria for Nuclear Criticality Safety Controls in Operations with Shielding and Confinement. Each is briefly discussed below.

- ANSI/ANS-8.1. 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 described in the topical report for criticality analyses external to a waste package (both near-field and far-field locations) uses and is consistent with much of the methodology provided in this standard. The guidance in this standard is followed in establishing critical limits. [3] Its guidance for establishing bias by correlating the results of

[3] 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

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. 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 features, events, and processes that pose the potential for criticality but will not do so using the double-contingency criterion.

- ANSI/ANS-8.15. This standard addresses isotopes of actinide elements, other than those isotopes addressed in ANSI/ANS-8.1, that are capable of supporting a chain reaction and that may be encountered in sufficient quantities to be of concern for criticality. It addresses these isotopes in a manner similar to that by which ANSI/ANS-8.1 addresses ^{233}U, ^{235}U, and ^{239}Pu. The single-parameter limits of ANSI/ANS-8.15 are not applied to disposal criticality analysis, for the same reason as discussed above for ANSI/ANS-8.1. Because ANSI/ANS-8.15 refers to the methodology discussed in ANSI/ANS-8.1, the methodology in this topical report is consistent with ANSI/ANS-8.15 to the same extent it is consistent with ANSI/ANS-8.1, as previously described.

- ANSI/ANS-8.17. This standard provides guidance for criticality safety for a specific waste form, light water reactor spent fuel, as opposed to the more general scope of ANSI/ANS-8.1. ANSI/ANS-8.17, which is intended to provide supplemental guidance for ANSI/ANS-8.1, 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 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. Also, 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 (Lichtenwalter et al. 1997) for establishing subcriticality, with certain differences respective of the differences between the deterministic storage analyses and risk-informed disposal analyses.

The risk-informed, performance-based methodology described in this Topical Report defines a CL that establishes systems that have the potential to be critical. Past applications of ANSI/ANS-8.17-1984, which were deterministic, defined an upper subcritical limit that used an arbitrary subcritical margin. The CL values described in this report do not include an arbitrary subcritical margin (i.e., Δk_m as defined in ANSI/ANS-8.17-1984). Elimination of this

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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.

arbitrary margin is consistent with the elimination of the requirement in the NRC's proposed 10 CFR Part 63. That proposed regulation, like DOE's planned 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's approach in the proposed regulation. DOE's disposal criticality method is intended to address the proposed 10 CFR Part 63, on the assumption that it will ultimately be issued in a form similar to the draft regulation. DOE's planned method will contain appropriate conservatisms for a risk-informed, performance-based approach. DOE therefore believes that the 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.

The DOE has not yet evaluated the need for burnup verification through physical measurement of each spent fuel assembly, vs. an alternative and less resource-intensive method, perhaps one involving statistical sampling. This matter will be addressed in a future revision to this topical report, in which DOE will propose an alternative to physical measurement of every spent fuel assembly.

- ANSI/ANS-8.10. 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 requires designing for one, rather than two, unlikely events as required by ANSI/ANS-8.1 and ANSI/ANS-8.17. The approach described in ANSI/ANS-8.10 is consistent with the methodology presented in this topical report.

2.3.3 Regulatory Guide

NRC Regulatory Guide 3.71, *Nuclear Criticality Safety Standards for Fuels and Materials Facilities*, was also used in developing the methodology. This Regulatory Guide endorses 15 ANSI/ANS standards, including the four identified in the previous section as useful in development of disposal criticality analysis methodology.

However, the Regulatory Guide takes exception to certain aspects of the standards. The exception pertinent to this topical report is that 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. As noted in the previous subsection, the methodology presented in this report is consistent with ANSI/ANS-8.17, which allows measurements or analyses to verify burnup. The need for burnup verification of every fuel assembly is considered an open issue in NRC's SER (Reamer 2000b), because the DOE has not yet determined whether such measurements are needed for all spent fuel bundles, for suitable samples, or are not needed. The DOE may propose that burnup of bundles not subjected to flux measurements be inferred from measurements of burnup of a statistically significant set of assemblies with similar design and power histories, as discussed in this topical report. With the exception of physical measurements of burnup, the planned implementation of the methodology presented in this report is consistent with Regulatory Guide 3.71 to the same extent it is consistent with the four ANSI/ANS standards discussed in Subsection 2.3.2.

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3. METHODOLOGY

This chapter presents the methodology for performing criticality analyses for waste forms emplaced in the proposed repository at Yucca Mountain for long-term disposal. This methodology applies to the time period of regulatory concern after the repository is permanently closed (postclosure). Although the methodology will apply to the entire postclosure period, the application of the individual models will vary as conditions, events of interest, and levels of uncertainty change. Acceptance of the principles of the risk-informed, performance-based approach discussed in this chapter is sought in this report. In addition, specific aspects of the methodology for which NRC acceptance is sought are noted throughout Chapter 3.0. The full list of items for which acceptance is being sought are listed in Section 1.2.

Chapter 3 is divided into 8 sections. An overview of the overall methodology is provided in Section 3.1. Section 3.2 discusses design 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 features, events, and processes. 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 analysis components of the methodology are described in the remaining sections of this chapter. Each section is divided into subsections that present the analysis process or methodology, the modeling approach, and the validation approach for the various models. Section 3.4 discusses the steps of the methodology to specify the configuration parameters, starting from the configuration classes and using a non-equilibrium geochemistry model as the principal evaluation tool. The modeling approach for the degradation analysis models (corrosion and geochemistry models) and the validation approach for these models are also presented. The neutronic methodology for evaluating criticality (k_{eff}) once the configuration has been completely specified is described in Section 3.5.

The last three sections are concerned with probability, consequence, and associated risk. Risk of criticality is defined as the product of probability of criticality multiplied by the consequence of the criticality. For the repository the most appropriate measure of consequence is the dose rate from the radionuclide increment and from other effects potentially resulting from the criticality. If there are several possible scenarios leading to criticality, then the total risk is the sum of the individual probability-consequence products from each of the scenarios. Section 3.6 gives the methodology for estimating the probability of the potentially critical configuration. The methodology is described with respect to probability distributions of the scenario-related parameters discussed in Section 3.3 and the configuration-related parameters discussed in Section 3.4. The methodology for estimating the consequences of criticality is presented in Section 3.7. Section 3.8 describes the methodology for combining probability and consequence estimates, which is part of the general TSPA methodology, including the modeling of radionuclide transport to develop an estimate of incremental dose at the accessible environment.

3.1 OVERALL METHODOLOGY

An overview of the disposal criticality analysis methodology 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. As the chart indicates, the input data includes the designs of the waste package (WP)/EBS (including the waste form characteristics), the characteristics of the site, and the degradation characteristics of the waste-package materials. In addition, a Master Scenario List with associated configuration classes is provided as input.

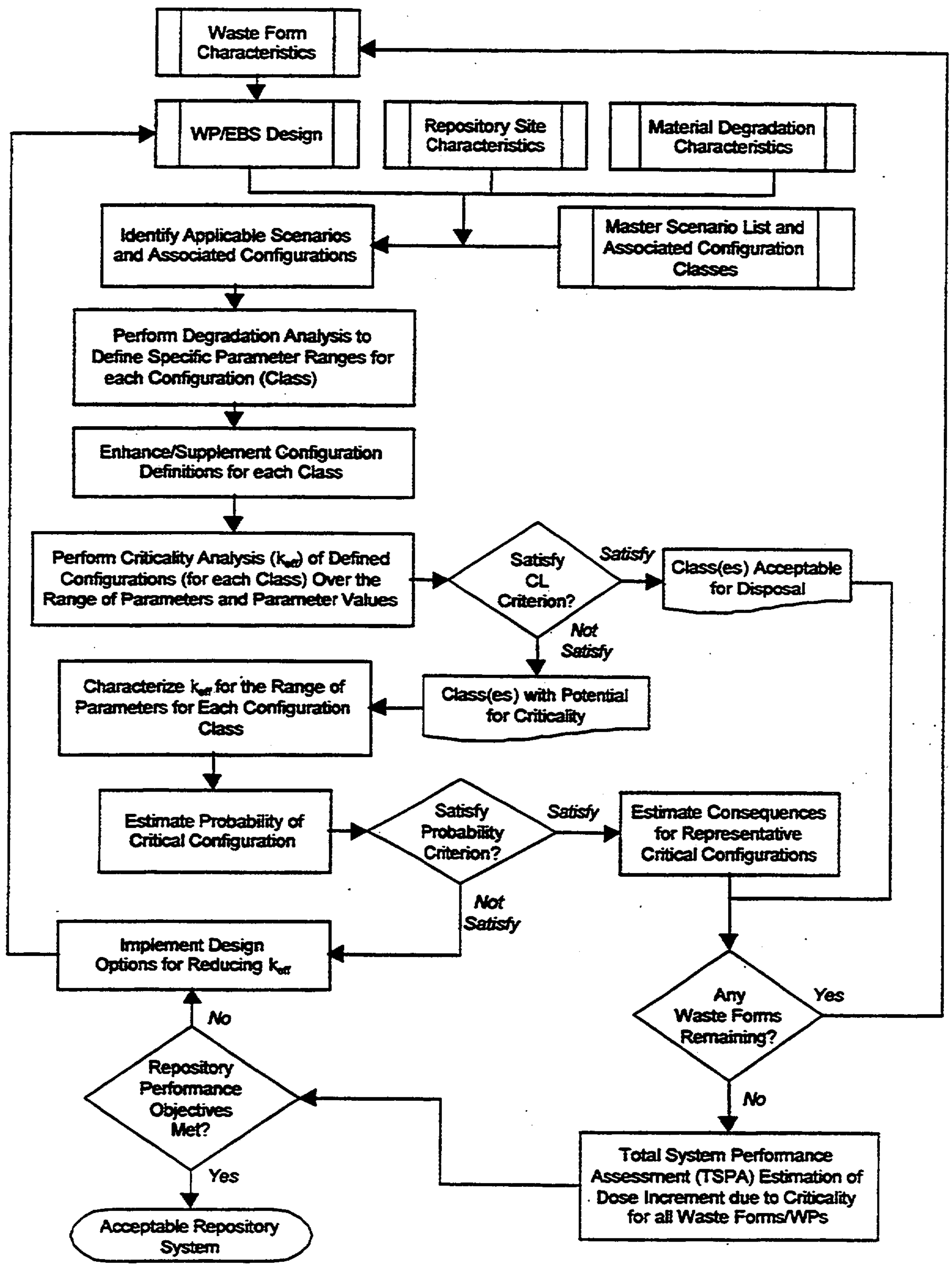


Figure 3-1. Overview of Disposal Criticality Analysis Methodology

The Master Scenario List (CRWMS M&O 1997d, pp. 13-45), 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, which are based on the features, events, and processes associated with Yucca Mountain, were developed at a workshop on postclosure criticality for the TSPA Viability Assessment (VA) abstraction/testing effort (CRWMS M&O 1997c).

The decision points represent design criteria that are imposed by the methodology and applied to ensure sufficient measures are implemented to limit the potential for, and consequences of, a criticality. These criteria include examining the significant contributing factors to the risk of criticality and implementing design enhancements to reduce the overall criticality risk, if the criteria are exceeded.

The process represents a logical, step-by-step approach. Moving through Figure 3-1, the process establishes how the waste package may degrade by examining the characteristics of the repository site and the types of likely conditions and anticipated interactions that could take place, and identifies applicable scenarios that result in degraded configurations. A configuration is defined by a set of parameters that characterize the amount and physical arrangement of materials that affect criticality. These parameters may include the amounts of fissionable material, neutron absorber material, corrosion products, reflecting material, and moderator. Similar configurations are grouped into configuration classes, where the composition and geometry of a configuration class are defined by specific parameters that distinguish one class from another.

After the applicable scenarios and configuration classes are identified, degradation analyses are performed to define specific parameter ranges for the configurations in each class, and the original configuration class definitions are reconsidered. For example, an original class of "partial basket degradation" may be split into two subclasses: one with the corrosion products fully distributed in the water surrounding the fissionable material, and another with the corrosion products settled to the bottom of the waste package but still contained within the package.

As noted in Figure 3-1, postclosure criticality evaluations are performed for these degraded configurations of the waste package and other materials. These criticality evaluations are performed for the defined configurations in each class over the range of parameters and parameter values. Configurations both inside and outside of the waste package that may have the potential for criticality are considered.

The first decision point in Figure 3-1 is the CL criterion. The CL is the value of k_{eff} at which the configuration is considered potentially critical as characterized by statistical tolerance limits. CL values are obtained by analysis of experimental systems with a range of neutronic parameters that are representative of the configuration parameters analyzed for the repository. Configuration classes that satisfy the CL criterion are considered acceptable for disposal, while those classes with k_{eff} values that are greater than or equal to the CL require further analysis. For the latter classes, the range of configuration parameters and parameter values are examined for potential design features that may be implemented to reduce k_{eff}. Further description of the CL criterion is given in Section 3.2. A discussion of the application of the critical limit criterion is presented in Section 3.5 and Figure 3-5. The process for calculating the CL is described in Subsection 3.5.3.2.

The probability of achieving a critical configuration is estimated for configurations that fail to satisfy the CL criterion. This probability is estimated for each configuration class, on a per package basis, as a function of the characteristics of the waste form (i.e., by looking at the characteristics of the waste form against the parameter ranges for the configurations in each class). The estimated probability is compared with the probability criterion as shown in Figure 3-1. If this criterion is exceeded, additional design options for reducing k_{eff} are implemented. When the probability criterion is satisfied, a criticality consequence evaluation is performed. Further description of the probability criterion is given in Section 3.2. The methodology for estimating the probability of critical configurations is presented in Section 3.6.

The criticality consequence analysis establishes the impact of potential criticality events on the radionuclide inventory, thermal effect, and mechanical failures in the repository. Changes in the radionuclide inventory may affect the source term considered in the TSPA. The thermal effect (temperature at the source as a function of time) may cause the removal of ambient ground water in the vicinity of the criticality and affect the migration of radionuclides. Mechanical failures, for example material degradation from corrosion enhanced by elevated temperatures or failures caused by a pressure pulse, may also affect the TSPA. The perturbation in the radionuclide inventory, the thermal effect, and the effects of mechanical failures are established by the criticality consequence analysis and treated as disruptive scenarios within the TSPA conducted for the repository. The entire process is repeated until all waste forms have been evaluated.

The TSPA estimates the dose increment due to criticality for all waste forms and waste packages and determines if the dose at the accessible environment or other locations is less than the regulatory limit (i.e., performance objectives of the repository are met). If the dose criterion (final decision point – repository performance objectives) is not satisfied, additional design options are implemented for reducing k_{eff}. If the performance objectives are met for all waste forms, the systems evaluated are acceptable for disposal.

3.2 DESIGN CRITERIA

The disposal criticality analysis methodology imposes three design criteria. These design criteria are decision points that are applied during the analysis to ensure sufficient measures are implemented to limit the potential for, and consequences of, criticality. As stated in Section 1.2, acceptance of the three design criteria is sought in this report.

3.2.1 Critical Limit Criterion

The CL criterion states that *the calculated k_{eff} for subcritical systems (configurations) for postclosure will be less than the CL.* The CL is defined as the value of k_{eff} at which the system is considered potentially critical as characterized by statistical tolerance limits. This k_{eff} limit includes all the appropriate biases and associated uncertainties for each in-package and out-of-package configuration analyzed for the repository. A presentation of the method for developing CL functions is provided in Subsection 3.5.3.2.6.

Specific CL values will be established by analysis of experimental systems with a range of neutronic parameters and parameter values that are representative of the configurations analyzed for the repository. Specific CL values and the accompanying range of applicability of these values for specific in-package and out-of-package configurations will be documented in validation reports and referenced in the License Application. The validation reports will also

confirm the conservative assumptions made in the neutronic model that will be used for waste package design. The modeling approach for calculating the CL values is presented in Subsection 3.5.2.2. The validation approach for the CL values and establishing their range of applicability is presented in Subsection 3.5.3.2.

3.2.2 Probability Criterion

The design probability criterion states that the average criticality frequency will be less than 10^{-4} per year for the entire repository for the first 10,000 years. This definition is equivalent to the statement that the criticality frequency will be less than 1 in 10,000 years for the first 10,000 years of repository operation, for the entire repository (all combinations of waste packages and waste forms).

This design probability criterion is established as a defense-in-depth measure to identify when the probability of criticality is so high that a redesign of the waste package or engineered barrier system is needed to reduce the probability of criticality. The criticality limit and probability criterion form design criteria for limiting the potential for criticality in the repository during postclosure (CRWMS M&O 1999j).

If any configurations were determined to be capable of supporting criticality events and found to have an estimated probability of occurrence below the design probability criterion, but contribute to a total probability of criticality for the entire repository inventory above the proposed 10 CFR 63.114(d) screening probability threshold of 10^{-4} in 10,000 years, consequence analyses would be performed. Only the criterion in proposed 10 CFR 63.114(d) will be used for screening criticality events from further consideration in the TSPA. The probabilities tested against this screening threshold will be the sum of the probabilities for all the scenarios that can lead to an individual criticality FEP.

3.2.3 Performance Objectives Criterion

The primary performance objective for the geologic 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 0.25 mSv (25 mrem) TEDE (total effective dose equivalent (10 CFR 63.113(b)). The waste package criticality performance objective is to ensure that the total effect of any criticalities will not significantly compromise the EBS, or the natural barrier system, with respect to the ability to inhibit the releases of radioactive materials to the accessible environment. Total effect will include all aspects of criticality events including, but not limited to, increase in radionuclide inventory, waste heat output, and any consequent degradation of the EBS. For purposes of this criterion, significantly compromise would be defined as that which could result in an increase of one percent in the dose at the accessible environment that would occur if no criticality had occurred. A one percent increase in dose is an order of magnitude smaller than the uncertainty in the TSPA. The satisfaction of this criterion will be determined by comparison of two TSPA runs: one with the full inputs from possible criticality events (probability and consequence), and the other without.

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 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. Features are defined as topographic, stratigraphic, physical, or chemical characteristics of the site that 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 physical or chemical interactions that can occur between the emplaced material and the surroundings. Examples of processes include groundwater flow, corrosion, and precipitation. Events are similar to processes, but have a short duration, and possibly a more extreme intensity or disruptive effect on the emplaced material. 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.

Scenarios based on the FEPs associated with the proposed repository at Yucca Mountain that may affect criticality have been reviewed as part of a workshop on postclosure criticality for the TSPA-VA abstraction/testing effort (CRWMS M&O 1997c). This workshop produced a standard set of degradation scenarios that must be considered as part of the criticality analysis of any waste form (Master Scenario List [CRWMS M&O 1997d, pp. 13-45]). This standard set is believed to be comprehensive with respect to the spectrum of scenarios that might occur in the repository and might affect criticality risk. Review and acceptance of the reports cited above (CRWMS M&O 1997c; 1997d) by the expert participants in the workshop constitutes validation of the scenario definition process. This report is seeking acceptance that the Master Scenario List (CRWMS M&O 1997d), discussed in this section and summarized in Figures 3-2a, 3-2b, 3-3a, and 3-3b, comprehensively identifies degradation scenarios based on FEPs associated with Yucca Mountain that may affect criticality. The report also seeks acceptance of the internal and external configuration classes, given in Subsections 3.4.1 and 3.4.2, respectively. These classes cover all of the criticality related FEPs from the comprehensive database (CRWMS M&O 1999a).

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 1997d). 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 SER (Reamer 2000b).

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 foldouts. In the sequence of Figures 3-2a and 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. Examples of this feedback are discussed further in Subsection 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.

In the discussion of scenarios and configurations given in the following subsections, the scenarios can be 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 external, and FF for far-field external) followed by a number. The configuration classes are identified in a similar manner, but with a lower case letter following the number. Each configuration also serves to define the standard scenario that leads directly to it. Many of the configurations can be reached by indirect scenarios routed through the triangle and circle connectors described in the previous paragraph.

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 Subsections 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 for the License Application.

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 License Application, so that this complete coverage can be demonstrated.

Note: WP = waste package
WF = waste form
FM = Fissionable material

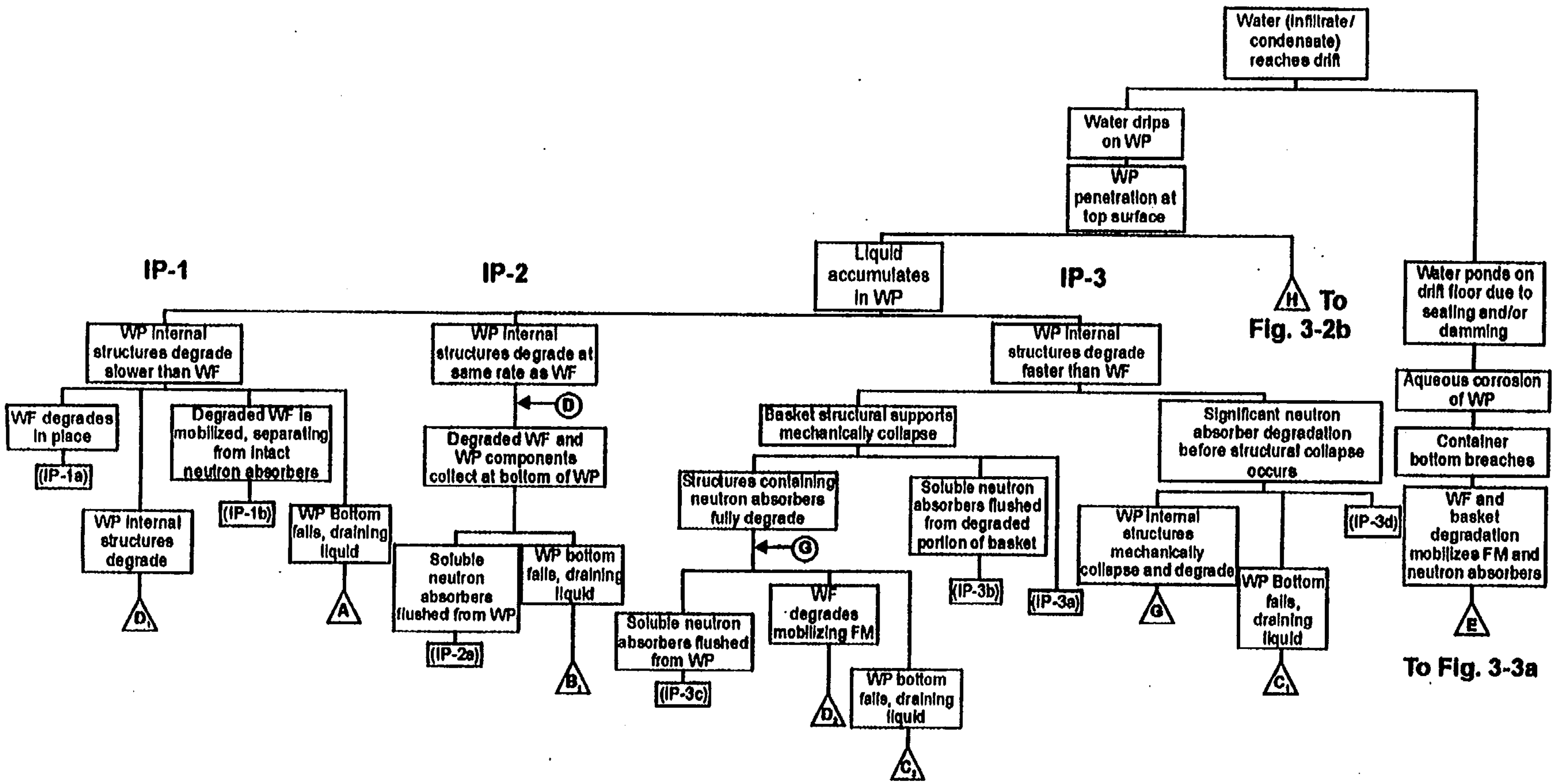
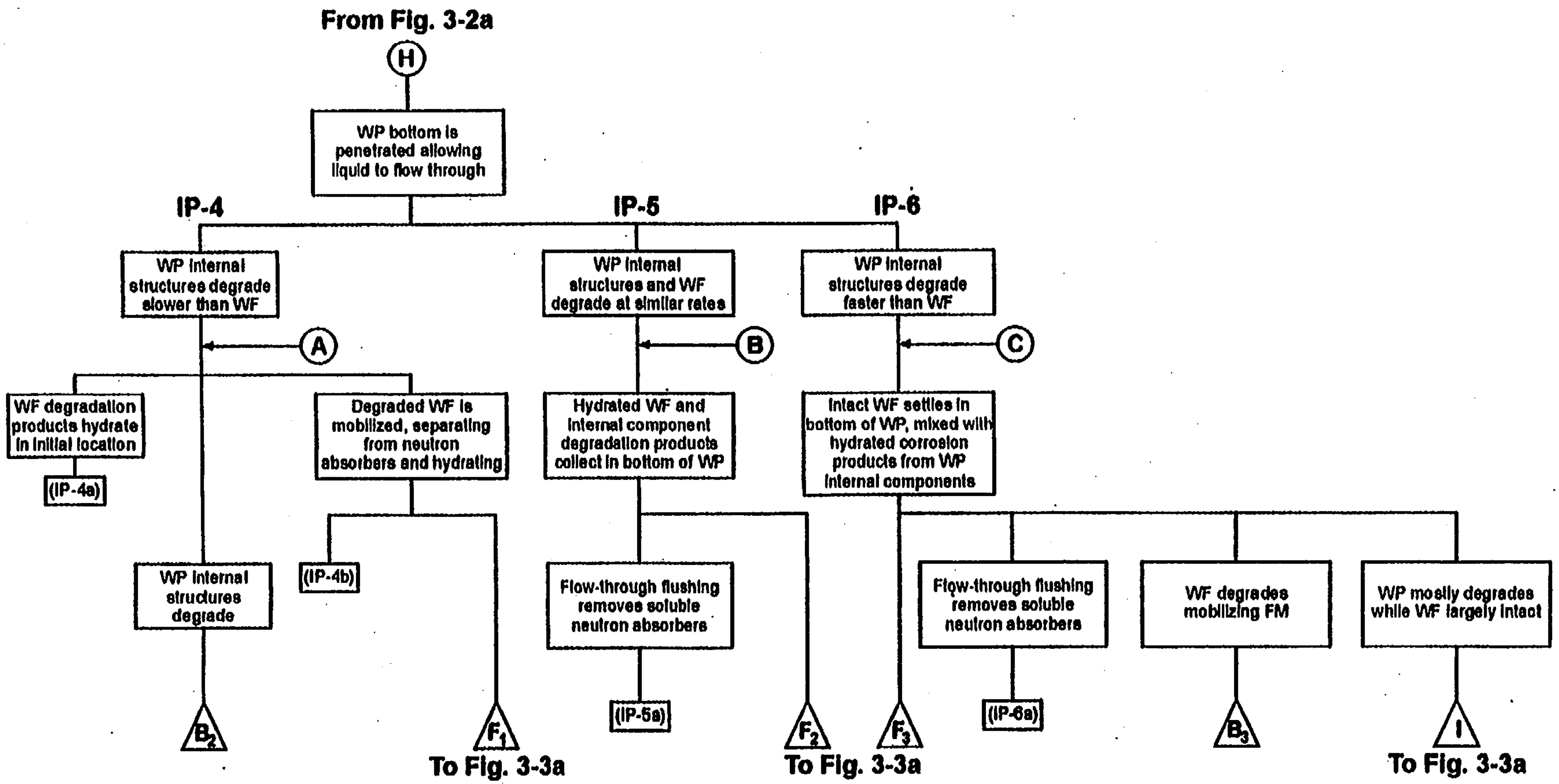


Figure 3-2a. Internal Criticality Master Scenarios, Part 1



<u>Note:</u> hydrated degradation products may include hydrated metal oxides, metal hydroxides, and clayey materials

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

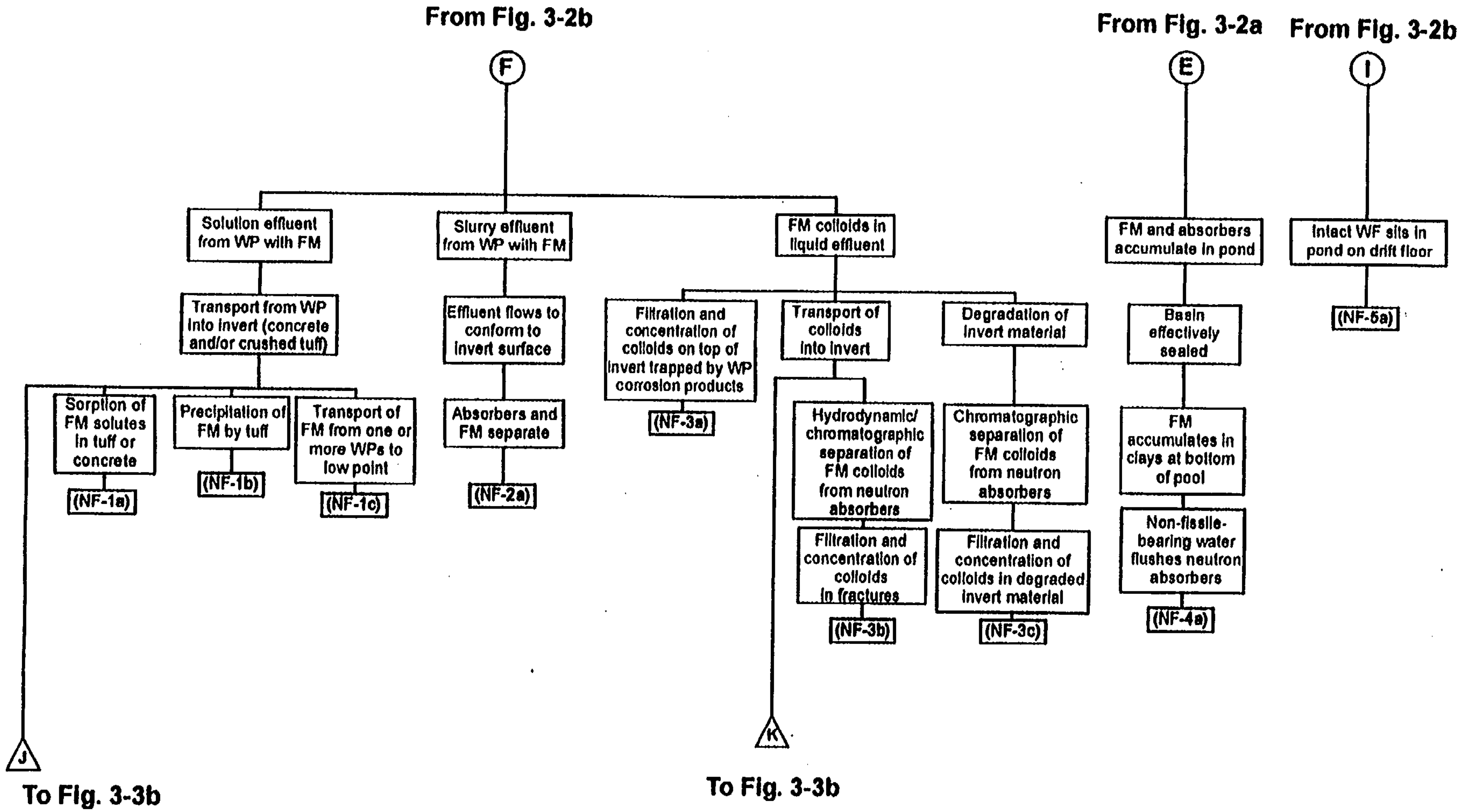


Figure 3-3a. External Criticality Master Scenarios, Part 1

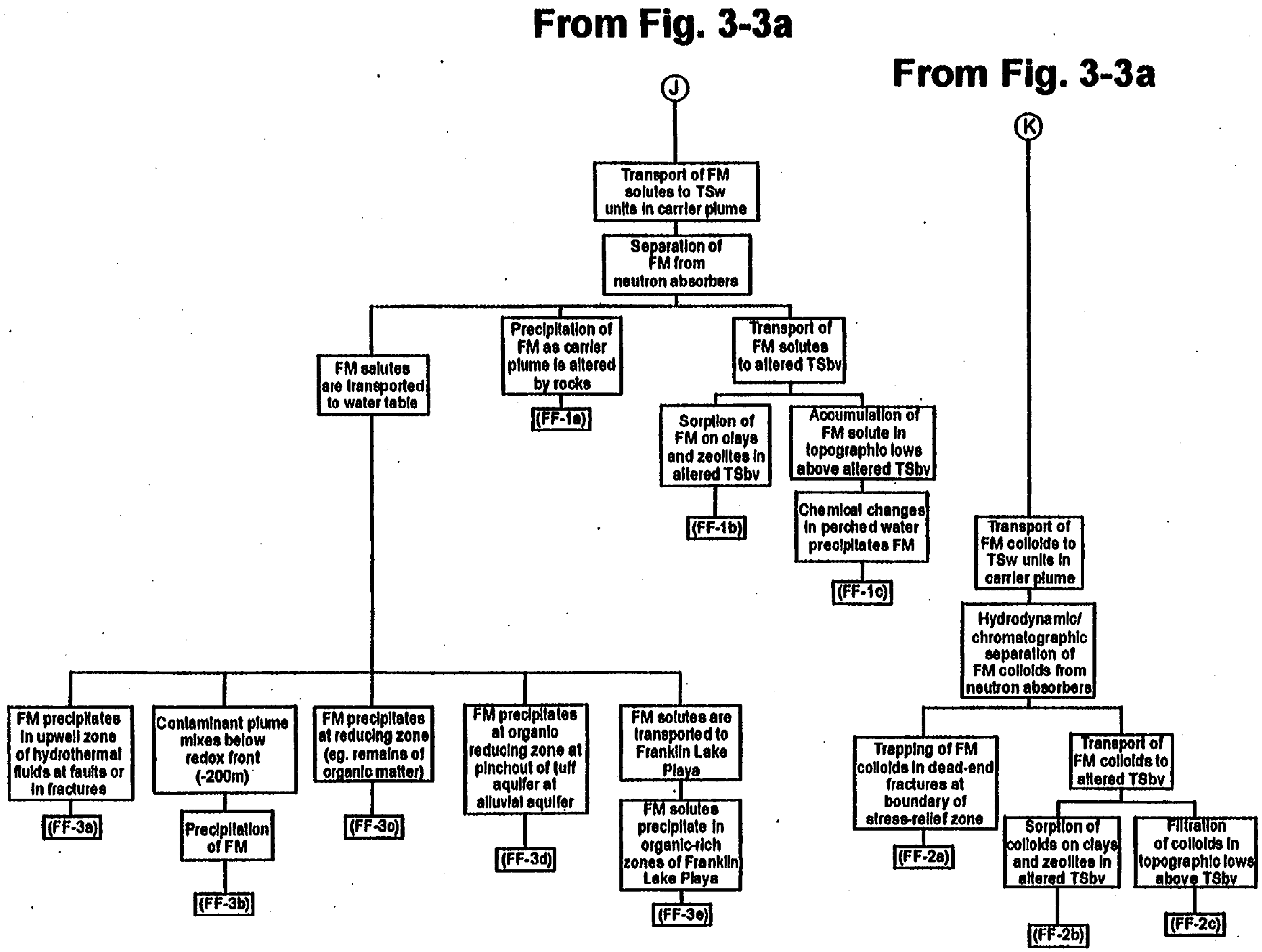


Figure 3-3b. External Criticality Master Scenarios, Part 2

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 fissile material will have high enough enrichment to support unmoderated (fast) criticality if the material can be concentrated beyond its 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 physically achievable concentrations of fissionable material, and will identify any possible fast criticality 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 (a) changes to a geometry having less neutron leakage, (b) accumulation/retention of moderator, and (c) 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 fissionable waste form(s) (FWF) and other internal components (OICs). 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 FWFs have the neutron absorbers designed into them, e.g., the plutonium immobilized in ceramic.

How the OICs degrade is an important aspect of the evaluation because 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 FWF and OIC's or both. This step of the methodology identifies the internal configuration classes (from Figure 3-2a or 3-2b) applicable to the waste form being evaluated. Additional details necessary to perform criticality analyses for the range of configurations in each class (i.e., the condition of the FWF; the amount of moderator; and the amount, composition, and physical distribution of the remaining FWF and OIC 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: the accumulation of water within the waste package, and the relative rates of the degradation processes affecting the FWF and the OICs. 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 FWF and OIC 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. The assumption that this potential removal of the neutron absorber occurs is conservative.

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 investigation. All of the configuration classes will be fully evaluated in the License Application.

1. The basket (OIC) is degraded, but the waste form is relatively intact (configurations IP-3a, b, c, d). 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 (configurations IP-3b, c, d). These configurations 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 FWF degrading at a much slower rate than the other internal components. Configurations IP-3b, c have been evaluated for commercial SNF (CRWMS M&O 1997a). This example uses a waste package design, in which the components supporting the FWF degrade and collapse before the neutron-absorber material degrades. This occurs because the supporting components are made of carbon steel and the neutron absorber is carried in stainless steel, which is much more robust with respect to corrosion than is carbon steel. Configuration class IP-3d could result if the neutron-absorber material degraded faster than the supporting components, but neither present nor contemplated waste package designs contain materials that would behave in this manner.

2. Both basket and waste form are degraded simultaneously with the same three additional conditions (water, absorber removal, and fissionable material remaining) as configuration #1 above (configuration IP-2a). In general, this configuration will result in the fissionable material accumulating at the bottom of the waste package. Since both FWF and OIC 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 FWF and OIC. The parameters of these configurations are determined by either 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 classes 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 largely intact basket (IP-1b). As with configuration #2, the fissionable material will most likely accumulate at the bottom of the waste package, but, unlike configuration #2, the physical opportunities for this transport and accumulation are limited because the basket is still largely intact. This configuration results from scenario group IP-1, which involves the FWF degrading faster than the basket (OIC). An alternative configuration having these relative degradation rates is IP-1a, in which the fissionable component of the FWF does not move significantly after degradation. This alternate configuration, particularly the variant with the fissionable material uniformly distributed throughout the waste package, has been analyzed for the aluminum-clad research reactor SNF (CRWMS M&O 1998b).

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

5. As with configuration #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 (IP-4a). This configuration class can only be reached if the FWF degrades faster than the OIC, so that the fissionable material remains in place to be locked in by its own hydration or by the hydration of OICs. Therefore, it is only reached by scenario group IP-4 (direct) or indirectly after IP-1. This configuration has been analyzed for the aluminum-clad research reactor SNF (CRWMS M&O 1998b).

6. Waste form has degraded in place with OIC intact (IP-1a). This configuration class is of interest if the degradation of the waste form (WF) can distribute the fissionable material into a more reactive geometry than the intact waste form. This can happen with the highly enriched research reactor SNF (CRWMS M&O 1998b).

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 (in largely intact SNF) simply remaining in place. 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 concrete or 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. The order of the list reflects the relative importance suggested by the preliminary evaluations performed. Therefore, the near-field and far-field configurations are intermixed.

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 (FF-3c, 3d, 3e, respectively). The combined probability of the existence of such a reducing zone and its being encountered by a flow bearing fissionable material is extremely low (CRWMS M&O 1996a).

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

3. Precipitation of fissionable material in fractures and other void space of the near-field. This configuration is obtained from processes such as adsorption or from a reducing reaction (configurations NF-1a, 1b, respectively). The two configurations are considered together because they are both limited by the same buildup of non-fissionable deposits in the fractures of the near-field.

4. Accumulation of fissionable material in a standing water pond in the drift. This configuration, 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 flowing from other dripping sites may collect around the bottom of the package during periods of high flow. A variant of this configuration class could have the intact, or nearly intact, waste form in a pond in the drift (configuration NF-5a). Such a configuration would be evaluated for waste forms that could be demonstrated to be more robust with respect to aqueous corrosion than the waste package. The detailed analyses for the License Application will evaluate the probability of occurrence for a pond of sufficient depth to cover enough assemblies to result in criticality, while the assemblies are stacked in a geometry favorable to criticality.

5. Accumulation by processes involving the formation, transport, and eventual breakup (or precipitation) of fissionable material containing colloidal particles. It has been suggested that the colloid-forming tendency of plutonium will enhance its transport capability, providing the potential for accumulation at some significant distance from the waste package. Such transport and accumulation could lead to far-field configurations FF-2a, 2b, 2c, for final accumulation in dead-end fractures, clay or zeolites, and topographic lows. It could also lead to the near-field configurations NF-3b, 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 NF-1c. The scenario leading to this configuration must have a mechanism for sealing the fractures in the drift floor so that the effluent from individual waste packages can flow to, and accumulate at, a low point in the drift or repository, possibly in combination with effluent from other waste packages. As with the discussion of NF-4a, above, such a pond would be expected to occur only within a short time (weeks or less) following a high infiltration episode. It should be noted that the repository design is currently being re-evaluated with respect to the possibility of maintaining a zero slope in the emplacement drift so there could be no significant accumulation from effluent that may flow out of multiple waste packages.

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), configurations FF-3a, 3b, respectively. This configuration is considered unimportant because there is no evidence for any such bodies below Yucca Mountain that would have sufficiently different chemical or redox characteristics to significantly concentrate fissionable material from the contaminant plume (CRWMS M&O 1997a).

8. Accumulation at the surface of the invert due to filtration by the degradation products, or remnants, of the waste package and its contents (configurations NF-2a, 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 FF-1c). This case will be evaluated for License Application to see how much fissionable material can be accumulated before the chemistry of the perched water is changed to that of the carrier plume. A variation of this configuration could support accumulation over several cycles of filling and dryout of the perched water zone.

10. Accumulation by precipitation from the chemistry changes made possible by carrier plume interaction with the surrounding rock (configuration FF-1a). It is possible that the amount of material that could be precipitated in this manner is limited by the fact that chemistry changes in the carrier plume itself would precipitate non-fissionable material from the carrier plume before any precipitation of fissionable material from the waste package plume (CRWMS M&O 1997e). The result would be fracture filling with non-fissionable material, as in configuration #3, above.

3.3.3 Effect of Seismic Events

Configurations having k_{eff} above the critical limit will also be evaluated to determine whether they can be reached from a configuration having k_{eff} below the critical limit by sudden reactivity insertion due to a seismic disturbance. This evaluation will consist of identifying representative configurations (called seismic predecessor configurations) that could be transformed to the subject configuration by a seismic event. A representative configuration 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). The predecessor configurations will have significantly higher gravitational potential energy than the subject final configuration. 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 configurations will be evaluated together with the probability of the seismic event of sufficient magnitude to take such configuration to criticality. The combined probability will then be used with the estimated transient criticality consequences to develop a transient criticality risk. This risk will be summed over a representative set of seismic events to arrive at an expected risk, incorporating the effects of large seismic events, weighted by the appropriate probability for each such event.

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

1. Mostly degraded basket, with only partly degraded waste form (principally spent fuel assemblies), reachable from scenarios IP-3a, b, c, d. Two types of configurations will be examined for predecessor configurations. The first type of final configuration reachable from a higher energy predecessor configuration has waste forms (e.g., assemblies) stacked in their lowest potential energy configuration with little, or no, basket steel between the assemblies. The potential predecessor configurations 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 and calculating the probability of occurrence of the predecessor configuration.

   The second type of final configuration represents a somewhat more degraded configuration 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 is just above this gap at the top and has one waste form stacked above the water level, a seismic disturbance could cause the stacked waste form 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 configurations in this class are identified as having k_{eff} greater than the critical limit, the search for predecessor configurations will include two types of configurations. Both types of predecessor configurations would have the same composition of solid degradation products as the final configuration, as determined by the geochemistry calculations. The first type of predecessor configuration would differ from the final configuration 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 would be further evaluated as a potential sudden-insertion predecessor, including estimation of the probability of occurrence of the predecessor configuration.

   The second type of predecessor configuration could be conceptualized as having the same geometry as the final configuration 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 IP-1a, b. Most of these configurations would have some neutron absorber in the basket material, and such a configuration 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 CL. If such configurations are identified, the search for predecessor configurations will include configurations 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, which 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 configurations 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 configurations 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 will be similar to the initial configuration (which could, presumably, become more uniform following some shaking).

3.3.4 Effect of Volcanic Events

The portion of the methodology for identifying potential critical configurations following a volcanic event will generally consist of the following steps:

1. Evaluate the potential for waste package breach due to a volcanic event as a function of the magma temperature and the degree of existing degradation of the waste package barriers. This will include consideration of the probability distributions of all the determining parameters.

2. Evaluate the potential patterns for transport, by magma, of the fissionable material, including consideration of the probabilities of patterns that confine the magma flow versus patterns that disperse the flow.

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

4. 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.

Step 1 has already been applied to give the range of volcanic characteristics in the Process Model Report (PMR) for Disruptive Events (CRWMS M&O 2000a) in support of TSPA-Site

Recommendation (SR). This analysis identified two types of damage to the waste package: (1) Those waste packages lying within the conduit of a sudden eruptive event may be thrown about so violently that they impact each other, which may result not only in the breach of a waste package, but also the dispersal of the waste package contents. This is called complete destruction. (2) The magma flow in any drift contacted by an igneous intrusion could cause some waste package breach due to overpressure (either internal or external). This is called partial destruction.

The application of step 2 to the complete destruction scenario is expected to show two types of potentially critical configurations. The first has the fissionable material from several waste packages piled against each other as they block the drift opening (which is also a very conservative application of step 3). 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 2 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.

Application of step 2 to the partial destruction scenario is expected to show that the volcanic event that fractures a limited number of welds will leave the waste package in a state that is similar to one following a localized breach of aqueous origin (e.g., IP-1, 2, 3). Subsequent filling of the waste package with water and the ensuing degradation of the waste package internal materials is expected to be similar also. Therefore, the standard scenarios and configuration classes can be applied directly to such configurations starting with igneous intrusion. Nevertheless, the geochemistry degradation analysis will consider any significant changes in J-13 water chemistry that could result from flow through the ash and fractured lava remaining in the drift following the volcanic event. These water chemistry changes are not expected to be great, however, since the volcanic material remaining in the drift would be expected to have a composition similar to the tuff already surrounding the repository.

3.4 POTENTIALLY CRITICAL CONFIGURATIONS

Degradation analysis models provide the raw data for specifying the range of parameters that characterize the degraded configurations. This raw data may be used to develop parameters for heuristic models that are implemented in the configuration generation code (CGC, described in Subsection 3.6.3.3). The CGC is, in general, the primary tool for determining the parameter ranges that characterize the potentially critical configurations. It consists of routines for quantifying the mobilization and transport of fissionable material from the degraded waste forms. In some cases the degradation analysis models themselves may cover enough of the varying parameters to characterize the configurations requiring criticality evaluations, so that there is no need to adapt and run the CGC. Acceptance is sought for the model validation process portion of the methodology described in Subsections 3.4.1.1 and 3.4.2.1, for the environment of the proposed repository site at Yucca Mountain over the range of environmental conditions currently expected in the repository. Specific examples of the application of this model validation process for the industry standard geochemistry codes, EQ3/6 and PHREEQC are discussed in Sections 3.4.1.3 and 3.4.3.

This section describes the portion of the methodology for quantifying the parameter ranges of the potentially critical internal configurations; it is these parameter ranges that determine the inputs to the criticality model. 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 configurations are identified and evaluated. Acceptance is sought for this portion of the methodology for developing comprehensive sets of internal configurations. The 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

This section describes the portion of the methodology for quantifying the parameter ranges of the potentially critical internal configurations; these parameter ranges determine the inputs to the criticality model. Acceptance is sought for this portion of the methodology for developing comprehensive sets of internal configurations. The following subsections also describe the models used in implementing the methodology and the validation of these models.

3.4.1.1 Methodology for Internal Configurations

There are 10 essential steps to specify the geochemical process (briefly discussed below). These steps have been used in the analyses discussed in this document, and will be applied further in the refined analyses for the License Application.

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 with the License Application will utilize corrosion rates officially accepted in the CRWMS database on the subject. This database is expected to always 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 UZ (unsaturated zone) flow model.

3. Identify the range of dripping water chemistry parameters, which will cover the officially approved range 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 parametric EQ3/6 flow-through mode 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 (i.e., is it simply a chemical alteration of the original solid material without changing the shape, flocculent, and easily disturbed, or gel-like and immediately mobilized?).

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 FWF (if nondegraded).

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 FWF, 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 (CRWMS M&O 2000b, 2000c) and from published results of other testing programs (e.g., Hillner et al. 1998 and Rishel et al. 2000 for Zircaloy and Hafnium) for each of the materials that make up the waste package barriers, internal components, and contained waste forms. 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. Version 3.06, CSCI:30048, of WAPDEG (CRWMS M&O 1998f) was used for the VA design. The output of the TSPA waste package degradation model is a distribution of breach times at various locations on the waste package (top, bottom, sides) for a given set of environmental conditions (temperature history, relative humidity history, exposure to drips, etc.). Disposal criticality analyses will primarily utilize the "base 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. Sensitivity studies will be performed to determine the effects of any alternative case waste package breach distribution on the probability of exceeding the CL. Validation of the TSPA waste package degradation model, and the individual material corrosion models which support it, will be performed as part of the TSPA submittal for License Application, and thus will not be addressed as part of the disposal criticality analysis for a particular 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 for License Application as part of the TSPA submittal, and thus will not be addressed as part of the disposal criticality analysis for a particular package design. The range of degradation rates considered for the other internal components of 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 the License Application for any material corrosion model, which is not already considered as part of the TSPA submittal for License Application. 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 initial version of the internal geochemistry model consists of the industry standard reaction path geochemistry code EQ3/6 (Wolery and Daveler 1992) plus special software (external data transformation routines) to chain together a sequence of runs (transforming the output of one run into the input for the next run) to create a "pseudo flow through" model. The methodology has been used for the geochemistry analysis preparatory to several degraded waste package criticality evaluations, where it is described in detail (CRWMS M&O 1998b). The calculations are performed for a unit mass of solution, typically 1 kilogram, within the waste package. Amounts of reactants to be input for this unit mass are determined by scaling the total waste package inventory (and reactant surface areas) according to the amount of water calculated to be in the waste package. This mass of water will generally vary with time; a typical value of

4.55 m^3 has been used for most of the calculations thus far (CRWMS M&O 1998b), but sensitivity to this mass will be evaluated for License Application. The results of the calculation are then re-scaled back to waste package totals. Reactants are input in two modes: (1) initial amounts of solute for each dissolved species, and (2) reagents which are added continuously (actually in discrete increments at each time step), primarily to simulate the elements which can go into solution as the solid materials, WF and OIC, degrade.

EQ3/6 has been enhanced in EQ3/6v7.2bLV to incorporate a solid-centered-flow-through mode, which automatically adjusts the water volume at each timestep so that it returns to a constant value at the beginning of each timestep. This enables the modeling of water inflow and outflow to track the timestep adjustment process exactly, thereby ensuring not only that the chemical changes are accurately resolved in time, but that they also accurately reflect the volume of water (constant) in the waste package at any given time. The documentation for this new version of EQ6 (CRWMS M&O 1998a) includes tests of the solid-centered flow-through method. The tests include comparisons against analytical solutions, and also comparisons against results obtained by chaining several thousand individual EQ6 runs (with adjustment of the water mass between each run).

It should be noted that the above approximation neglects the effects of evaporation. Analysis of evaporation has been performed in connection with steady-state criticality. This is summarized in Subsection 3.7.2.1, as part of the discussion of criticality consequences.

The output of the internal geochemistry model includes concentrations of solutes and amounts and chemical composition of solid precipitates in the waste package. The successive runs provide these results as a function of time over simulated periods that may be as long as several hundred thousand years. Of particular importance are the concentrations and solid amounts of fissionable materials and neutron absorbers.

The internal geochemistry model is nominally run with the assumption of constant degradation rates for the solid components, and under the assumption that the degradation products for all these components feed into the same solution which is well mixed on a geologic time scale. Potential deviations from these assumptions have been considered in recent geochemistry analyses (CRWMS M&O 1999k) and will be quantitatively evaluated in the more detailed analysis planned for the validation reports.

In the nominal geochemical analysis, upwards of 100 species are considered simultaneously. Additional cases involving only subsets of the degrading components are used to test the sensitivity to this assumption. It should also be noted that this methodology is applicable to both of the waste package flushing schemes: circulation in a nearly filled waste package, and direct flow-through of a waste package with penetration on the bottom. In the latter case there will be no standing water in the waste package.

3.4.1.3 Validation of Degradation Methodology and Models for Internal Criticality

Validation of the technique of in-package geochemistry, specifically the solid-centered-flow-through model, has been provided thus far by hand calculations to verify the correctness of the computer code that has been added to adjust the solute amounts downward from the end of one EQ3/6 timestep to the beginning of the next, thereby canceling the effect of the water that has been added during the timestep (CRWMS M&O 1998a).

With respect to the validation of the simpler static fixed fluid volume model, several studies have presented data on the comparison between EQ3/6 predictions and experiments or observations of natural systems. The most complete comparison cases are summarized in Table 3-1. They demonstrate the validity of the code, particularly the computation of concentrations of solutes over a wide range of total dissolved solids.

Table 3-1. Quantitative Comparison between Experiment and EQ3/6 Predictions

Case Modeled	Parameters Compared	Goodness of Match	Reference
Alkalinity in river water, low concentrations of solutes	pH and alkalinity	Within about 4%	Wolery and Daveler 1992, pp. 156-166
Solubility of gypsum in NaCl solutions, dilute to concentrated solutions.	Concentrations of Ca and sulfate, i.e., solubility of gypsum adjusted to 25°C.	Within about 4% up to about 4m[a] NaCl, and within 10% up to 6m NaCl at 25°C	Wolery and Daveler 1992, pp. 144-156
Solubility of gypsum and anhydrite in NaCl solutions up to 6m.	Concentrations of Ca and sulfate, i.e., solubility of gypsum at elevated temperatures.	Within about 12% for 6m NaCl at 35°C Within about 11% for 6m NaCl at 50°C	Zen 1965[b]

[a] molal
[b] This reference gives experimental results which have been approximated with EQ3/6.

Additional comparisons for chemistry conditions typical of a geologic repository at Yucca Mountain are summarized in Table 3-2. Analyses of the first three cases show that suitable choices of reaction rates permit accurate modeling of solution compositions. The solids are well predicted in any case. Because suitable reaction rates are not well known, models used for waste package calculations utilize a range of rates to identify the most conservative cases.

Table 3-2. Comparison between Observations and EQ3/6 Predictions: Conditions Similar to Repository Chemistry

Case Modeled	Parameters Compared	Goodness of Match	Reference
Experimental hydrothermal alteration of Topopah Spring Tuff with J-13 Well Water[a]	Precipitates formed, solution composition, including pH	Accurate prediction of mineral types: clays and calcite[b]	Wolery and Daveler 1992, pp. 166-179
Degradation of borosilicate (HLW) glass with J-13 Well Water[a]	Precipitates formed, solution composition, including pH	Accurate prediction of mineral types: clays and uranyl silicates[b]	Bourcier 1994
Degradation of spent fuel with J-13 Well Water[a]	Precipitates formed, solution composition, including pH	Accurate prediction of mineral types: clays and uranyl silicates[b]	Bruton and Shaw 1988
Natural geothermal alteration of welded tuff, (Wilder 1996)[c]	Precipitates formed, solution composition, including pH	Accurate prediction of mineral types: clays and zeolites	Wilder 1996, Volume II, Chapter 3.4.2

[a] Experimental conditions intended to model the expected repository environmental parameters and degraded waste package component chemistry.
[b] For some reaction times quantitative agreement requires downward adjustment of reaction rates.
[c] Natural analog, also demonstrating conservative behavior with respect to high temperatures (up to 250°C).

The validity of the geochemistry calculations depends as much on the quality of the thermodynamic data as on the model itself. Some initial sensitivity analyses for those data of greatest importance have been done. Specifically, these involved sensitivities to the "hard core" radii of ions such as $UO_2(CO_3)_3^{4-}$, and equilibrium constants for $Pu(OH)_4$ (CRWMS M&O 2000i). Sensitivity to partial pressures of CO_2 was addressed in CRWMS M&O 1999k. By varying the partial pressure of CO_2 the effects of different values of carbonate equilibrium constants were evaluated. Sensitivity to thermodynamic data for Gd carbonate species was addressed in CRWMS M&O 1999k.

3.4.2 Configurations with the Potential for External Criticality

This section describes the portion of the methodology for quantifying the parameter ranges of the potentially critical external configurations; these parameter ranges determine the inputs to the criticality model. Acceptance is sought for this portion of the methodology for developing comprehensive sets of external configurations. The following subsections also describe the models used in implementing the methodology and the validation of these models.

3.4.2.1 Methodology

The external criticality methodology 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:

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 of deposits of zeolites and other adsorbing materials.
4. 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 by combining the geochemical and physical flow analyses of Subsection 3.4.1.1. 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.
3. Determination of mineral precipitates from reactions of the waste package plume with the host rock fracture walls, using EQ3/6 and/or PHREEQC (described in Subsection 3.4.3.1). The calculation must account for both fissionable and other materials because they compete for the limited fracture voidspace.
4. Determination of alternate paths, or spreading, when the primary fractures are filled. This step includes consideration of the possible collection of the source terms from several waste packages.
5. Determination of reaction products, from the plume encountering a reducing zone, using EQ3/6 and/or PHREEQC. This step will include consideration of the following limiting factors: (1) voidspace available in the reducing zone for product precipitation, and (2) low flow rate of waste package plume. Acceptance is sought for the use of EQ3/6 and/or PHREEQC for this purpose.

For those configurations found to have criticality potential (according to the portion of the methodology 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.

3.4.3 External Geochemistry Model

The possibility of accumulating a critical mass of fissionable material outside of a waste package is evaluated by EQ3/6 and/or PHREEQC (CRWMS M&O 1999d) analysis of the

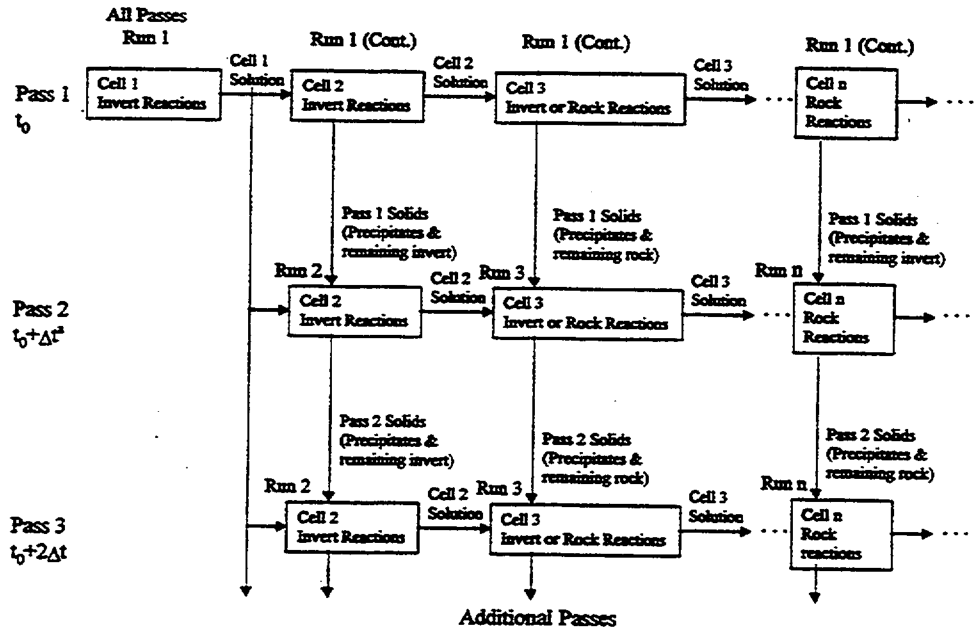
chemical processes that can precipitate dissolved fissionable material from the carrier plume of the source term. The code is used in an "open system" mode in which the reactions of an initial parcel of solution are traced as the parcel passes through the external reacting material *Report on External Criticality of Plutonium Waste Forms in a Geologic Repository* (CRWMS M&O 1998g). Since the EQ3/6 code is actually zero-dimensional, the simulation of one-dimensional flow is accomplished by mapping reaction end time into distance traversed at the nominal groundwater flow rate. The PHREEQC code treats this mapping of time into distance with explicit representation of discrete cells along the pseudo-flow path. Any precipitation, or adsorption, of fissionable materials transported as colloids reported in the TSPA will be added to the accumulations of dissolved material calculated by EQ3/6 and/or PHREEQC.

Cell or layer boundaries are then determined by distances (times) at which there is a change in the principal mineral being deposited. The process starts with the reacting material closest to the waste package, the invert (e.g., crushed tuff) and any remaining drift liner; the passageway for flow through this layer is primarily the connected fractures and space between rock fragments. Beyond the drift-wall, the reacting material is in the walls of the fractures in the host rock, and these fracture walls define the passageway, under the assumption that the major portion of the flow is in fractures (which is consistent with the rationale for the *Controlled Design Assumption* TDSS 026 [CRWMS M&O 1998d]). A complete traversal of a parcel through all the cells (or layers) is called a pass.

The first pass consists of a single run, of duration corresponding to the time for a parcel of solution to traverse all of the cells. The times at which the depositing mineralogy changes significantly are used to define the cell (or layer) boundaries by mapping such time of change into distance along the flow path using the groundwater flow or percolation rate. It is nominally assumed that the flow rate is the same in all layers, but the methodology can accommodate variations in this parameter, including the possibility of intermediate ponds along the path. The source term flowing from the waste package defines the initial solution in the first cell. This complete calculation methodology is shown in Figure 3-4. The first pass, consisting of a single run, is shown as the first line of this figure. The first pass starts at time t_0, and the time evolution is shown as mapped into a spatial sequence of cells, from one ton. Since the reaction rates are slow, the mineralogy changes only a few times during several thousand years. Typically, five cells, or fewer, are determined in this manner.

The mass of solution in the parcel is usually taken to be 1 kilogram, as in the internal criticality geochemistry model. The input and results are scaled to correspond to the actual flow out of the waste package in some specified period of time, Δt, which is set equal to the time required for the flow to traverse a cell. This Δt is also the time offset between successive passes, as indicated in Figure 3-4. The more complete analysis for License Application will determine the optimum value for this parameter.

Passes following the first must be broken up into a sequence of runs, so that for each pass the solid contents of any cell can be set equal to the total precipitate left in that cell from the previous pass. For the first pass there are no precipitated solids with which to pre-load each cell; however, the environment must still be updated to reflect the movement of a parcel of water into a new cell which has no prior depositions. This is accomplished by assigning the precipitated solids to a "physically removed subsystem" where they no longer react with the solution. This is done periodically by the code as the movement of the water (simulated as time or "reaction progress") proceeds. This simulates the movement of the specific kilogram of solution through the system, leaving behind it the precipitated material.



NOTE: [a] Δt is the time difference between successive passes, which is also the time to traverse the principal cell (or layer)

Figure 3-4. Information Flow for External Geochemistry Model (open-system)

3.4.3.1 Validation of the Methodology and Models for External Criticality

Since the external criticality analysis starts with the fissionable material flow out of the waste package source term, this part of the external criticality methodology validation is covered by the internal criticality validation in Subsection 3.4.1.3.

The principal tool for estimating external accumulation of fissionable material is the geochemistry-transport code PHREEQC. The PHREEQC family of software products originated in the late 1970's and was developed by the U.S. Geological Survey. PHREEQC Version 2.0(beta) contains capabilities such as speciation-solubility and kinetically controlled reaction pathway features, which are found in many geochemical software packages, but also includes surface complexation, ion exchange, absorption and solid solutions, and a very versatile treatment of rate laws. In addition, PHREEQC has transport features with handling of dispersion and diffusion in a double-porosity medium, and can handle a variety of models of adsorption. The thermodynamic database used by PHREEQC in this work is a direct transcription of the EQ6 database, translated into a PHREEQC-readable format as described in CRWMS M&O 1999d, Section 5 and Attachment II. PHREEQC handles advective transport by moving aqueous solutions from one cell to the next, allowing the contents of each cell to reach equilibrium (or not) with the solids and surface features present in the cell, as described in Figure 3-4.

The validation of the accumulation part of the methodology rests primarily on the validation of this code.

The validation of PHREEQC for external accumulation has been documented in the *Validation Test Report for PHREEQC* (CRWMS M&O 1999d). In order to make maximum use of the benchmark comparisons already done for EQ3/6, many of the test cases in CRWMS M&O 1999d are comparisons with EQ3/6 calculations. However, there are also direct experimental comparisons, including some for temperatures other than 25°C. For example, test case E6 of CRWMS M&O 1999d compares the kinetics of quartz precipitation at 105 °C with experimental results. The results (particularly case 2E of Figure 2 of that reference) show that PHREEQC reproduces the time variation of solution silica concentration within 1%.

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 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 approach, and the approach for validation of the models that are used for criticality evaluations are described in this section.

3.5.1 Methodology

An overview of the criticality analysis methodology is presented in Figure 3-5 and discussed in the following three subsections. These subsections address the material composition from the degradation analyses, the k_{eff} evaluation, and the regression analysis for developing regression expressions or look-up tables as a function of parameters that affect k_{eff}. Figure 3-5 provides an expansion of the criticality evaluation component of the disposal criticality analysis methodology that was presented in Figure 3-1.

3.5.1.1 Material Composition

Material composition and geometry of this material (i.e., waste form configuration) determine the potential for nuclear 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. The methodology for determining material composition for naval SNF is described in the naval addendum (Mowbray 1999). 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 nuclear criticality will change during the disposal time period because of this change in material composition and geometry.

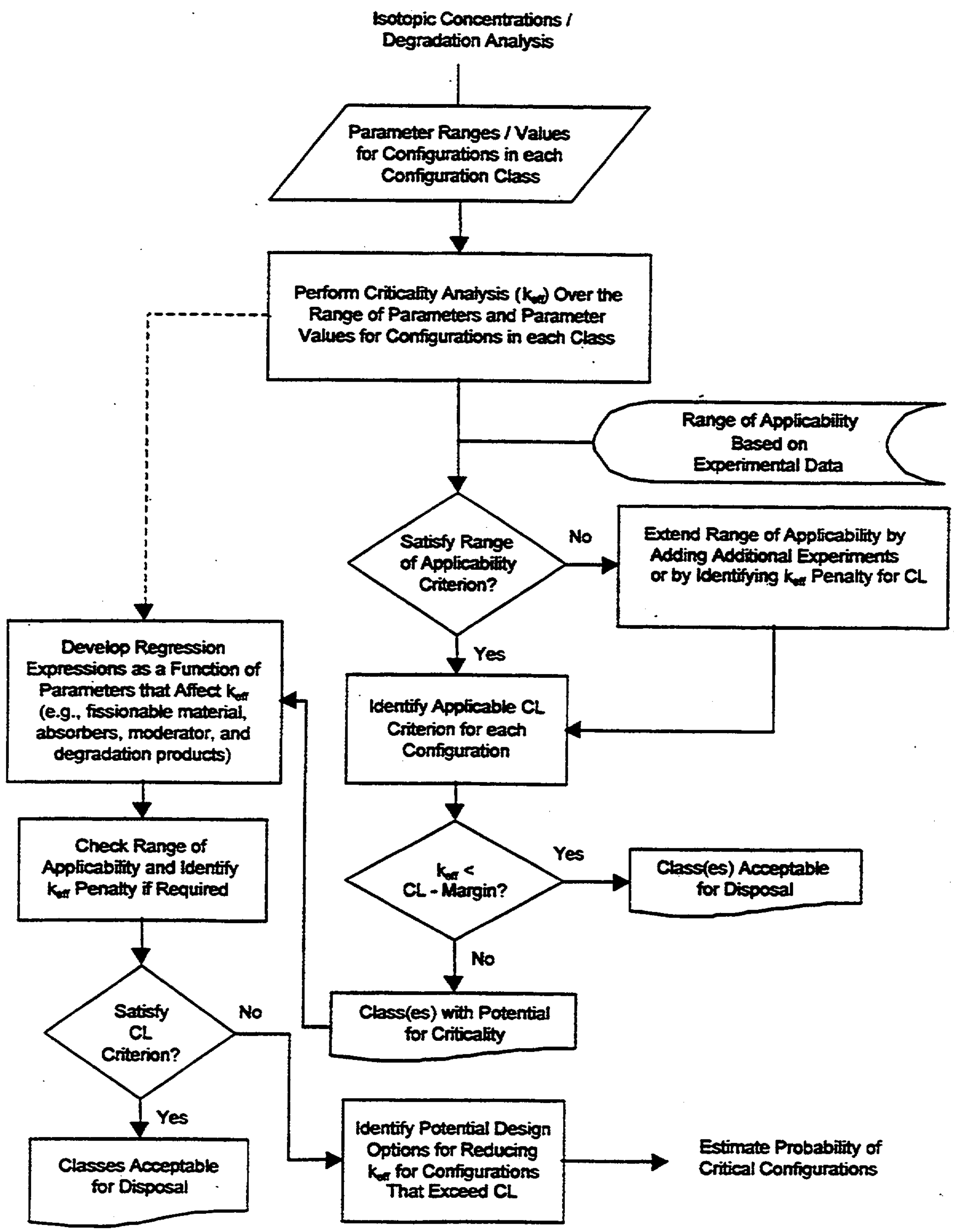


Figure 3-5. Criticality Analysis Methodology

For commercial SNF, credit is sought for the reduced reactivity associated with the net depletion of fissionable isotopes and the creation of neutron-absorbing isotopes during the period since nuclear fuel was first inserted into a commercial reactor. 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.

The range of parameters and parameter values that define configurations in each class represents the material composition and geometry. As shown in Figure 3-5, the parameters and parameter values used in the criticality evaluations are obtained from the degradation analysis. This includes results from corrosion, geochemistry, and configuration generation models, as well as isotopic inventories for the waste forms. The isotopic inventories for commercial SNF are established using the isotopic modeling approach discussed in Subsection 3.5.2.1 and are provided as input to the degradation analysis. For waste forms other than commercial and naval 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. Degraded material composition will include situations where the fuel remains relatively intact but includes pinholes and cracks in the cladding. For these situations, the availability of isotopes used for burnup credit will be established by assuming that an appropriate percentage of the SNF contains pinholes and cracks in the cladding at the start of the degradation analysis. 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 3-5, k_{eff} evaluations are performed over the range of parameters and parameter values for configurations in each class. 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 CL) is placed on the calculated value of k_{eff} for the configuration analyzed. This CL, 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 CL. This is represented in Figure 3-5 by the range of applicability criterion. The modeling approach for the k_{eff} evaluations is discussed in Subsection 3.5.2.2. The process for establishing CL values (and hence the CL criterion) and the process for validating the CL values are discussed in Subsection 3.5.3.2. A description of the process for defining the range of applicability of the CL values based on the experimental database used in establishing the CL values is also presented in Subsection 3.5.3.2. As shown

in Figure 3-5, when the range of applicability criterion is not satisfied, either additional experiments are required to extend the range or a k_{eff} penalty is applied to the CL. In either case, a CL is established that is applicable to the range of parameter values that are used in the k_{eff} evaluation. The procedure for extending the range of applicability of the CL is described in Subsection 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 define the regions of parameter space where criticality may be a concern. For example, a configuration class of intact commercial SNF in a waste package may be evaluated for an initial enrichment of 5 weight-percent (wt%) ^{235}U fuel for a range of parameter values representing configurations within this class. If the k_{eff} values for configurations within this class satisfy the CL 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. As shown in Figure 3-5, a k_{eff} margin is subtracted from the CL to provide assurance that the configuration classes or configurations within a class are not prematurely omitted from further evaluation. Specific values for this margin will be established as part of the criticality model validation and will be documented in the validation reports, which will be referenced in the License Application.

When the range of applicability criterion is satisfied and an applicable CL criterion is identified, the calculated k_{eff} value for each configuration evaluated is compared with the applicable CL less the conservative margin. If the calculated k_{eff} is less than CL minus the margin for all configurations within a class, the configuration class is acceptable for disposal. A configuration class with one or more configurations that have calculated k_{eff} values that are greater than or equal to CL minus the margin has the potential for criticality, and further evaluations are required. For those configuration classes requiring further evaluations, regression expressions or look-up tables are developed as a function of parameters that affect k_{eff}. The regression analysis methodology is discussed in Subsection 3.5.1.3.

3.5.1.3 Regression Analysis

As noted in Subsection 3.5.1.1, the material composition and geometry of this material 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 time period. These configurations may occur either inside or outside of the waste packages and may involve material from more than one waste package. The criticality evaluation process for the many possible configurations is facilitated by the use of regression expressions or look-up tables that are developed as a function of parameters that affect k_{eff}.

Parametric criticality evaluations are performed using the criticality modeling approach described in Subsection 3.5.2.2. Results from the parametric evaluations and the previous criticality evaluations (dashed line in Figure 3-5) are used to identify configuration classes with the potential for criticality. Tables of k_{eff} values are constructed as a function of parameters that affect criticality for configurations in each class. These parameters will include the amounts and arrangement of fissionable, neutron absorbing, and neutron scattering materials. The tables

of data are then used to develop regression expressions of k_{eff} as a function of these parameters or are used for linear interpolation of k_{eff} between parameter values. The modeling approach for the regression expressions and the interpolation tables is presented in Subsection 3.5.2.3. The validation approach for the regression analysis and the look-up table (with interpolation) analysis is presented in Subsection 3.5.3.3.

As shown in Figure 3-5, the regression expressions or look-up tables are developed for configuration classes that show a potential for criticality. When applied to configurations within a class, the range of parameter values used in the regressions or look-up tables are checked against the range of parameter values used in developing the corresponding CLs. If the regressions or look-up tables are beyond the range of applicability of the CLs, the range of applicability is extended using the method described in Subsection 3.5.3.2. The uncertainty in k_{eff} values obtained from the regression expressions or look-up tables will be established during the validation process. This uncertainty will be added to the k_{eff} value obtained for the configuration being analyzed prior to comparison with the CL criterion. This ensures that appropriate allowances are made for the uncertainties associated with the regression expressions or look-up tables in analyzing degraded configurations of SNF or HLW.

If the k_{eff} values from all configurations within a class satisfy the CL criterion, then that class is acceptable for disposal, as illustrated in Figure 3-5. For those classes that fail to satisfy the CL criterion, the region of parameter space where the CL criterion is exceeded is established and design options for reducing k_{eff} are identified. As shown in Figure 3-5, for configurations showing potential for criticality, an estimate of the likelihood (probability) of the configuration is made. The methodology for estimating the probability of occurrence of potential critical configurations is described in Section 3.6.

3.5.2 Modeling Approach

The modeling approach for the neutronic models used in assessing the criticality potential of waste forms during the postclosure period of the geologic repository are described in the following three subsections. First, the approach for modeling isotopic concentrations from the waste form is described. Second, the approach for criticality modeling (k_{eff} calculation) of configurations of SNF and HLW is presented. Finally, the approach for developing regression expressions or look-up tables (with interpolation) of criticality data as a function of parameters that affect k_{eff} is described.

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 time 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 isotope 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., fuel where significant plutonium has been generated, and a scenario where the plutonium and uranium may be separated).

For commercial SNF, burnup credit is sought for the net effect of depleting fissionable isotopes and creating neutron-absorbing isotopes during the period since the nuclear fuel was first inserted into a reactor. The isotopic model determines the concentrations of these isotopes that are present in the SNF and subsequently used in the criticality evaluations. The isotopic modeling approach for naval SNF was provided in a classified addendum (Mowbray 1999). Thus, 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, and the availability of the commercial SNF isotopes. The nuclear properties considered are cross-sections and half-lives 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-fissile absorbers. Thus, the selection process is conservative.

This process results in selecting 14 actinides and 15 fission products (referred to as "Principal Isotopes") as the SNF isotopes to be used for burnup credit. Table 3-3 lists these isotopes. The actinide ^{233}U from this table is not present in current generation commercial SNF. However, for long disposal time periods (tens of thousands of years), ^{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 1998c). 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 Disposal Criticality Analysis Methodology* (CRWMS M&O 1998e, pp. 40-42).

Table 3-3. 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	

Acceptance is sought that the principal isotopes selected to model burnup in intact commercial SNF, presented in Table 3-3, may be used for disposal criticality analysis provided that:

1. The bias in k_{eff} associated with predicting the isotopic concentrations is established in the validation reports as described in Subsection 3.5.3.1.

2. Deviations from the predicted concentrations because of radionuclide migration from intact fuel assemblies through pinholes and cracks in the cladding are addressed in the geochemical analysis.

The k_{eff} values from criticality evaluations of intact commercial SNF with pinholes and cracks 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. The applicability of the principal isotopes for intact commercial SNF will be demonstrated in validation reports, which will be referenced in the License Application.

Acceptance is also sought that the process for selecting isotopes from the list of principal isotopes for degraded commercial SNF presented in Subsection 3.5.2.1.4 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 validation reports, which will be referenced in the License Application. NRC acceptance of the application of the selected isotopes to postclosure repository conditions will be sought in the License Application.

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 fuel that is initially loaded into the reactor is in the form of ceramic UO_2 pellets that are 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 isotope 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 decrease with irradiation.

Establishing accurate initial isotopic concentrations 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. 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. The sensitivity of the calculated isotopic concentrations to the modeling approximations will be quantified during model validation. The validation approach for the isotopic model, including the treatment of neutron spectrum effects and modeling approximations, and the establishment of an isotopic bias for k_{eff} based on analysis of radiochemical assay data are discussed in Subsection 3.5.3.1.

The modeling approach for the isotopic model applies a combination of one-dimensional neutron transport with spatial and neutron spectrum adjusted cross sections in a point-depletion calculation, a two-dimensional neutron transport-depletion calculation, and a three-dimensional neutron diffusion-depletion calculation. The one-dimensional neutron transport with point-depletion calculation has an extensive cross section library covering all isotopes of significance in commercial SNF. The accuracy of this calculation is directly dependent upon the accuracy of the spatial and neutron spectrum weighting of the cross section data used in the depletion calculation. The two-dimensional neutron transport-depletion calculation provides a more accurate representation of spatial effects. Thus, variations in fuel enrichment across an assembly and the presence of control rods, control blades, or burnable absorbers can be represented more accurately. The number of isotopes considered by the two-dimensional neutron transport-depletion calculations is less than that considered by the one-dimensional neutron transport with point-depletion calculation. The two-dimensional calculation considers all of the important actinides and most of the fission products that are important for commercial power reactor applications. The remaining fission products are combined and treated as one or more "lumped" fission products. This method for treating fission products provides accurate results for power reactor applications but may be limited for SNF waste disposal applications. The treatment of SNF isotopes by the three-dimensional diffusion-depletion calculation is similar to the two-dimensional neutron transport-depletion calculation. This includes the combining of certain fission products and treating them as one or more "lumped" fission products.

The modeling approach for the isotopic model uses one-dimensional neutron transport with point-depletion as the base model. The two-dimensional neutron transport-depletion model is used to verify the homogenization approximations made by the one-dimensional model. Core-follow data from the three-dimensional diffusion-depletion model are used in providing realistic operating history (burnup, fuel temperature, moderator temperature and density, etc.) of fuel samples for model validation (e.g., radiochemical assays). The three-dimensional diffusion-depletion model also provides axial and radial burnup profiles. Further discussion of the use of the three models for isotopic model validation is provided in Subsection 3.5.3.1.

3.5.2.1.3 Postclosure Isotopic Concentrations Considering Isotopic Decay

This section discusses the modeling approach for addressing isotopic decay for postclosure. An overview of this process is presented in Figure 3-6. As shown in this figure, the evaluation starts with the initial isotopic concentrations. For commercial SNF, the modeling approach described in the previous subsection is used in establishing the initial isotopic concentrations.

For other waste forms, except naval SNF, design values for fissionable isotopic concentrations or the technical specification limits for fissionable 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 3-6, a base criticality calculation is then performed using the isotopic concentrations from the decay calculations and a base reactivity is 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 3-6, this process is repeated until the desired confidence level is achieved. 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.

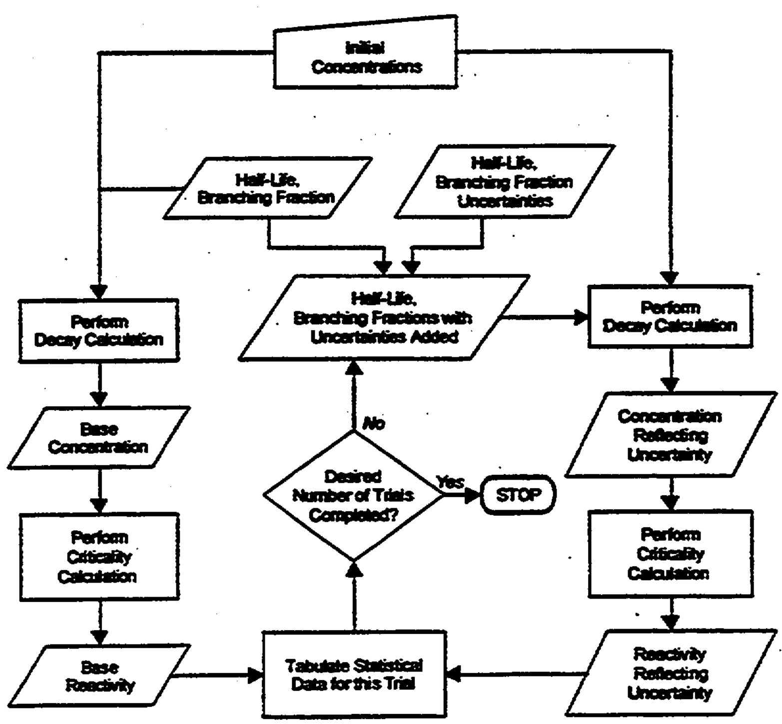


Figure 3-6. Modeling Approach for Postclosure Isotopic Decay

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. These evaluations, as well as the application of the bounding margin, will be documented in the validation reports for each waste form and referenced in the License Application.

3.5.2.1.4 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 that are evaluated for criticality. This includes configurations ranging from intact commercial SNF with pinholes and cracks in the cladding to fully degraded configurations. Thus, the effects of radionuclide migration from intact fuel assemblies through pinholes and cracks in the cladding are considered. The isotopic model establishes the initial concentration for each of the principal isotopes. The model uncertainty in calculating these concentrations for each of the principal isotopes is established based on analysis of radiochemical assay data. This uncertainty is applied to the initial isotopic concentrations used in the geochemical analysis. 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.

The isotopic concentrations from the geochemical analysis are used along with configuration parameters in the regression expressions or look-up tables (with interpolation) for k_{eff}. A single regression expression or set of look-up tables for k_{eff} represents a configuration class. Values of k_{eff} for configurations within a class are obtained by varying the values of the independent variables (parameters) in the regression expression or look-up table set. As noted in Section 3.6, probability distributions are developed from the uncertainty associated with these parameters. Thus, uncertainty in initial isotopic concentrations that are used in the geochemical analyses is contained in the final concentrations that are used in the regression or look-up tables and are represented in the probability distributions for the configurations analyzed for criticality.

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

Subsection 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 simulates and records the behavior of individual particles within a system. The behavior of simulated particles is assumed to describe the average behavior of all of the particles within the system. 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 including 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 validation reports that will be referenced in the License Application.

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

3.5.2.3 Regression Analysis Modeling

Regression analysis modeling starts with the identification of configuration classes for each waste form. Parameters that affect criticality are identified for each class, and ranges of values for these parameters are established based on degradation analyses. These parameters characterize the isotopic concentrations and geometry of the waste form materials, other waste package materials, and moderating and reflecting materials. The regression analysis modeling facilitates the criticality evaluation process for the many possible configurations that may occur inside and outside of the waste package, including configurations containing material from more than one waste package.

The first step in the process is to identify configuration classes inside the waste package along with the parameters that describe the material composition and geometry of each class. The initial configuration class for a specific waste package is the intact waste package (no degradation), where configurations within this class are described by variations in material content of the waste form. For a waste package containing commercial SNF fuel assemblies of a particular design, the burnup and initial enrichment of the SNF assemblies along with the time since the assemblies were discharged from the reactor may be used to describe configurations within this initial class. However, criticality evaluations should show that the configurations within this initial configuration class are subcritical. For this example, the waste package must be breached and a neutron moderator (e.g., water) must enter the package before criticality would be a concern. The next configuration class for this waste package would be identical to the initial class with the addition of various amounts of moderator (water). From Figure 3-2a in Section 3.3, this would correspond to waste package penetration at the top with the water accumulating in the waste package. The parameters characterizing configurations within this class are burnup, initial enrichment, time since discharge, and the amount of water present in the waste package. A table of k_{eff} values is constructed from k_{eff} evaluations, where these parameters are varied over the range of possible values for each of the parameters. Data from this table are used to develop regression expressions of k_{eff} as a function of these parameters or may be used for linear interpolation of k_{eff} between parameter values.

Proceeding with the illustration of commercial SNF inside the waste package, the next configuration class may correspond to the scenario group where the waste package internal structures degrade faster than the waste form. If the neutron absorber material in the basket degrades faster than the supporting components several configuration classes may arise. A configuration class may exist with intact waste form and intact internal support components but with different amounts of absorber material removed from the basket and suspended uniformly in the water. Another configuration class may exist with different amounts of the neutron absorber material removed and settled to the bottom of the waste package. Configuration classes may also exist with different amounts of neutron absorber material removed and various combinations of absorber material suspended in the water and settled to the bottom of the waste package.

Consider the configuration class where various amounts of neutron absorber material are removed from the basket and this absorber material is suspended in the water. The parameters characterizing configurations within this class are burnup, initial enrichment, time since discharge, amount of water present in the waste package, and the fraction of neutron absorber material suspended in the water. Criticality evaluations are performed for the range of possible values for these parameters, and a table of k_{eff} values constructed. Regression expressions of k_{eff} as a function of these parameters may be developed from this table or linear interpolation of k_{eff} between parameter values may be made.

For the process illustrated with the simplified examples above for commercial SNF, configuration classes and the parameters that affect criticality and define configurations in each class are identified. Criticality evaluations are performed over the range of parameters and parameter values. Tables of the k_{eff} values are constructed and used in developing regression expressions of k_{eff} as a function of these parameters. This process is applicable for all configuration classes identified for all waste forms and waste packages that may occur inside and outside of the waste package, and includes configuration classes identified that may contain material from more than one waste package. The methodology for identifying internal and

external configuration classes is given in Subsections 3.4.1 and 3.4.2, respectively. The validation approach for the regression analysis model is presented in Subsection 3.5.3.3.

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 geologic repository are described in the following three subsections. First, the validation approach for the isotopic model is described. Second, the validation approach for the criticality model used for assessing criticality potential of configurations of SNF and HLW is presented. Finally, the approach for validating the regression analysis model used to facilitate the criticality analysis process is discussed.

3.5.3.1 Isotopic Validation

Isotopic model validation is performed for commercial SNF where burnup credit is sought. Validation of the isotopic model for naval SNF is described in the naval addendum (Mowbray 1999). Other waste form types will use the design values for fissionable isotopic concentrations or the technical specification limits for fissile isotope concentrations in establishing the initial isotopic content of the waste form. 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 Subsection 3.5.3.1.1. Acceptance of the described validation process is sought in this report. The applicability of this bias and uncertainty for postclosure repository conditions will be demonstrated in validation reports, which will be referenced in the License Application. Thus, acceptance is not sought in this report for specific values of bias and uncertainty related to the isotopic model.

Additional requirements imposed for modeling burnup of commercial SNF for waste package design applications are presented in Subsection 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. Acceptance is sought in this report that these requirements are sufficient, if met, to ensure adequate conservatism in the isotopic model for burnup credit. Confirmation of the conservatism in the application model will be demonstrated in validation reports and acceptance of the confirmation for postclosure repository conditions will be sought in the License Application.

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 Subsection 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 Subsection 3.5.2.1.3 will be used to establish this uncertainty, and the results will be documented in the validation reports. The isotopic model validation will consider the remaining principal isotopes.

The validation approach for the isotopic model uses radiochemical assay data from both PWRs and BWRs. The radiochemical assay data is applied in model validation to establish the bias in k_{eff} values predicted by the isotopic model and to establish the uncertainty in the principal isotope concentrations predicted by the isotopic model. The bias in k_{eff} values will be incorporated in CL values established for commercial SNF as described in Subsection 3.5.3.2.10. The principal isotope concentrations used in the regression expressions or look-up tables will contain the uncertainty established by analysis of the radiochemical assay data for those isotopes affected by geochemical processes. The uncertainty in the isotopic concentrations from the geochemical analysis along with the uncertainty (for the same isotopes) from the radiochemical assay analysis will be represented in the probability distributions for the configurations analyzed for criticality.

The bias in k_{eff} values are 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 isotopic model. The fuel pellets from which the samples are taken started their irradiation cycle as fresh fuel (only uranium isotopes with no higher actinides or fission products). Calculations for the assay samples are establishing the reactivity effects due to irradiation of the fuel samples in a commercial reactor. The length of the irradiation time affects the reactivity of the fuel sample 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 k_{eff} established for the isotopic model is based on the capability of the model to predict the changes in the isotopic concentrations with increasing irradiation time (burnup) in the commercial reactor.

The isotopic concentrations from the assay samples will be compared to the isotopic concentrations calculated using the isotopic model. The uncertainty in the calculated concentrations will be established for each of the principal isotopes. As noted above, this uncertainty will be combined with the uncertainty from the geochemical analyses for those isotopes affected by geochemical processes and will be represented in the probability distributions for configurations analyzed for criticality.

The modeling approach for the isotopic model uses one-dimensional neutron transport with point-depletion as the base model. This model will be used to analyze samples of fuel pellets that have been irradiated in commercial reactors. Radiochemical assay samples are from several PWR and BWR cores and cover a range of initial fuel enrichments and burnups that are representative of the current inventory of commercial SNF. For the analyses of SNF assay samples, burnup history parameters such as power densities, moderator temperatures and densities, fuel temperatures, and soluble boron concentrations (for PWRs) affect the neutron spectrum that the fuel sample experiences. This in turn will affect the isotopic concentrations of the fuel sample. Thus, appropriate values for these parameters will be used in the analysis of the samples for isotopic model validation.

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. The process for reconstructing burnup history parameters and establishing the uncertainty introduced by the process will be documented in the validation report for the isotopic model.

Radiochemical assay samples are generally taken from a single fuel pellet in a burned fuel assembly. This fuel pellet may not be representative of the many fuel pellets contained in the fuel assembly. Thus, the one-dimensional neutron transport-depletion model will contain additional uncertainty because of the limited capability to represent individual fuel pellets and the neutron spectrum associated with fuel pellet samples. 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 one-dimensional neutron transport-depletion model. These uncertainties will be documented in the validation report for the isotopic model.

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. This report is seeking acceptance that these requirements for modeling burnup of commercial SNF for design applications, when met are sufficient to ensure adequate conservatism in the isotopic model for burnup credit. Confirmation of the conservatism in the bounding isotopic model used for burnup credit for commercial SNF will be demonstrated in validation reports, which will be referenced in the License Application. Acceptance of the confirmation of the bounding isotopic model for postclosure repository conditions will be sought in the License Application.

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 for individual fuel assemblies from the commercial reactor criticals (CRCs) database used for criticality model validation. The isotopic concentrations for these fuel assemblies are 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 for individual assemblies from the CRC database, along with the bounding parameter values to represent reactor operating histories and conditions will be used to verify that the isotopic model for waste package design is conservative with respect to criticality. As part of the process, the sufficiency of the fuel assembly database used in satisfying the first requirement will be demonstrated.

The second requirement addresses the problem of using integral experiments (CRCs) 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 Subsection 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 Subsection 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 address 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 computer codes used to calculate the criticality of a waste package. It is organized as follows: 1) selection of

benchmark experiments, 2) calculation of the bias and uncertainty, and critical limits associated with the computer codes used to calculate criticality, 3) establishment of the range of applicability of the benchmark experiments, and 4) the acceptance criteria used for criticality.

Figure 3-7 shows the approach presented, starting with benchmark experiments and the Master Scenarios (CRWMS M&O 1997d) for internal and external waste package configurations. This is the same general approach to validation of calculational methods for criticality given in Dyer and Parks (1997, pp. 15-19) and Lichtenwalter et al. (1997, pp. 139-182).

In this approach criticality experiments are selected from a group of experiments that include laboratory critical experiments (LCE) 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 its Range of Applicability (ROA).

Similarly, a set of waste package configurations that are to be analyzed will be selected from the Master Scenarios (CRWMS M&O 1997d). The Range of Parameters (ROP) of the waste package configuration chosen 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 acceptance criteria. From there, critical limits will be determined and other margins or penalties will be used to determine if a particular system is critical. The term "penalty" is used in conjunction with extension of the Range of Applicability. The term "margin" is used to denote further reductions in the critical limits.

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, acceptance criteria, using critical limits penalties and margins will be applied, as described in subsection 3.5.3.2.10, to determine criticality.

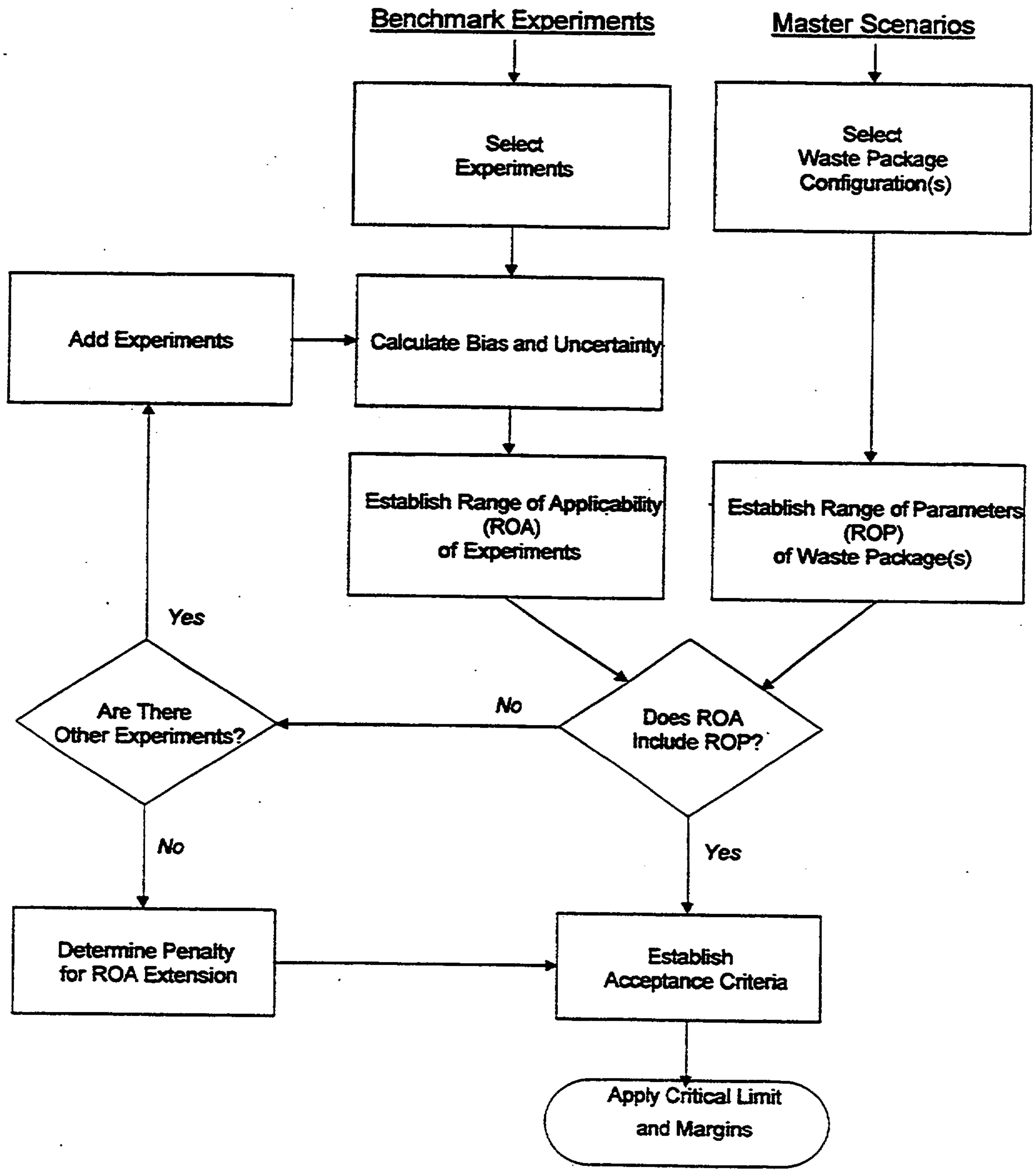


Figure 3-7. Process for Establishing Criticality Acceptance Criteria

3.5.3.2.1 Selection of Experiments

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

In the past, nuclear 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 fissile-isotope-mass were used. Other parameters included: fuel lattice pitch and parameters that described either material concentrations, geometry, or ratios of moderator to fissile-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 single global parameters for correlating experiments to evaluations of systems of similar fissile 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 in Lichtenwalter et. al. (1997, pp. 139-182) and Dyer and Parks (1997, pp. 15-19).

The benchmark experiments will be selected from a set of experiments, which consists of LCEs, PWR CRCs, and BWR CRCs for each applicable scenario/waste class from the master scenario list. 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 (ROA) 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. Usually, it is difficult to distinguish between bias and uncertainty or the difference between measurement and calculational bias and uncertainty, therefore they are all taken together.

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 Master Scenarios (CRWMS M&O 1997d).

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 with 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 are identical. This is not usually practical, 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 geological 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 concentration 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 the form of margin-to-criticality. In these cases, there may be an extension of the Range of Applicability to cover the Range of Parameters of the system.

In those cases where biases are exhibited, the area of applicability can be extended by the use of 1) expert judgement, 2) sensitivity analysis, 3) statistical evaluation of the importance of these parameters or 4) comparison with other credible methods (code-to-code comparisons). In some cases, the probability of occurrence or risk of occurrence (probability times consequence) can also be used to evaluate configurations and their impact on the repository.

The means used to extend the range of applicability will depend on a number of factors. Some of these are: 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, 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 step wise 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 an ROA is extended, where there is a trend in the data, without the use of additional experiments, additional penalty will be added to the acceptance criteria used to determine if a system is critical. The same techniques described above for extending the ROA 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 (ROA). If the extension of the ROA 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 CL and an appropriate penalty. If the extension is not small, then more data, covering the ROA, will be necessary. When more data are obtained, the process of Figure 3-7 must be applied to the new data set. This applies when the ROA for fundamental parameters (material concentrations, geometry, or nuclear cross sections) does not cover the ROP 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 (LCEs) and commercial reactor criticals (CRCs). Various

parameters will be trended with the k_{eff} values from the LCEs and the CRCs. These trends will be used to establish biases and uncertainties of the criticality model.

The CRCs represent intact commercial SNF in known critical configurations. Although the CRC evaluations provide integral criticality benchmarks for SNF in a reactor, they do not provide separate benchmarks for isotopic concentration of individual isotopes. The CRCs are used to provide reasonable assurance that the initial isotope concentrations of SNF are known and they will be used as criticality benchmarks for SNF in an intact form.

Radiochemical assays (RCAs) are used to validate the isotopic model for SNF. These are used to provide further assurance that the initial isotope concentration of SNF is known. The biases and uncertainties from the CRCs, lattice LCEs, and the RCAs will be used to establish acceptance criteria for the neutronic model that will be used to determine if a system containing commercial SNF in the intact state is critical.

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

3.5.3.2.5 Determination of Bias and Uncertainty

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 CL. The CL is derived from the bias and uncertainties associated with the criticality code 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 CL for a waste package is a limiting value of k_{eff} at which a configuration is considered potentially critical. The CL is characterized by statistical tolerance limits that account for biases and uncertainties associated with the criticality code trending process.

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.

A CL is associated with a specific type of waste package and its state (intact or various stages of degradation described by the Master Scenarios (CRWMS M&O 1997d). The CL 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 CL function may be expressed as a regression-based function of neutronic and/or physical variable(s). In application, a CL function could also be a single value, reflecting a conservative result over the range of applicability for the waste form characterized.

Other margins may be applied to reduce the CL. Subsections 3.5.3.2.5 through 3.5.3.2.9 do not address margin; they address the statistical methods to account for differences of 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 CL 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 CLs 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 CL function.

The determination of CL 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 CL function for a waste form results from the process shown in Figure 3-8. The data set and the resulting k_{eff} values produced by the criticality code are assumed to be appropriate and valid for the waste form. This is fundamental to the development of the CL function. The objective of this process is to produce CL's that are statistically meaningful and practical in application.

The purpose of the CL 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 acceptance criteria for criticality. 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 is an assumption, as explained above. The CL 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.

Figure 3-8 displays two general statistical methods for establishing CL 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 Subsection 3.5.3.2.3.

If no trend is identified, a single value may be established for a CL 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 CL. For purposes of differentiation, this technique will be described as "non-trending". The normal distribution tolerance limit (NDTL) method and the distribution free tolerance limit (DFTL) method, described below, are "non-trending" methods.

The regression or "trending" methods (Subsection 3.5.3.2.7) use statistical tolerance values based on linear regression techniques to establish a CL 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 may be used to determine the value of the CL. The lower uniform tolerance band (LUTB) 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 tolerance-limit CL function. In either single or multiple situations, the regression trend that produces the lowest CL 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 CL 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. Subsection 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 NDTL. Subsection 3.5.3.2.9 describes the DFTL method. The DFTL 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 of the underlying probability model. Assumptions about the randomness of the process and the data as representing a random sample from the population of interest are necessary.

In all calculations of CL 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 CL for cases in which the best estimate of the bias trend would result in a CL greater than 1.0. The treatment of this element is discussed below in the context of each method used to establish the basic CL function.

The critical limit is estimated such that a calculated k_{eff} below this limit is considered subcritical, and a system is considered acceptably subcritical if a calculated k_{eff} plus calculational uncertainties lies below this limit. In equation notation,

$$k_S + \Delta k_S < CL \qquad \text{(Eq. 3-1)}$$

k_S = the calculated multiplication factor of a system to be considered for criticality,

Δk_S = the uncertainty in the value of k_S.

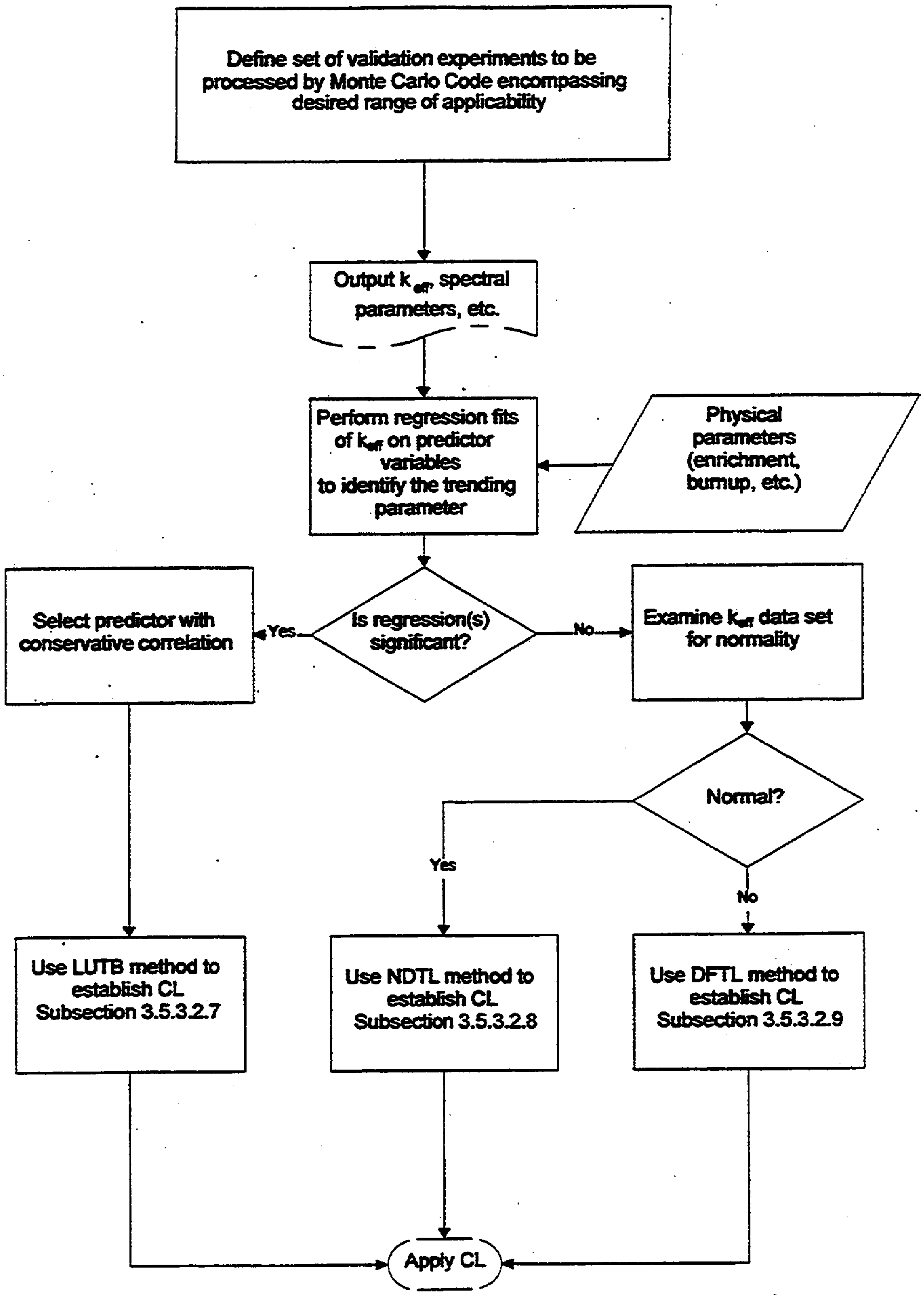


Figure 3-8. Process for Calculating Critical Limits

The CL function is defined as,

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

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, CL is estimated as a function (f (CL)) of a parameter(s). Because both Δk_C (x) and k_C (x) can vary with this parameter, the CL 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 CL is further reduced by a positive bias adjustment. The positive bias adjustment sets k_C = 1.0 when k_C exceeds 1.0. This provides further assurance of subcriticality and represents additional conservatism.

The following sections discuss the various methods for estimating a CL function. Subsection 3.5.3.2.7 presents the regression method for trending k_{eff} versus a parameter vector. Subsections 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.

Acceptance of these methods for estimating bias and uncertainty, and establishing the CL function for a waste form is sought. Acceptance of specific CL values will be sought as part of the License Application.

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 CL function of some neutronic or physical parameter. The statistical tolerance limit method, discussed in Lichtenwalter et al. (1997, p. 157-162) 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 Lichtenwalter et al. (1997, p. 157-162) is found in 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 CL function as a statistically meaningful result that yields a conservative CL over the ROA 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 Subsection 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 provide 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 CL function. From these results, the conservative value may be selected as the CL. 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 CL function uses a tolerance band approach referred to as a single-sided, uniform width, closed interval, approach in Lichtenwalter et al. (1997, pp. 160-162). This will be referred to as the LUTB 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 CL 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 CL is the one that 1) exhibits a meaningful correlation, 2) has a meaningful interpretation, and 3) results in a conservative CL function. A detailed description of the basic LUTB method is given in Lichtenwalter et al. (1997, pp. 160-162), Bowden and Graybill (1966, pp. 182-198), and Johnson (1968, pp. 207-209).

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

The CL function is the lower bound of a tolerance limit for the critical system. There is a specified confidence that, at least, a specified percentage of the systems that are above the CL are critical systems. Consequently, there is also this same confidence that a small portion of the systems with a k_{eff} less than the CL function value are critical systems.

3.5.3.2.8 Normal Distribution Tolerance Limit

The NDTL method is one of two techniques for estimating a CL 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 NDTL 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 NDTL 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 NDTL.

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

$$CL = k_{ave} - k(\gamma, P, df) \bullet S_P \qquad \text{(Eq. 3-4)}$$

where:

k_{ave} is the average of the k_{eff} values, unless k_{ave} is greater than unity (1.0), in which instance the appropriate value for k_{ave} should be 1.0 to disallow positive uncertainty; $k(\gamma, P, df)$ is 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 df is the number of degrees of freedom. The term S_P is 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

$$k(\gamma, P, df) \bullet S_{CCave}$$

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 DFTL 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 CL 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 Natrella (1963, pp. 1-14, 1-15, 2-15); and Hogg and Craig (1966, pp. 182-185).

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 2. 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 ($3^*\sigma$) 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,

$$k_{eff1} < k_{eff2} < k_{eff3} < \ldots < k_{effN} \quad \text{(Eq. 3-5)}$$

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

$$CL = k_{eff\,I} \quad \text{(Eq. 3-6)}$$

is the CL with the characteristics of confidence and population coverage available for the data set of interest.

3.5.3.2.10 Criticality Acceptance Criteria for the Isotopic and Criticality Models

The bias and uncertainty associated with the isotopic model (Δk_I) will be subtracted from the CL calculated for SNF using the CRCs and LCEs as benchmark critical experiments. The penalty for extending the range of applicability (Δk_{EROA}), if applicable, will also be subtracted from the critical limits. The determination and justification of all of these biases and uncertainties will be documented in validation reports applicable to different waste packages under various stages of degradation.

The acceptance criteria for a waste package system for intact SNF will be as follows:

$$k_S + \Delta k_S < CL - \Delta k_{EROA} - \Delta k_I \quad \text{(Eq. 3-7)}$$

3.5.3.3 Regression Analysis Validation

The process for constructing tables of k_{eff} values for configuration classes and developing regression expressions of k_{eff} as a function of parameters that affect criticality was provided in Subsection 3.5.2.3. The accuracy of these regression expressions must be established prior to their application for disposal criticality evaluations in the repository. This section describes the validation approach for the regression expressions. For certain situations it may be desirable to use linear interpolation between k_{eff} values in the table constructed for a configuration class instead of developing regression expressions. The validation approach for the linear interpolation modeling is also described in this section.

Validation of the regression expressions establishes the uncertainty in k_{eff} values obtained from the regression expressions compared to k_{eff} values obtained from direct evaluations that use the criticality model. Values of k_{eff} are obtained from criticality evaluations for the range of independent parameter values represented by the regression expressions. These k_{eff} values provide a base set of data for comparison with the k_{eff} values obtained from the regression expressions at identical values of the independent parameters. Additional k_{eff} evaluations are performed for values of the independent parameters that are different from those used in developing the regression expressions. These k_{eff} values are added to the base set of data and used in the validation. Comparisons of fitted k_{eff} values obtained from the regression expressions are made with values from the calculated set of data, and the uncertainty in the fitted data is established as characterized by statistical tolerance limits. This uncertainty is added to the k_{eff} value obtained from a given regression expression for a potentially critical configuration prior to comparison with the critical limit.

A similar validation approach is used for the situations where k_{eff} values for a configuration are obtained from linear interpolation between k_{eff} values in the table constructed for a

configuration class. Additional criticality evaluations are performed for values of the independent parameters that are different from those in the table. Values of k_{eff} obtained from linear interpolation between independent parameter data points in the table are compared with values of k_{eff} obtained from the additional criticality calculations for the same values of the independent parameters at the fitted points. The results of these comparisons are used to establish the uncertainty in the fitted data as characterized by statistical tolerance limits. This uncertainty is added to the k_{eff} value obtained for a configuration evaluated using linear interpolation prior to comparison with the CL. Validation of the regression expression method and the linear interpolation method will be documented in validation reports that are referenced by the License Application.

3.6 ESTIMATING PROBABILITY OF CRITICAL CONFIGURATIONS

This section describes the general methodology for estimating the probability of occurrence of critical configurations with fissionable material in the repository. It is this methodology for estimating the probability of occurrence for potentially critical configurations for which acceptance is sought. Acceptance is also sought for the use of the multivariate regression model, or the table lookup and interpolation from a discrete, but large, number of criticality calculations, as a significant component of this methodology. This mapping from a discrete set of criticality calculations to a continuum of parameter values is used with continuous probability distributions of those parameters to estimate overall probability of 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 and the effect on the dose at the accessible environment. The second objective is to provide an estimate of the effectiveness of the variety of measures used to control or limit postclosure criticality.

3.6.1 Criticality Probability Methodology

The first step in estimating criticality probability is to identify the configuration classes that are critical, which, in turn are developed from the standard scenarios. Probability will be estimated for all configuration classes that have a k_{eff} exceeding the CL over a portion of their parameter range. Therefore, the first step in applying the methodology is to identify the range of parameters that will result in calculated k_{eff} greater than the CL. This screening is applied to each configuration class. The potentially critical configurations are characterized by parameters having a range of values. 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).

It would be impractical to subject all of the possible combinations of parameter values to reactivity calculations. Therefore, a table of k_{eff} values for representative parameter values is used to determine k_{eff} values for any given set of parameters. Either of two techniques is used for this purpose. The table of k_{eff} values can be used to construct a regression for k_{eff} as the dependent variable, with the configuration and waste form parameters as independent variables. The goodness of fit is dependent on the data being modeled; regression analyses thus far for k_{eff} have suggested that to get a good fit, the regression should be non-linear with terms up to the third power are needed in the individual parameters and cross products of different parameters. If the regression fit is good, it can be used to calculate k_{eff} for any values of the parameters that fall within the range of the table. Alternatively, the table can be used directly for a multidimensional lookup and interpolation. The latter technique is more accurate, since the

regression may introduce anomalous behavior, but it also requires more computation if the number of parameters is large. The number of computations for a regression with cubic cross terms could increase as the third power of the number of parameters while the number of computations for an n-parameter interpolation would increase as 2^n.

Probability distributions are developed from the uncertainty associated with these scenario and configuration parameters. Then the Monte Carlo technique is used to estimate criticality probability. The Monte Carlo process consists of a series of random selections (called Monte Carlo trials, iterations, repetitions, or realizations) from these distributions, and determination of whether the selected set of parameter values satisfies the requirements for criticality. The probability of criticality is then determined by dividing the number of trials, which satisfy the requirements for criticality occurrence, by the total number of trials. A confidence limit equal to 0.95 or 0.98 will generally be appropriate for such a parameter estimate. This confidence limit will correspond to a confidence interval of $\pm 1.98\ \sigma$ or $\pm 2.33\ \sigma$, respectively.

The value of the standard deviation, σ, will reflect principal uncertainties associated with the Monte Carlo simulation: (1) the random fluctuations due to the limited number of samplings, (2) errors inherent in the regression or table lookup and interpolation process, and (3) uncertainty in the configuration parameters for processes that will take place over long time periods. For the first two uncertainty types the error can be driven as small as desired by increasing the number of repetitions or the number of points in the lookup table. For the third uncertainty type, the contribution of configuration parameter uncertainty to the overall standard deviation is determined by the probability distribution of such parameters. A recent calculation (CRWMS M&O 1999b) used 30,000 trials. Even the slower table lookup and interpolation technique could handle 100 million trials in a reasonable computation time.

There are two general types of parameter 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 Subsections 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) Base Case distribution of breach times developed using WAPDEG (WAste Package DEGradation model, developed by PA) for waste packages under drips. The WAPDEG 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. Essential inputs to WAPDEG come from the PA probabilistic climate model for the water drip rate as a function of time and the PA probabilistic model for dripping flow and fraction of waste package being dripped on as a function of infiltration rate. 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 FWF or OIC. 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 which can arise, and with the subrange(s) that can lead to a critical configuration. Generally, criticality is determined by several configuration parameters acting together so whether a configuration is critical is determined only after all the parameters have been selected. The criticality-determining relationship among the configuration-related parameters is best expressed by the regression for k_{eff} as a function of parameters describing the potentially critical configuration. 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 FWF remaining intact.

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

4. Parameters characterizing the amount of neutron-absorber material remaining in its intact carrier.

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 very 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 assumption that the waste forms are loaded into the proper waste package. For commercial SNF there may be several different designs or means of limiting criticality potential to correspond to different ranges of burnup and initial enrichment.

The results of these probability calculations are expressed in the following forms: (1) frequency of criticality per year (equivalent to a probability density function, in time, for the occurrence of a criticality); (2) the probability of criticality before some time (equivalent to a cumulative distribution function); and (3) the expected number of criticalities, (on a per year and a cumulative basis) for the waste form type and for the entire repository.

3.6.2 Design Criticality Probability Criterion

The calculated probability per waste package is compared with the waste package design criticality probability criterion, which is derived from the repository design criticality probability criterion, according to the procedure described in this section, below. The repository design criticality probability criterion was defined in Section 3.2.2 as that the average criticality frequency will be less than 10^{-4} per year for the entire repository for the first 10,000 years. This is equivalent to the statement that the expected number of criticalities will be less than one in 10,000 years. The reason for choosing this value is that an expectation of less than one criticality in 10,000 years implies that there will be few or no criticalities during the first 10,000 years following emplacement, which is the assumed regulatory period of principal concern, although criticality, like performance assessment, may remain of concern for much longer times.

The allocation of the repository probability criterion to a per-waste-package and per-year basis is complicated by the following factors:

1. Less than 10 percent of the waste packages will have sufficient fissionable material, at sufficient enrichment to be able to support a criticality. It would be unnecessarily conservative to burden these potentially critical waste packages with the small probability allocation that would result from simply dividing the repository probability criterion by the total number of waste packages.

2. The probabilities of waste package breach and loss of neutron absorber increases with time (analogous to a very long lifetime or wear-out process) so there can be no formula for allocating the 10,000 year regulatory time period to a per-year basis.

3. There is a possibility of common mode failure. In particular, for external criticality, there is a possibility of multiple packages contributing to the accumulation of fissionable material at a single location. It is expected that the License Application document will demonstrate such occurrences to be of negligible probability, but they cannot be completely rejected at the present time.

The above reservations notwithstanding, the methodology will initially apply a design guideline determined by allocating the repository probability criterion (expected number of criticalities less than one in 10,000 years) among the approximately 10,000 waste packages to obtain a derived waste package design probability criterion of less than approximately 10^{-4} expected criticalities, per waste package in 10,000 years.

This derived design probability criterion is not proposed for regulatory purposes, and will only be used to guide decision processes internal to waste package design. The only probability criterion to be applied in licensing documents will be the TSPA screening threshold of 10^{-4} in 10,000 years for the entire repository, given in 10 CFR 63.102(j) and 10CFR 63.114(d).

3.6.3 Probability Calculation Model

This section presents a discussion of the Monte Carlo method of criticality probability calculation and the model for determining the probability distributions that are used for the random selections of the Monte Carlo method. This section also provides an overview of the

configuration generator code, which is used to track the specific parameters of the processes that make up the scenarios.

The mass balance equations of the configuration generator code are used to calculate the parameters that serve to specify the potentially critical configurations for which k_{eff} will need to be evaluated. Acceptance is sought for the concept that probability of criticality can be estimated and for the Monte Carlo methodology based on random sampling from probability distributions of individual parameters. The mass balance equations of the configuration generator code are presented for illustration only; their exact form will be determined for License Application.

3.6.3.1 Probability Concepts

The Monte Carlo methodology involves the concept of random sampling from a set of probability distributions for values of a set of parameters. An understanding of the mathematical form of the probability distribution most often used for this purpose begins with the probability density function (pdf), which is defined in terms of the probability that a random variable, T, falls in the interval t to t+dt, where t is some value which can be assumed by T, and dt is some small increment in t:

$$\Pr\{t \le T \le t+dt\} = f(t)dt \qquad \text{(Eq. 3-8)}$$

Where Pr indicates probability, and $f(t)$ is said to be the probability density function with respect to the independent variable, t, and has units that are the reciprocal of the units of t. Related to the pdf is the cumulative distribution function (CDF) that can be defined in either of two equivalent ways:

$$F(t) = \int_0^t f(\tau)d\tau \qquad \text{(Eq. 3-9)}$$

or

$$F(t) = \Pr\{T \le t\} \qquad \text{(Eq. 3-10)}$$

where τ is used as the variable of integration to distinguish it from the variable t which is a limit of the integration, so that it can be the independent variable for the integral function F(t). It should be noted that the CDF, F(t), is a function of t, and this functional relationship is important for generating Monte Carlo random values for parameters having distributions other than uniform, as described in the following subsection. In general, this functional relationship provides a one-to-one mapping of the range of the random variable into the 0 to 1 domain of the CDF.

3.6.3.2 Monte Carlo Model

The random selection of sample values is determined by the following algorithm:

A. Sample a random number from a uniform distribution between 0 and 1; this is the same as, or can be derived from, the random number generator supplied with most technical system software (e.g., FORTRAN or C compilers).

B. Set the CDF for the random variable of interest equal to the random number selected, and solve the resulting equation for the specific value of the random variable (corresponding to this random number). This process is called inverting the function. Since the CDF determines a one-to-one mapping from the random variable to the domain of 0 to 1, the

inverse relation maps the random numbers from 0 to 1 into the random values for the random variable.

C. Repeat the above steps for each parameter having uncertainty represented by a CDF.

The Monte Carlo technique is used to develop statistics by randomly tracing through the steps of the scenarios leading to a potentially critical configuration. In this process care will be taken that there is no multiple, or redundant, sampling of individual uncertain parameters. For example, the probability distribution of waste package breach times is taken from the latest TSPA calculation. On the other hand, the distribution of subsequent process parameters is developed as part of the waste package disposal criticality analysis process, according to the methodology of this Topical Report.

The sequence of steps in the application of the Monte Carlo technique is shown in Figures 3-9a and 3-9b for internal and external criticality, respectively. This is an application of the well-known set of system simulation techniques. Each sequence starts by incrementing the number of realizations (also called trials or iterations); the sequences leading to a criticality event will end by incrementing either the internal or the external criticality counters. The probability of a criticality event is then determined by dividing the number in the criticality counter by the number in the realization counter. The following is a brief description of the major probabilistic considerations for the individual steps.

Internal Criticality

A. Sample from the distribution of barrier lifetimes. This distribution is obtained by (a) first applying the PA program WAPDEG to obtain waste package failure distributions under always dripping and no-dripping conditions, and (b) then applying the TSPA program GoldSim to combine the WAPDEG output with the value for drip rate sampled in the previous step. It should be noted that both the WAPDEG and GoldSim computer programs are validated as part of the performance assessment methodology, as explained in Section 3.8.1.

B. Sample from the distribution of the possible locations of significant penetrations of the waste package barriers. This distribution of penetration locations is also generated by the WAPDEG program. The lowest penetration on the waste package will determine the depth of water standing in the waste package, which, in turn, will determine the number of assemblies covered by water and the potential for the occurrence of a criticality event.

C. Sample from distribution of drip rates. The distribution of seepage fraction, seepage rate and their temporal variation will be obtained from a drift-scale seepage model, which will include the effects of thermal reflux. These seepage rates are used as inputs to the degradation calculations (particularly EQ3/6), which will develop the distribution of degradation parameters.

D. Sample from the range of waste form parameters (e.g., burnup and enrichment for commercial SNF), and test whether they could produce a criticality event under the worst case degradation conditions, if such worst case conditions can be defined (e.g., loss of all neutron absorbers and the time of peak criticality potential). If there can be no criticality event occurrence for these waste form characteristics, the realization is ended, saving the additional computation required for the following steps. This step of the methodology is

most applicable to commercial SNF, which has a range of burnup and enrichments, which, in turn, leads to a large range of criticality potential. The test for sufficient fissionable material to support criticality will consider external, as well as internal, configurations.

E. Sample from the distribution of degradation parameters for the WF and OIC, and calculate the amounts of neutronically significant material remaining in the waste package. These calculations are made with the mass balance equations of the configuration generator code (described in Subsection 3.6.3.3), that uses the sampled degradation parameters as coefficients in the equations. The distributions of the degradation parameters are consistent with degradation parameter distributions used for the TSPA. There will be Monte Carlo selection of environmental parameters having some influence on the transport and accumulation processes. The CDFs for these Monte Carlo selections will coincide with those used in the TSPA process, or will be abstracted from the results of calculations for the TSPA. Examples of such parameters are given in items C and D above.

F. Evaluate criticality of the configurations defined by the previous step, using the k_{eff} regression or table lookup. If $k_{eff} \geq CL$, increment the internal criticality counter and end the realization and start another (until the desired number of realizations is reached).

G. If the configuration is not critical, test whether the ending condition has been reached, usually a time limit (upwards of 100,000 years) or loss of moderating water from the waste package. If the ending condition has not been reached, increment the time and calculate a new concentration of degradation products. If the ending condition has been reached, end the realization.

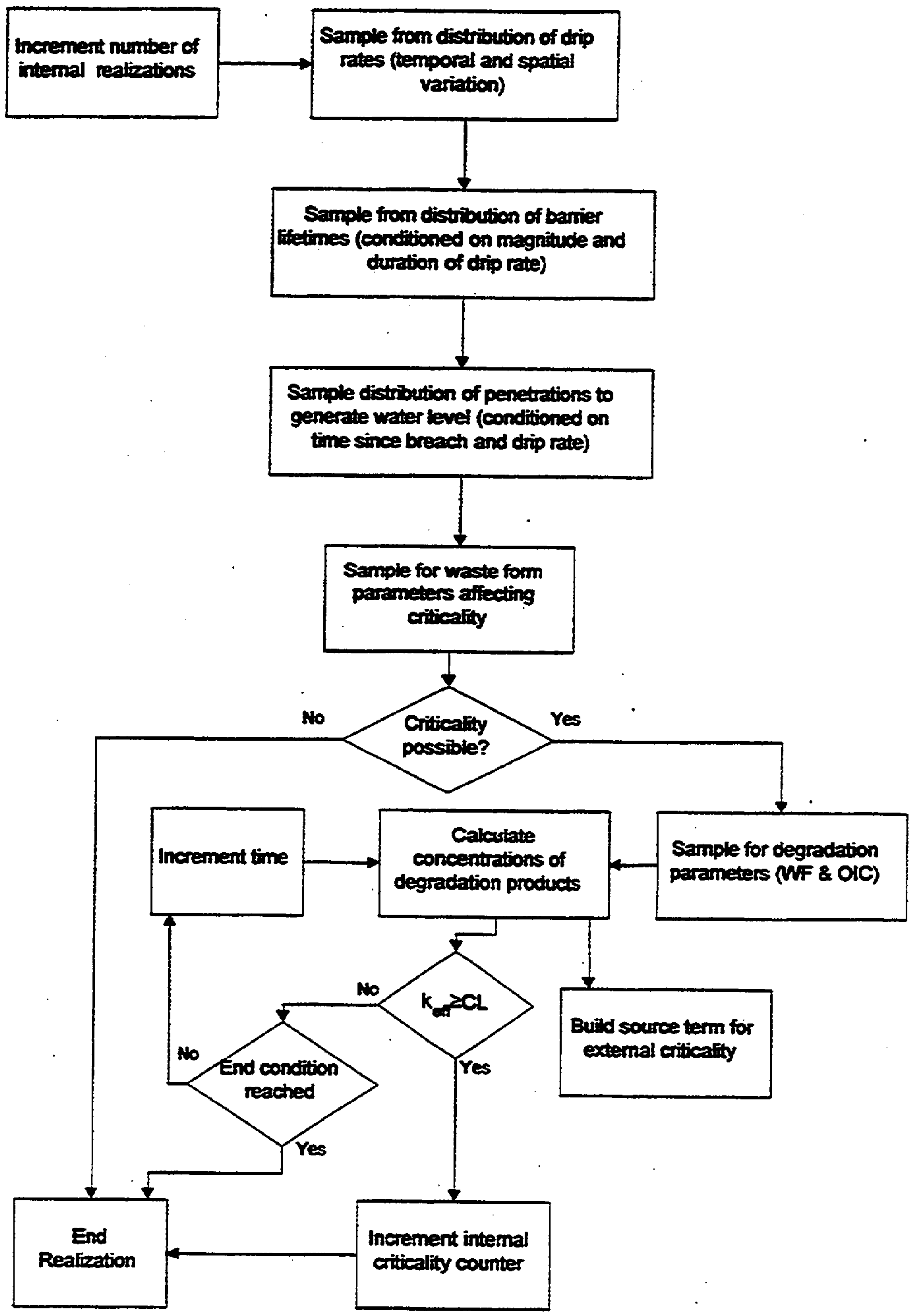


Figure 3-9a. Monte Carlo Technique Informational Flow, Internal

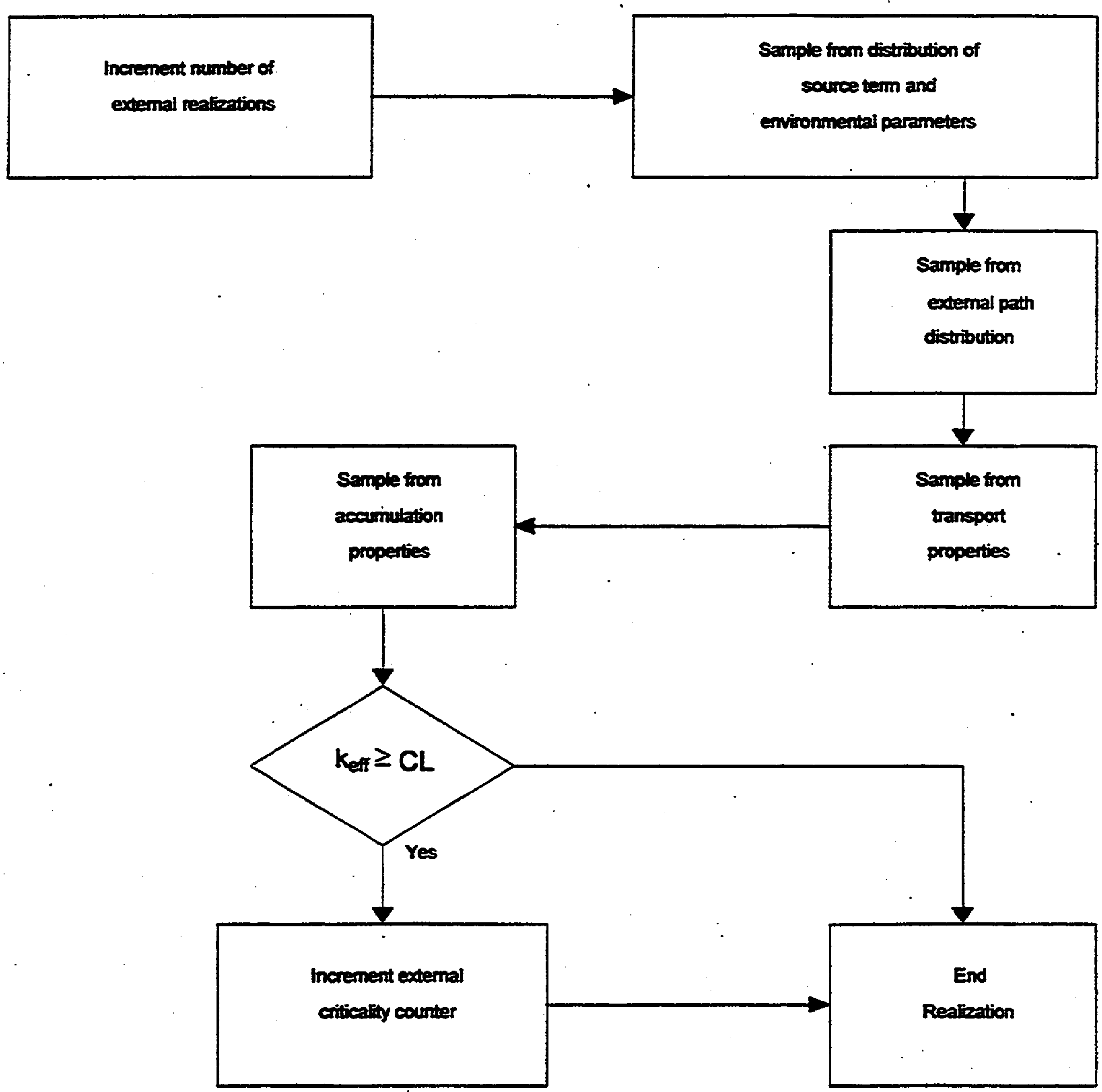


Figure 3-9b. Monte Carlo Technique Informational Flow, External

External Criticality

A. To develop the source term for external criticality, sample from the distributions for the flow rate, concentration of fissionable elements and associated solution characteristics (e.g., pH, Eh, ionic strength, concentration of major solution ionic components). The flow rate out of the waste package is taken to be the same as the drip rate (flow rate in), and the distribution is also the same. The distributions of the solution characteristics parameters are abstracted from the various EQ3/6 runs that use the sampled drip rates as input. In both cases the drip rate distribution is the same as that used for the latest version of the TSPA.

B. Randomly select the external path from among those leading to one of the standard set of external criticality locations, with the selection process weighted according to the probability of such a location existing and being encountered. Such parameters will include the groundwater flow rate, the rock porosity, and the fracture density. In this manner both the matrix and fracture transport can be evaluated. The standard external locations will be established as part of the analysis for License Application. Preliminary analyses (CRWMS M&O 1998g) suggest that the locations will fall into the following general categories: (1) coating the fracture walls of the drift invert and nearby host rock, (2) deposits of adsorbing material, and (3) deposits of reducing material.

C. Sample from the distribution of transport parameters, which are taken to be those used in, or generated by, the TSPA. Calculate the amounts of fissionable material transported through that portion of the external environment that contains little material with the capability for removing fissionable material from the flow. Such portions of the external environment are identified by prior geochemical analysis (EQ3/6). These calculations will be accomplished by the transport mass balance equations from the configuration generator code, with Monte Carlo selection of those parameters that have significant uncertainty.

D. Sample from the distribution of accumulation parameters, which are taken to be those used in, or generated by, the TSPA. Such parameters will include the adsorption coefficients for the fissile elements in solution.

E. Calculate the amounts of fissionable material removed from the flow at that portion of the external environment, which contains sizeable amounts of material with the capability for removing fissionable material from the flow. Such portions of the external environment are identified by prior geochemical analysis (EQ3/6). These calculations will use the mass balance equations from the configuration generator code. There will be Monte Carlo selection of parameters having significant uncertainty.

F. Evaluate the k_{eff} of the configurations having a significant accumulation of fissionable material. If this is above the CL, a potential external criticality has been identified, and the external criticality counter is incremented (for the specific location), as indicated in Figure 3-9b. In either event, this realization is ended and a new one begun. Allowing only one path for external criticality for each realization may appear to be non-conservative, since it is theoretically possible for a single source term to feed more than one external criticality location. However, it is expected that the probability of a single external criticality will be so small that the probability of multiple criticalities from a single source term will be completely insignificant. This expectation will be demonstrated to be correct as part of the License Application.

The application of the Monte Carlo technique outlined above shows a strong dependence on the inputs used by, and results from, the TSPA. This is justified because the TSPA reflects the most complete and consistent application of the scientific and engineering capabilities of the M&O to the relevant issues.

3.6.3.3 Configuration Generation Code

The CGC has been developed for the waste forms examined thus far. Further versions will be developed by modifying the existing version(s); all the versions will be demonstrated to be valid as part of the License Application process. The purpose for the CGC is to track the concentrations (or amounts) of neutronically significant isotopes (either fissionable or neutron absorbing) and chemical species which can effect the solubility of the neutronically significant elements. The concentrations, or amounts, are tracked by time-dependent first-order differential equations, which are solved by numerical integration. Some of these differential equations represent chemical transformations of elements or compounds. These equations form heuristic model(s) with coefficients determined by fitting data from the detailed EQ3/6 geochemistry calculations described in Subsection 3.4.1.2.2 for internal degradation, and from PHREEQC abstractions as described in Section 3.4.3 for external transport and accumulation. For some waste forms the geochemistry calculations using EQ3/6 are sufficient to characterize the contents of the waste package, so the CGC does not need to be used for internal criticality. The appropriate balance between the use of EQ3/6 and the CGC will be demonstrated for each major waste form category as part of the License Application process.

In summary, it can be stated that the CGC will generally be used for two purposes: (1) to provide bookkeeping for the transport between sites of application of EQ3/6, such as the interior of the waste package where the source term for external criticality is generated, and the external location where a chemistry change might cause significant precipitation, as may be determined by PHREEQC; (2) to provide more rapid calculation of Monte Carlo statistics in situations where the EQ3/6 and PHREEQC results can be used to develop heuristic models for the few most significant ions for a few solution parameters, such as pH.

For the CGC, at each time step the update process for each numerically integrated differential equation consists of the following:

I. For the waste package:

   A. Increment water in the package according to the difference between inflow and outflow from package.

   B. Compute the increment to the solution from each solid being dissolved at this time step, according to the intrinsic dissolution rate and the solid surface remaining.

   C. Compute the decrement to each element and isotope due to the amount of solution removed at the previous time step.

   D. Compute pH and solubilities as a function of the concentration of species which can effect pH and solubility (e.g., chromate, carbonate), including the effect of pH on solubility.

E. Compute the precipitation or dissolution of the various species being tracked, according to the above determined solubilities for this time step; for elements with more than one neutronically significant isotope (e.g., ^{238}U and ^{235}U in the current model implementation) the following refinement is implemented:

1. The relative isotopic concentrations going into solution from the dissolution of the several possible source terms at this step and those isotopic concentrations already in solution are recorded (stored).

2. The isotopic concentrations are combined to update the amounts of each element or each chemical species in solution according to the maximum concentration permitted (solubility limit) for the combined isotopes; the increment of the combined isotopes (or decrement) to the amount in solution is recorded.

3. The amounts of the individual isotopes in solution and precipitate are re-calculated according to the previously recorded isotopic percentages and the combined decrement (or increment) to the amount in solution.

II. For the invert:

A. Accept outflow from the package, augmented by any inflow from the drift (including dissolution from depleted uranium backfill, if any).

B. Decrement by outflow and compute new concentrations.

C. Compute pH and solubilities as a function of pH and other solution characteristics identified by abstraction from geochemistry code analysis (e.g., EQ3/6 or PHREEQC).

D. Compute precipitation into, or dissolution from, the various solids in contact with solution, according to the above determined solubility for this time step. If there is an inflow from the drift containing depleted uranium backfill, the isotopic composition can change with time, so the special bookkeeping of individual isotopic species used for the waste package solution will have to be repeated for the invert.

E. Compute the concentrations in the outflow for this time step.

III. For a designated path through the rock beneath the invert to the next pond location:

A. Accept the outflow from the invert and store in array element for this time.

B. Compute fracture travel time (which is the same for all dissolved species, since they are transported in the same solution).

C. Compute matrix travel time for each species (primarily Pu and U), using species-specific retardation coefficients.

D. Compute outflow for this time from inflows at this time minus corresponding travel times.

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

3.6.4 Validation of the Criticality Probability Calculation Models

The validation approach of the criticality probability calculation models is conveniently divided into three parts: (1) the Monte Carlo framework for calculating probability follows well established Monte Carlo principles and needs no further validation, (2) several submodels, dealing primarily with environmental and material performance parameters, abstracted as part of the TSPA process, and (3) the configuration generator code, which incorporates (a) the TSPA developed sub-models, (b) mass balance time-dependent differential equations, and (c) the k_{eff} regression expression or table lookup based on criticality calculations. The validation approach for item (2) is provided separately by the TSPA process. Since the submodels dealing with the environmental and material performance parameters are the principal use of probability distributions, their validation approach also constitutes a validation of the CDFs used to generate the particular random variable values used in the Monte Carlo technique. The validation approach of item (3), configuration generator, is highly dependent on the specific waste form/waste package combination; it has been provided in the individual waste form criticality evaluations thus far.

The most comprehensive implementation of the configuration generator, applicable to both internal and external criticality, has been in the software routine *generate.c*, which is described in CRWMS M&O 1997b; a major specific application was for the immobilized plutonium waste form, for which the software routine was modified to *pugdcr.c*, described in CRWMS M&O 1997d. For these reasons, the probabilistic model validation given here is focused on the Monte Carlo framework, item (1). This is also appropriate because the Monte Carlo framework is the "analytical engine" responsible for manipulating the model inputs and the outputs of the submodels. A more recent application of the probabilistic criticality evaluation portion of the methodology for the commercial PWR SNF is given in CRWMS M&O 1999c.

Examples of hand calculations that would be compared to the Monte Carlo calculation for validation activities include modeling of the waste package degradation process. The degradation process of the commercial SNF waste package is characterized as (1) the steel corrodes to iron oxide, and (2) the boron is removed as the basket is corroded. The MathCAD calculation of criticality probability is given in CRWMS M&O 1998h, Attachment IV, and summarized in Table 3-4. The rows of the table represent parameters that are either factors in the final probability calculation (last row) or factors in the calculation of the time to corrode all the borated stainless steel.

The cumulative probability was estimated to be approximately 8.2×10^{-4} per PWR waste package (last item in above table), for 100,000 years, which agrees very closely with that inferred from the Monte Carlo results presented in Figure 6-1 of CRWMS M&O 1998h. It should be noted that this probability is much larger than for more recent calculations that use a more robust, waste package design. These more recent calculations are given in CRWMS M&O 1999c, particularly Table 6-1 and Figure 6-1 of that document. Since the more recent calculations make more conservative assumptions with respect to the failure of criticality control measures (including significant loss of iron oxide), they are not directly comparable to this calculation.

Table 3-4. Parameter Values for Validating Monte Carlo Calculations

Parameter	Value	Variable Name	Source[a]
Mean Percolation Drip Rate	38.8 mm/yr		Subsection 5.1.1
Mean Probability that a Waste Package Gets Dripped On	0.26446	P_{drip}	Table 5.1.2-1 (This is a function of the percolation rate.)
Probability that Waste Package Under a Drip is Breached	0.4	P_{breach}	Figure 5.1.4-1 (determined at 100,000 years)
Probability that Breached Waste Package will Accumulate Water	0.4775	P_{bath}	Subsection 5.1.5
Mean Stainless Steel Corrosion Rate	1×10^{-4} mm/yr	SS	Figure 5.1.6-1
Multiplier From SS Corrosion Rate to B-SS Corrosion Rate	2.5	B_{fac}	Subsection 5.1.6
Mean Boron Factor	2.5	B_{fac}	Subsection 5.1.6
Mean Time to Corrode 7 mm of B-SS from Both Sides	1.4×10^{4} yr		7 mm/ (2 x B_{fac} x SS)
Probability that Waste Package Flooding Lasts Longer than Mean Time to Corrode B-SS	0.65	P_{dur}	Figure 5.1.5-1
Probability that waste package contains fuel that will exceed k_{eff} of 0.98 when flooded and all boron is removed	0.025	P_{crit}	Curve in Attachment IV, page 2 at 100,000 years
Estimate of Probability that Waste Package will Exceed k_{eff} of 0.98 in 100,000 years	8.2×10^{-4}		$P_{drip} \times P_{breach} \times P_{bath} \times P_{dur} \times P_{crit}$

[a] All Section, Table, and Figure references are from CRWMS M&O 1998h unless otherwise stated.

3.7 ESTIMATING CRITICALITY CONSEQUENCES

This section describes the portion of the methodology for estimating the consequences of potentially critical events internal and external to the waste package. The need to perform criticality consequence calculations for intact naval SNF are discussed in Mowbray 1999. Acceptance is sought for this portion of the methodology for estimating the consequences of potential criticality events with the criticality consequence models. As shown in Figure 3-1, Overview of Disposal Criticality Analysis Methodology, when the k_{eff} resulting from the degradation of a waste package design exceeds the CL, the consequences of the resulting criticality will be estimated. The estimated probabilities and consequences of criticality events will be input to the TSPA process according to the procedures indicated in Section 3.8.

The objective of the consequence evaluation is to identify and quantify the important parameters affecting the risk associated with criticality events and to provide this information to TSPA as input to the repository risk assessment evaluation. 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 is given in Subsection 3.7.1 and a discussion of specific models within the methodology in Subsection 3.7.2. Methods for validation and verification of the specific models are described in Subsection 3.7.3.

3.7.1 Criticality Consequence Methodology

The general criticality consequence 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 EBS degradation that can affect the radionuclide transport mechanisms, and their effects are also considered in the consequence methodology.

It should be noted that the CL may be significantly less than 1.0 (reduced by the bias and uncertainty, [Section 3.5]) prior to performing a criticality consequence analysis. Criticality consequences may then be estimated for configuration parameters with a k_{eff} significantly less than 1.0. This makes no difference for steady state criticality, where the consequences are determined by the power level that is determined by the seepage or percolation rate into the system or by other critical configuration parameters. The reactivity values (Δk) utilized for transient analyses are relative changes from a base configuration that is assumed to be critical. The configuration parameters for the transient criticality evaluation must be adjusted in a logical manner relative to the actual criticality state point.

3.7.1.1 Type of Criticality Event

The consequence of a criticality event depends upon the type of event and the configuration in which the criticality event occurs. Before describing the methodology for evaluating possible criticality events that might occur in, or near, the Yucca Mountain repository, 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 only very slow reactivity insertion (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 possible phenomena may include, but are not necessarily limited to, seismic events or rockfalls (CRWMS M&O 1997a, p. 60).

Steady-state versus transient events. A steady-state criticality produces energy at a constant rate, and most of that energy is quickly converted to heat. Criticality transients that can occur in the repository will be sufficiently slow that significant kinetic energy release will not likely

occur. 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 License Application. In order to produce a sufficiently rapid transient releasing an amount of kinetic energy sufficient to cause the movement of material within or outside the canister, the fissionable mass would have to

1) be confined either externally or by inertia

2) have a reactivity sufficiently above critical that the rate of increase of neutron density and power generated (proportional parameters) produces a doubling time of less than 1/1000 second.

The steady-state methodology 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 consequences resulting from a steady-state criticality are due to the incremental increase in the radionuclide inventory over the duration of the event. A second consequence that can exacerbate the radionuclide mobility for internal criticalities is an increase in the corrosion rate of the EBS resulting from increased local temperatures. The increase in the nuclide mobility could result from path alteration and/or chemical alteration of the environment.

The transient methodology uses codes that model 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 the 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 (Subsection 3.7.2.2), but evaluation of such effects will continue as part of the methodology. 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 transient criticalities can lead to an increase in the radionuclide mobility. The specific models for evaluating consequences of steady-state and transient criticality events are discussed in Subsection 3.7.2, Criticality Consequence Modeling.

Under-moderated versus over-moderated configurations. For thermally critical configurations, 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 at the same time, and there is still enough 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 MGR 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 efficient moderators. Since they are much less effective moderators than water, they are unlikely to produce a critical mass, as explained in Subsection 3.7.2.

3.7.1.2 Evaluating Direct Criticality Event Consequences

Steady-state and transient 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 the same initial conditions.

The steady-state analysis estimates the power and duration of a steady-state criticality event using a zero-dimensional model. 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 compute the total burnup for this power level and duration, using a point-depletion analysis model to estimate the increment in 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 for the EBS that might subsequently lead to increased nuclide releases (DOE 1998, Figures 3-45 and 3-46); (e.g., the estimated rate enhancement for Alloy 22 is about a factor of three from 40 °C to 80 °C). Since the consequence methodology proceeds in an explicit manner, coupled processes must be evaluated through sensitivity analyses.

The transient analysis models both the neutronic and other physical responses of the system to the temperatures and pressures generated if a rapid energy release results during a criticality. Identifiable mechanisms leading to possible transient criticality events without water moderation are limited to situations involving highly enriched fissile material. These situations are all very unlikely, requiring large accumulations of fissile material or special circumstances such as volcanic intrusion. Thus, the transient criticality methodology utilizes hydraulic mechanisms to couple processes. 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, EBS 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, and thus nuclide mobility. Longer-term consequences resulting from elevated temperatures may include, for internal criticality events, effects such as enhanced corrosion rates (DOE 1998, Figure 3-45). However, the duration of elevated temperatures from a transient criticality event is short which will mitigate effects on the corrosion rates for such events. Both immediate and long-term consequences to the physical system will be evaluated, as appropriate, although any significant mechanical consequences are expected to be very unlikely. The next step in the analysis is to compute the total burnup for the power history, using a point-depletion analysis model, consistent with the zero-dimensional

power and burnup modeling, to estimate the increment in radionuclide inventory caused by the criticality event.

Potential critical configurations in the MGR 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 accurately 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 timestep 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) will be used in the averaging process for input parameters to the zero-dimensional models (point reactor kinetics, steady-state power estimations, and incremental radionuclide inventories) 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 Subsection 3.7.1.2 for high enrichment fissile 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 License Application. 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} very 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 MGR 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 MGR 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 1998i, 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 1998i, Table 7.4-8). The steady-state criticality portion of the methodology will additionally incorporate equations for static heat and mass transfer. 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 2 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. The insertion rate distinguishing between these two regimes is often parameterized by the reactivity inserted in excess of a delayed critical state using units ($) that are multiples of the total delayed neutron fraction (ß). The possibilities and consequences for attaining specific reactivity insertion rates that enable either transient regime will be determined by the analyses for License Application.

Both transient and steady-state models will be developed for three general locations where a criticality event may occur: internal to the waste package, external in the near-field (i.e., drift), and external in the far-field. The status of the development of these models is indicated in the following subsections. The models will all be refined by the time of the License Application, so that the region of applicability can be demonstrated.

3.7.2.1 Steady-State Criticality, Internal

The steady-state internal criticality methodology assumes 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 ability 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 just equal to the total (net) water infiltrating into the waste package. If the temperature were to increase beyond this point, the net decrease in moderator would shut down (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 conservatively bounded by the length of the high moisture part of a climatological cycle, which might be as long as 10,000 years (DOE 1998, Vol. 3, p. 3-13). The subsequent return of a moist cycle, upwards of 10,000 years after the shutdown, would be very 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 fissile 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 assuming 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 a point-depletion code with a given initial set of isotopes for a criticality event (or process) of a specified power level and duration. The isotopic concentrations used in the point-depletion code are those which lead to the criticality event. 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 CL 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 for License Application 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 (Subsection 3.7.1.2 and 3.7.3.1).

The following results from steady-state criticality calculations are described as a demonstration of applying the steady-state criticality consequence analysis methodology and are for illustration only. No acceptance is being requested for these example calculations. The examples considered thus far are based on the maximum wet cycle duration of 10,000 years as postulated above. Analysis showed that even a conservatively high flow rate supports a power level of only a few kilowatts (CRWMS M&O 1996b, p. 55 and CRWMS M&O 1999e, p. 27). Under these conditions, the increments in the nuclides important for long term MGR performance (^{99}Tc, ^{129}I, and ^{237}Np) were each less than 5 percent of the pre-criticality amounts of these three nuclides from low enriched uranium SNF (CRWMS M&O 1996b, p. 61) and less than 8 percent from MOX SNF (CRWMS M&O 1999f). The total increment for all the nuclides considered in performance assessment, measured in curies at the time of criticality ending, ranged from 25 to 100 percent for this extreme case. Note that these increments apply to a single waste package and that multiple criticalities, including those initiated by common mode failures, will be considered in application of the methodology. If a more conservative model of the hydrologic environment were developed, the wet cycle duration and/or flow rate would be increased, resulting in a corresponding increase in radionuclide inventory at the end of the criticality. The small radionuclide increments calculated for the nominal case leave a considerable margin for more conservative models of the hydrologic parameters.

3.7.2.2 Transient Criticality, Internal

The transient internal criticality methodology assumes 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. Critical internal configurations without water moderator are unlikely for SNF, which cannot sustain fast criticality. However, configurations allowing fast criticalities will be considered for SNF and other wastes, and will be evaluated if identified as credible. Most cases of relevance will involve water moderation, and the methodology 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 such as, for example, the RELAP5/MOD3.2 code (INEEL [Idaho National Engineering Laboratory] 1995, p. 1-1). 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 Subsection 3.7.3.2.

The transient internal criticality methodology includes both slow and relatively rapid reactivity insertion mechanisms such as described in Subsection 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 mechanism 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 is applicable to configurations having a wide variation in fissile content that primarily affects 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 CL screening process. These may include but are not necessarily be 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 3 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.

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 therefore re-criticality) between the episodic moderator losses (CRWMS M&O 1999e, 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 following results from the transient criticality analyses for commercial PWR SNF (CRWMS M&O 1997g; CRWMS M&O 1999e, Section 6; CRWMS M&O 1999g, Section 6) are qualitatively described to demonstrate the application of the transient criticality consequence analysis methodology and are for illustration only. No acceptance is being requested for these example calculations. These analyses produce a number of direct consequence measures, including the cumulative energy release, incremental radionuclide generation, time history of temperature, reactor power, and neutron flux, but particular emphasis was given to the time history of overpressure and waste package egress mass flow rate. For relatively rapid criticality events, negative thermal reactivity feedback effects in the fuel will halt the power rise but generation of negative void reactivity is necessary to terminate the event. The void reactivity results from pressurizing the waste package and reducing the water moderator inventory through the egress flow rate, which is sensitive to the aggregate package penetration area. The moderator expulsion process continues until criticality cannot be maintained. For relatively slow transient criticality events, the negative fuel temperature and moderator reactivity effects can terminate the criticality event for the full spectrum of penetration areas with only a minor overpressure in the waste package.

The additional analysis for License Application 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 Subsection 3.7.2.4.

3.7.2.3 Steady-State Criticality, External

The external steady-state criticality methodology assumes 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 ability 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, Vol. 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 Subsection 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.

Results from an external steady-state criticality calculation of fissile material deposited in an fracture network (CRWMS M&O 1998g, Section 9) are described as a demonstration of the methodology and are for reference only. No acceptance is being requested for these example calculations. The calculations were based on a conservatively high percolation flux of 50 mm/year that replenished evaporation at a moderate steady power. The neutronic basis for the criticality consequence analysis was a critical configuration of ^{239}Pu in a cubic volume of wet tuff (CRWMS M&O 1998i, Table 7.3-5). Criticality evaluations were performed for several fracture size, water content, and fissile material combinations. Extreme assumptions concerning the accumulation of fissile material and fracture aperture (0.01 cm), and moderate assumptions for water content (~ 10 % by volume) and fracture pitch (3 cm), were required in the model to achieve criticality. The calculated criticality endured for 4,000 years, with the consequence of a terminal radionuclide inventory increment exceeding the inventory that would be present in the absence of criticality by only 14%.

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 for License Application). 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 fissionable material to support autocatalytic criticalities will be evaluated using geochemistry codes such as EQ3/6 (Wolery and Daveler, 1992). 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 designed to calculate the time dependent evolution of nuclear reactivity and fission power for fissile 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 analysis for the License Application will reflect the actual characteristics of the rock (particularly compressibility) that would regulate any mechanical effects of the criticality. The code used in analysis for the License Application 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 calculates 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 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 from a point-depletion code 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 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 nuclide inventory and possible pathway alteration information.

3.7.3 Validation of Criticality Consequence Methodology

Acceptance is sought for the validation approach of the methodology for the steady-state consequence models (equations representing physical material and heat balance processes). Acceptance is sought for the validation process of the methodology for the consequence evaluation of transient criticality events. 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 Methodology Validation Approach

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 Subsections 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. Point depletion codes, such as ORIGEN-S (part of the SCALE package [NRC 1995]) will be used to calculate the radionuclide inventory for a specified exposure history. Burnup and decay calculations in the particular code sequence will be validated by comparing calculated values with results of radiochemical analyses (as, for example, in the ORIGEN-S code qualification, CRWMS M&O 1997f, p. 38). 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 this methodology must be made by 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 methods 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. The particular experiments selected for validation cases will collectively include important parameter ranges for possible critical configurations in the repository. Examples of such experiments include:

1) Steady-state criticalities in solution-fueled systems characterized by moderate fissile material enrichments with homogeneous compositions and fast neutron spectra, such as the Solution High-Energy Burst Assembly (SHEBA, 2nd experimental version) Experiments. Fission power levels in these experiments were predominately regulated by the neutronic consequences of solution voiding.

2) Steady-state criticalities in systems characterized by heterogeneous fuel compositions and thermal neutron spectra, such as the Boiling Reactor (BORAX-I) Experiments. Fission power levels in these experiments were predominately regulated by the moderator boil-off and replenishment rates, analogous to the processes affecting potential steady state criticalities.

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 2000h, pg. 3-33 and Fig. 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 pathways characterizing the interiors of swollen and cracked fuel pellets would limit mass transport to diffusive modes. The relevance of diffusion-limited pinhole releases is explained below and will be demonstrated as part of the steady-state criticality consequence model validation.

The basis for validation of the mass transport part of the consequence methodology is comparison of modeling results with experimental measurements. For conservatism and relevance, experiments identified for validation cases will involve mass releases from commercial SNF with perforated cladding. Aqueous experiments, such as those performed in the Nevada Nuclear Waste Storage Investigations (Wilson 1990) to establish the technical requirements for successful SNF disposal in an MGR, quantify the fractional releases of soluble fission products and actinides from SNF segments with engineered cladding perforations. For SNF segments with perforations of ~200-micro-meter diameter, the experiments indicate that reductions in actinide mass release may exceed a factor of 3000 as compared to situations with unclad fuel. Typical values of the fractional reductions observed for pinhole releases of soluble fission products (Wilson 1990, pp. 3.47 and 3.50) are ~1/44 for Sr and ~1/74 for I. The accuracy or conservatism of assumptions for the following issues will be demonstrated as part of the steady-state criticality consequence model validation:

1) the statistical bases for the distributions of defective cladding inventory, defect size, and spatial density

2) the relative magnitudes of the experimental defect sizes to the actual sizes of defects from reactor operations

3) determinations for (a) the applicability of pinhole release reduction factors that are derived experimentally for high solubility fission products to specific fission products that have potential neutronic significance and that are less soluble (e.g., Rh-103, Nd-143, Sm-149, Eu-153, and Gd-155) or for (b) the applicability of low-mobility assumptions concerning specific low solubility fission products of neutronic significance.

3.7.3.2 Transient Criticality Consequence Methodology Validation Process

The consequence portion of the methodology 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. As an example of the validation process, results from models of appropriate experiments applicable to waste package applications have successfully tracked the measured data (CRWMS M&O 1999i).

A number of transient criticality codes exist that can be adapted for internal waste package criticality analyses. All of the codes receiving consideration couple the neutronic, thermal, and hydraulic phenomena associated with a criticality. One such code, for example, is the RELAP5/MOD3.2 code (INEEL [Idaho National Engineering Laboratory] 1995), utilized here for illustrative purposes. The particular code used for criticality consequence evaluations will have similar or equivalent characteristics.

The RELAP5 computer code is a light water reactor transient analysis code developed by the NRC for use in rulemaking, licensing audit calculations, and evaluation of operator guidelines. A criticality event in a breached but otherwise intact PWR SNF waste package is similar to $k_{eff} > 1$ events in a power reactor and/or other thermal-hydraulic transient events which RELAP5 has been designed to analyze. Typical analysis configurations for RELAP5 include PWR and BWR reactor systems. The SNF waste package systems are modeled with SNF assemblies immersed in a water system that, except for orientation, are similar to typical RELAP5 core analysis configurations. The models provide interaction between energy generation, energy redistribution, and negative feedback to the energy generating mechanism.

The waste package 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 control rods

4) For the PWR waste package, a major portion of the flow during a criticality will be across the assembly pins, rather than along them.

State properties in the RELAP5 code extend to the low pressure and low temperature state conditions, so the code, as used in waste package analyses, is within the range of thermal-hydraulic design conditions.

The principal limitation of codes such as RELAP5 that affects the waste package analyses is that the flow system is primarily one-dimensional. To extend the flow system to cover limited two-dimensional capability, the RELAP cross flow junction model was invoked in the representative waste package analysis. In such situations, momentum flux terms in the mathematical models are normally neglected, because their vectorial characteristics are no longer unidirectional, thereby diminishing any net effect from resultant forces in the flow.

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). Additional multipliers can be included for conservatism as in the example consequence analyses for a PWR SNF waste package. However, as a sensitivity analysis (CRWMS M&O 1999g) has shown, peak pressures in PWR SNF analyses are not very sensitive to the loss coefficient values in the numerical range above approximately 20.

A different type of code is used for analyzing the direct consequences of transient criticalities external to the waste package. The code is an enhancement to a computational framework that was developed and demonstrated for a hypothetical external fissionable material deposit developed for exploratory purposes (Gratton et al. 1997). This code is particularly useful for evaluating the relevance of external configurations exhibiting the autocatalytic effect, should such configurations be identified. As described in Subsection 3.7.2.4,the code simulates the dynamics of coupled physical and nuclear processes for systems composed of fissile material, water, and rock. The model implementation couples transient fission power, non-equilibrium multi-component thermodynamics, and rock-mechanical effects into 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 included in the consequence models. A comprehensive set of internal nuclear reactivity feedback mechanisms that influence the transient power trajectory are quantified for consequence evaluations of transient external criticalities.

The transient criticality consequence methodology 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 methodology will utilize a number of cases to span the various phenomena as well as the expected parameter ranges. Examples of transient experiments and incidents that can be used as validation test cases for the internal criticality consequence methods are as follows:

1) A multi-phase transient hydrodynamic experiment demonstrating choking phenomena in a fixed-aperture relief for pressurized systems with initial no-flow conditions, such as Marviken III Test 24. For this particular test, the vessel contains a region of saturated liquid at ~5MPa, extending for approximately 2 m with the remainder subcooled liquid reaching approximately 32K subcooling at the exit line in the vessel bottom. The experiment simulates a large break and terminates fairly rapidly (at ~ 50 seconds). This type of experiment provides a means of evaluating the influence of uncertainties in the critical mass flux model (for two-phase critical fluxes in the range 2 to 7 $kg/cm^2/s$ – disregarding that choked flow conditions are not phenomena inherent to credible events within the waste package, these critical flux magnitudes bound those applicable to internal criticalities with pressures < 500 kPa). Critical flux variation over a range of liquid subcooling levels is considered experimentally. Additionally, such experiments provide a means of evaluating the impacts of uncertainties in the estimation of phasic mass densities, phasic velocities, and energy fluxes at non-equilibrium conditions.

2) An experiment incorporating the effects of non-condensable gases in transient, multiphase flows in pressurized systems, such as the Loft Test L3-1 Accumulator Blowdown. For this particular test, the accumulator contains low temperature water (~ 305K), pressurized to ~ 4.5 MPa with the non-condensable gas, that is injected into the cold leg of a PWR primary coolant loop (~ 556K). The experiment simulates a small break (~ 2 cm^2 – comparably too small a breach to admit waste package flooding for criticality in less than 1 million years), terminating after ~ 1500 seconds. This type of experiment provides a means of evaluating the impacts of uncertainties for the hydrodynamic and thermodynamic modeling of multiphase conditions involving non-condensable gases at low

temperatures, and at system pressures that are nominally a factor of 10 greater than the peak transient values for internal criticality.

3) An experiment combining the effects of natural circulation flow and convective heat transfer in a confined system, such as the Semi-Scale Natural Circulation Experiment. This type of experiment involves low flow rates (under ~½ kg/s), high fluid pressures (~ 10 MPa) and moderate driving temperature differentials (< 38 °C), especially as steady-state is approached. For this particular test, the power source is held constant while the system approaches steady conditions. The test is repeated at different power levels up to 100 kW and approximates natural convective heat transfer conditions that can accompany evaporative loss at atmospheric pressure during a momentary (< 7 minutes) power plateau for a transient in-package criticality. Therefore, this type of experiment is useful for validation of the heat transfer models employed in the dynamic simulations for internal criticalities where comparable mass circulation rates and temperature gradients are involved. Additionally, this type of experiment provides a means of evaluating the effects of uncertainties in natural circulation computations requiring widespread integration of models.

4) An experiment incorporating the effects of multiphase flow and condensation heat transfer in a pressurized system with initial no-flow conditions, such as the MIT Pressurizer Experiment where local fluid properties vary dynamically from vapor to liquid. This particular experiment consists of cold water (294 K) injected into saturated water at 423 K over a 40 second period and at pressures (> 500 kPa) bounding those likely for in-package criticality. This time period is less than ¼ of the time necessary for termination of a rapid internal criticality transient following a significant nuclear reactivity insertion. This type of experiment provides a means of evaluating the influences of uncertainties in the inter-phase mass and energy exchange, buoyancy induced stratification processes within individual phases, and the evaporation and condensation heat transfer models within experimental temperature ranges that are applicable to internal criticalities.

5) An experiment or incident involving coupled thermodynamic, hydrodynamic, and nuclear processes in a neutronically over-moderated and mechanically confined heterogeneous fuel assembly with low fissile material enrichment, such as the NRX Reactor Incident of December 12, 1952. This particular incident involves an ~20 second power surge caused partially by positive void reactivity effects at low flow rates. The large magnitude of the power peak (~ 100 MW) and brief duration of the power surge for this incident constitute a limiting impulsive energy release analog for internal criticality. This class of experiment provides a means of evaluating the impacts of uncertainties in the power calculation and reactivity effects from fuel temperature and moderator density changes allowing k_{eff} to peak near 1.006. Information from such tests can also assist in validating models for multiphase mass and momentum transfer and evaporative heat transfer processes occurring on ~20 second time scales.

6) An experiment involving coupled thermodynamic, hydrodynamic and neutronic processes in a mechanically confined heterogeneous fuel assembly with high fissile material enrichment, such as the Boiling Reactor (BORAX-I) or Special Power Excursion Reactor Test (SPERT-I, plate assembly) Experiments. This class of

experiment provides a means of assessing the effects of uncertainties on power calculations with peak levels as high as 2 GW and reactivity effects from fuel temperature and moderator density changes in pooled coolant systems with initial reactor periods ranging from 14 to 0.005 seconds and with short (~ 65 micro-second) neutron lifetimes. Experimental information from such tests can also assist in validating the equation of state and models for evaporative heat and mass transfer accompanying rapid reactivity insertions and dynamic coolant pressurizations from atmospheric levels to peak values approaching ~5 atmospheres.

Examples of transient experiments and incidents that can be used as validation test cases for the external criticality consequence methods are as follows:

7) An experiment involving coupled thermodynamic, hydrodynamic, and neutronic processes in unreflected and mechanically unconfined homogeneous fuel assemblies with high fissile material enrichments, such as the Lady Godiva Experiments. This type of experiment provides a means of evaluating the impacts of uncertainties in the coupling between power (peak levels of ~10 GW) and reactivity feedback effects for fast neutron spectra allowing ~7 nanosecond neutron lifetimes and 12 microsecond initial reactor periods. The reactivity feedback effects result from fuel density changes with temperature increases approaching 100 °C in a solid homogenous core. This type of experiment also allows evaluations for couplings among power, the equations of state for the fuel materials, the mechanical strain model, and the typically small fission-to-kinetic energy conversion efficiencies (from 0 to 4 %).

8) An experiment involving coupled thermodynamic, hydrodynamic, and neutronic processes in an unreflected and mechanically confined homogeneous solution fuel assembly with varying fissile enrichment, such as the Solution High-Energy Burst Assembly (SHEBA, 2nd experimental version) and the CRAC Solution-Criticality Experiments. This class of experiment provides a means of evaluating the impacts of uncertainties in the couplings between power and reactivity effects from fuel density, voiding and inventory in homogeneous pool reactors with initial reactor periods ranging from 20 to less than 1 second and peak powers exceeding 500 kW. The range of initial reactor periods for this class of experiments additionally admits variability in the relative magnitudes of couplings among power, fuel material equations of state, strain-rates, and evaporative heat and mass transfer.

9) An experiment or incident involving coupled thermodynamic, hydrodynamic, and neutronic processes in a neutronically over-moderated and mechanically confined heterogeneous fuel assembly with low fissile material enrichment, such as the NRX Reactor Incident of December 12, 1952. This type of experiment provides a means of evaluating uncertainties in the reactivity effects from material phase changes occurring in less than 1 minute and leading to mechanical disassembly of the core. This type of experiment involves instances where as much as ~¼ of the accumulated reactivity inserted during a transient arises from positive reactivity feedback. This category also permits assessments of the influences of uncertainties in couplings among the mechanical strain rate modeling for fuel, moderator, coolant and confining materials and fission-to-kinetic energy conversion efficiencies of less than 0.02 %.

10) An experiment involving coupled thermodynamic, hydrodynamic, and neutronic processes in a mechanically confined heterogeneous fuel assembly with high fissile material enrichment, such as the Boiling Reactor (BORAX-I) or Special Power Excursion Reactor Test (SPERT-I, plate assembly) Experiments. Destructive experiments that involve large initial reactivity insertions (~3.5$), peak power levels above 2 GW, peak core pressures above 200 atmospheres, and steam explosions reveal up to ~20 millisecond separations between the neutronic and thermodynamic responses for the systems. For modeling external criticality situations with rapid transients (~ 15 millisecond power pulse) and temporal lags between nuclear and thermodynamic processes, the experiments assist in establishing quantitative bounds for the influences of uncertainties in mechanical strains, material failure thresholds, and fission-to-kinetic energy conversion efficiencies.

The preceding list of example experiments and incidents is intended to illustrate the steps of a comprehensive validation effort for the transient criticality methodology and does not constitute an exhaustive set of cases that can be used as part of the validation process for the methodology.

3.8 ESTIMATING CRITICALITY RISK

The risk of criticality is ultimately measured by the increase in dose at the accessible environment, which is computed as part of TSPA. The incorporation of criticality risk into the TSPA process is described in the following subsections.

3.8.1 Criticality Risk Methodology

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, per se, is the subject of other documents. The principal document in this regard will be the TSPA Model Document (CRWMS M&O 2000f). Increased radionuclide inventory potentially increases the dose at the accessible environment. This section presents the portion of the methodology for estimating the potential increased dose at the accessible environment and the portion of the methodology for incorporating the result into the total system performance assessment and using it for design guidance. The TSPA calculates a dose at the accessible environment for comparison with regulatory standards to be specified by the EPA.
The risk associated with repository criticality is the product of the probability of criticality occurrence multiplied by the criticality consequence and summed over all credible criticality event categories (or probability-consequence pairs). In practice, the consequence will be measured by a parameter with significant health impact, such as radiation dose to the nearby population. Radiation doses will be estimated as part of TSPA, and will use, as primary input, the increased radionuclide inventory. If the mechanical effects of the criticality (e.g., elevated temperature for the duration of a stead-state criticality, or peak pressure pulse from a transient criticality) are significant, they will be reflected in the TSPA by modifying the degradation characteristics of the effected barriers.

Prior to completing the method described below, the features, events, and processes (FEPs) associated with criticality will be evaluated. The initial documentation of this effort is in The

Development of Information Catalogued in Revision 00 of the YMP Database (CRWMS M&O 2000e).

The dose increments will be calculated using the TSPA radionuclide mobilization and transport methodology, for the total expected radionuclide increment (from the sum over the probability-consequence pairs). Consistency with the current TSPA will be ensured by using the same calculations in both the TSPA and the criticality evaluation wherever there is a corresponding configuration. If these dose increments are determined to be insignificant (e.g., compared with the doses expected from the commercial SNF without a criticality event, and where significance is specified in the appropriate TSPA documents), no additional TSPA will be conducted. If the dose increments are determined to be potentially significant, the consequence will be evaluated as necessary at three locations: (1) within the failed waste package, (2) outside the waste package in the near-field, and (3) outside the waste package in the far-field.

The approach to evaluating the potentially significant consequence for each of these locations is the same. The initial step takes as input the previously defined potential criticality events, associated increments to the inventory of radionuclides, and the thermal effect from the criticality events (temperature at the source as a function of time). Then, the thermal effects are used to determine timing of the return of ambient groundwater flow conditions (if the event causes the removal of ambient groundwater) in the vicinity of the criticality. This serves to define the time when water can begin flowing back through the radionuclide inventory, now augmented by radionuclides produced by the criticality, if the region has been dried out by the extra heat from the criticality. Next, the waste form alteration and dissolution models are used to estimate the release rate of radionuclides from the location at which the criticality occurred. These models will provide the release rate caused by leaching, by the groundwater flow, of the inventory produced by the criticality. Finally, the criticality-produced source term is used in a TSPA model to evaluate the dose history at the accessible environment and other locations as required by regulations.

The approach to evaluating the potentially significant consequences applies to both the internal and external environments. The approach begins with the estimation of the increment in radionuclide inventory according to the steady state consequence methodology. Next, the geochemical models (specified in the TSPA documents) are used to estimate the release rate of radionuclides from the location at which the criticality occurred, due to leaching of the inventory by the groundwater flow (i.e., develop the source term for the inventory produced by the criticality).

Finally, the source term and the radionuclide inventory are used in a TSPA model to evaluate the dose history at the accessible environment and other locations as required by regulations. The TSPA model tracks radionuclides as they are leached from the inventory and transported through the unsaturated and the saturated zones (above and below the water table, respectively), and provides the concentration of radionuclides in groundwater at the accessible environment. For criticalities that occur within a failed waste package, or in the near-field, the source term is located in the unsaturated zone; for those occurring in the far-field, the source term is likely to be located in the saturated zone. The concentrations of radionuclides are decreased as they move over the transport pathway from the source to the accessible environment by processes such as retardation, dispersion, and dilution. Radioactive decay may either reduce or increase the concentration of a particular radionuclide over the transport path (the increase being produced by ingrowth of daughter products). It is assumed that at the accessible environment, a person uses the groundwater for drinking, or for both drinking and food production. The

radionuclide concentration at the accessible environment is converted to dose using a conversion factor that is derived using a dose model and a water use scenario (sources for drinking and agricultural use).

The performance assessment model used to evaluate the dose at the accessible environment can track several inventories simultaneously (e.g., commercial SNF, DOE SNF; immobilized plutonium; vitrified HLW; and the added increment from the location of a criticality). This capability allows the dose attributed to the criticality alone to be evaluated separately from that coming from the entire repository. Comparing these two doses then allows the investigator to determine the significance of the criticality event in terms of total dose at the accessible environment. The performance assessment model can also include a distribution of criticality events in time and space to evaluate the long-term effects that multiple cyclic events have on the total dose at the accessible environment.

3.8.2 Total System Performance Models (Risk Models)

This section describes the application of the current M&O performance assessment models to estimate the consequences of a criticality in the repository. The current versions of these models are described in detail in the TSPA-SR document (CRWMS M&O 2000g). Some, or all, of these models may be upgraded for License Application. Any implementation of the disposal criticality analysis methodology for License Application will utilize the most appropriate, OCRWM QA qualified versions of the performance assessment models and codes.

If the initial performance assessment evaluation indicates the need to conduct detailed TSPA calculations using the incremented radionuclide inventory, several models are required. Prior to using a TSPA model, the source term from the criticality event (i.e., the rate of release of radionuclides over time from the vicinity of the criticality) will be determined. This will be to evaluate the solubility and alteration of the inventory produced by the criticality event. The EQ3/6 code package is used to evaluate geochemical models of the criticality produced inventories. The result will be an estimate of the dissolved concentrations of radionuclides. The release rate over time as a function of groundwater flow and temperature, and the total inventory of radionuclides are then used in the TSPA model. If the mechanical effects of the criticality are estimated to have caused significant damage to any of the waste package barriers (including the fuel cladding), the effected parameters of the code will be modified accordingly. In cases where the conservative end of the parameter range must be applied, that conservatism will be judged with respect to the occurrence of criticality and its consequences.

Because of the variability and uncertainty in model input parameters, TSPA analyses will calculate numerous realizations of the processes comprising the scenarios important to repository performance. These calculations will provide a statistical representation of the effects of the variability and uncertainty.

The approach used in TSPA-SR (CRWMS M&O 2000g) for the potential radioactive waste repository makes use of the computer program GoldSim in conjunction with detailed process-level models. The methodology for this report will use the same codes. The GoldSim code and the detailed process models are described in documents for TSPA-SR (CRWMS M&O 2000g). The GoldSim code was specifically developed by Golder Associates Inc. (Golder Associates 2000). Its precursor, RIP was developed to evaluate the performance of a potential radioactive waste disposal facility at Yucca Mountain (Miller et al. 1992) and has subsequently been

applied to a wide variety of proposed radioactive waste disposal facilities both in the U.S. and abroad.

The major features of the four component models of GoldSim that comprise the performance assessment model are (1) waste package behavior and radionuclide release component model, (2) radionuclide transport pathways component model, (3) disruptive events model (which may include criticality), and (4) biosphere dose/risk model. The information flow between these models is indicated in Figure 3-10, and they are summarized briefly below. For evaluation of the consequences of a criticality event the waste package component model could be modified or replaced by the source term for the criticality event that is supplied to the TSPA.

The waste package behavior and radionuclide release component model input requirements are descriptions of the radionuclide inventories in the waste packages, a description of near-field environmental conditions (which may be defined as temporally and spatially variable), and subjective estimates of high-level parameters describing container failure, matrix alteration and dissolution, and radionuclide mass transfer. The waste package component model can simulate two layers of containment (e.g., waste package shell and fuel Zircaloy cladding). Waste package failure rates, along with matrix alteration and dissolution rates, are used to compute the rate at which radionuclides are exposed. Once the radionuclides are exposed, GoldSim computes the rate of mass transfer out of, and away from, the waste radionuclides. Exposure and mass transfer can be functions of near-field environmental conditions. The output from this component model (for each system realization) consists of time histories of release for each radionuclide from the waste packages (or from the vicinity of a criticality event), and acts as the input for the transport pathways component.

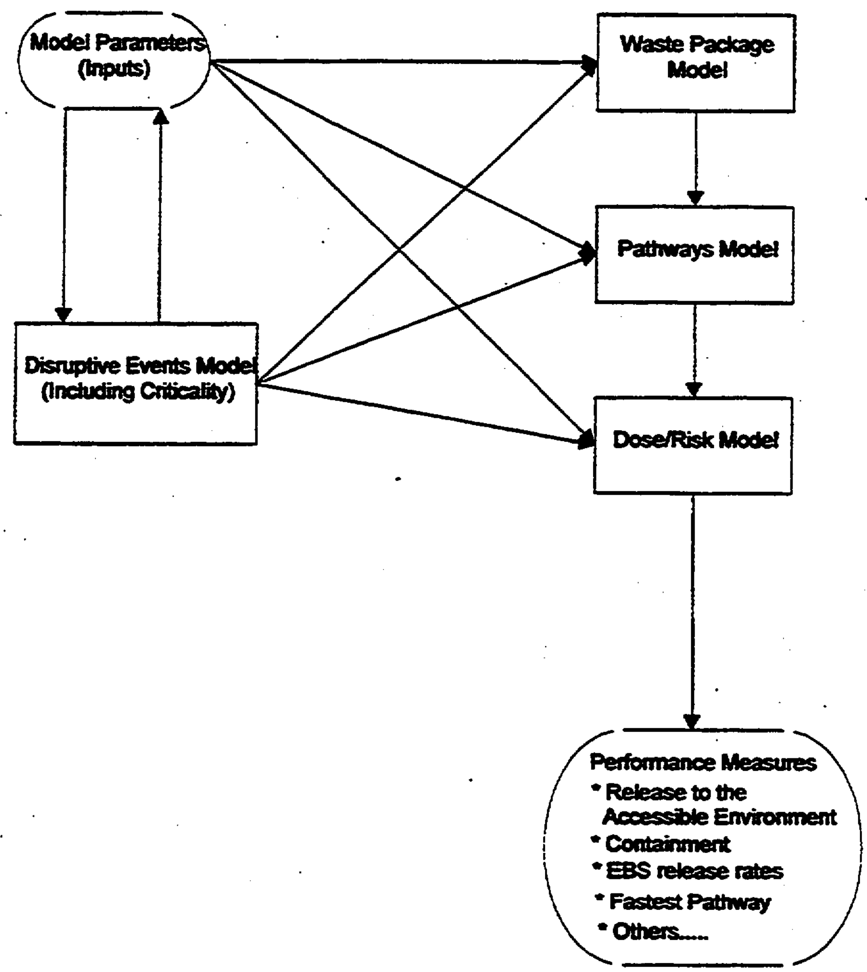


Figure 3-10. Components of GoldSim that are Used for Total System Performance Assessment

Geosphere pathways may be subdivided into flow modes, which address heterogeneity at the local scale. The radionuclide transport pathways component model simulates radionuclide transport through the near and far field in a probabilistic mode. The GoldSim model uses a phenomenological approach that attempts to describe rather than explain the transport system. The resulting transport algorithm is based on a network of user defined pathways. The geosphere and biocell pathways reflect the major features of the hydrologic system and the biosphere, and are conduits through which transport occurs. The pathways may be used for both flow balance and radionuclide transport purposes, and may account for either gas or liquid transport. The purpose of a pathway is to represent large-scale heterogeneity of the hydrologic system, such as geologic structures and formation-scale hydro stratigraphy (e.g., flow in rock matrix, flow in fractures). The flow modes are primarily distinguished from one another based on flow velocity, although retardation parameters may also differ between flow modes.

The transport of radionuclides along a geosphere pathway is based on a breakthrough curve, which is calculated as a cumulative probability distribution for radionuclide travel times along the pathway. The breakthrough curve combines the effects of all flow modes and retardation on the radionuclide travel time, and determines the expected proportion of mass that has traversed the pathway by any specified time. The breakthrough curve is computed based on a random process algorithm for back and forth exchange between different flow modes. For TSPA-SR, the UZ and saturated zone (SZ) transport is being simulated using the groundwater code FEHM (Zyvoloski et al. 1995).

The third performance assessment component model represents disruptive events. Disruptive events are defined as discrete occurrences that have some quantifiable effect on the processes described by the other two component models. Examples of disruptive events include volcanism, faulting, transient criticality and human intrusion. The user first identifies all significant events (i.e., events that are both credible and consequential). Having done so, each event is assigned a rate of occurrence and, if desired, one or more descriptor parameters, which define the characteristics and magnitude of the event. Descriptor parameters may be represented stochastically. Event occurrences are simulated as Poisson processes.

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

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

In summary, it should be noted that criticality may effect the performance assessment evaluations in two of the component models: waste package (where it may provide a radionuclide increment) and disruptive events (where it may effect subsequent repository hydrothermal behavior).

3.8.3 Criticality Risk Validation Approach

The incorporation of criticality probability and consequences into a total risk calculation will be described and validated in the TSPA Model Document (CRWMS M&O 2000f) and will be consistent with treatment in the TSPA of risks posed by other phenomena.

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4. SUMMARY AND CONCLUSIONS

The proposed methodology for performing criticality analyses for waste forms for long-term disposal in the potential monitored geologic repository at Yucca Mountain is presented in this report. The methodology presented is a risk-informed, performance-based methodology, which treats criticality as one of the processes or events that must be considered for the overall performance assessment. The methodology, 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, waste package /engineered barrier system designs, 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. The configurations 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. Criticality evaluations are then performed for configurations at various parameter values for the range of parameters characterizing each configuration class. Classes that show any potential for criticality are evaluated further. A table of k_{eff} values is constructed as a function of parameters that affect criticality for each configuration class. Regression expressions are developed that cover the range of parameter values where the peak k_{eff} may exceed the critical limit (CL) criterion. The CL is the value of k_{eff} at which the configuration of fissionable materials is considered potentially critical as characterized by statistical tolerance limits. The probability of exceeding the CL is estimated for each class as a function of the characteristics of the waste stream (i.e., by looking at the characteristics of the waste stream against the parameter ranges for the configurations in each class). Additional design features for reducing k_{eff} are implemented for those configurations that exceed the probability criterion. The CL and probability criteria form design criteria for limiting the potential for criticality in the repository for postclosure. The probability criterion is used to identify configurations that have a significant probability of exceeding the CL, thereby increasing criticality risk. For such identified configurations, 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 probability criterion is satisfied. 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 are provided as input for the TSPA. The TSPA determines if the risk to the health and safety of the public is acceptable, as stated in the repository performance objectives criterion. If this criterion is not satisfied, implementation of additional design features for reducing k_{eff} are required.

Although guidance documents from the NRC and various applicable industry standards (NUREGS, Regulatory Guides, and ANSI standards) have been used in developing the methodology presented in this report, none of the guidance documents or industry standards were written to specifically address disposal in a geologic repository. However, the proposed 10 CFR 63 was developed specifically for the potential repository at Yucca Mountain, Nevada. The methodology presented in this report starts with the guidance documents and industry standards discussed in Chapter 2 and extends their applicability to disposal while following the guidance of the proposed 10 CFR 63. It is concluded that the methodology presented in this report is fully compliant with the proposed 10 CFR 63.

For intact naval fuel, any processes, criteria, codes, or methods different from the ones presented in this report are described in a separate addendum (Mowbray 1999). This addendum employs the principles of the methodology described in this report as a foundation. Departures from the specifics of the methodology presented in this report are described in the addendum.

Aspects of the methodology for which NRC acceptance is sought are presented in Section 1.2 and repeated below. It is concluded that sufficient information is provided in this report to support this acceptance.

A. The following design 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 consequences of, criticality:

   1. The *Critical Limit (CL)* criterion discussed in Subsection 3.2.1: The calculated effective neutron multiplication factor (k_{eff}) for subcritical systems (configurations) for postclosure will be less than the CL. The CL is the value of k_{eff} at which the system is considered potentially critical as characterized by statistical tolerance limits.

   2. The *Design Probability* criterion discussed in Subsection 3.2.2: The average criticality frequency will be less than 10^{-4} per year for the entire repository for the first 10,000 years for all combinations of waste packages and waste forms. This criterion is intended to ensure that the expected number of criticalities is less than one during the regulatory life of the repository (10,000 years). It is used to define a waste package criticality control design requirement in support of defense-in-depth with respect to the Repository Criticality Performance Objective in item 3.

   3. The Repository *Performance Objectives* criterion discussed in Subsection 3.2.3: The ability to satisfy dose rate performance objectives will not be compromised by the radionuclide increment due to criticality events (if any).

B. The Master Scenario List (CRWMS M&O 1997d, pp. 13-45) presented in Section 3.3, and summarized in Figures 3-2a, 3-2b, 3-3a, and 3-3b, comprehensively identifies degradation scenarios based on features, events, and processes associated with the potential repository at Yucca Mountain that may significantly affect the potential for, and consequences of, criticality.

C. The portion of 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. Specifically, the 14 methodology steps specified for internal configurations in Subsection 3.4.1.1 and the five methodology steps specified for external configurations in Subsection 3.4.2.1 are acceptable as comprehensive.

D. The portion of the methodology for performing criticality evaluations of postclosure configurations and using critical limits discussed in Section 3.5 is acceptable in general for disposal criticality analysis.

E. The methodology for estimating the probability of postclosure critical configurations and using multivariate regressions, or table lookup and interpolation discussed in Section 3.6 is acceptable in general for disposal criticality analysis.

F. The portion of the methodology for estimating consequence of postclosure criticality events discussed in Section 3.7 is acceptable in general for disposal criticality analysis.

G. The validation approach for the isotopic, criticality, and regression models are acceptable in general for model validation. Specifically:

1. The isotopic model validation process described in Subsection 3.5.3.1 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 CL values for postclosure repository conditions will be demonstrated in validation reports, which will be referenced in the License Application. NRC acceptance of isotopic bias values for k_{eff} and their applicability for postclosure repository conditions will be sought in the License Application.

2. The criticality model validation process described in Subsection 3.5.3.2 is acceptable in general for model validation. Specifically, the process presented for calculating the CL values and the process presented for establishing the range of applicability of the CL values define the validation process for the criticality model. This validation process will be followed to calculate CL values for specific waste forms and waste packages as a function of degradation conditions. The applicability of the CL values for postclosure repository conditions will be demonstrated in validation reports, which will be referenced in the License Application. NRC acceptance of CL values and their applicability for postclosure repository conditions will be sought in the License Application.

3. The validation process for the regression analysis model for k_{eff} described in Subsection 3.5.3.3 is acceptable in general for model validation. The applicability of k_{eff} values obtained from the regression model for postclosure repository conditions will be demonstrated in validation reports, which will be referenced in the License Application. NRC acceptance of k_{eff} values obtained from the regression model and their applicability for postclosure repository conditions will be sought in the License Application.

H. The validation process for the degradation analysis portion of the methodology presented in Subsections 3.4.1.3 and 3.4.3.1 for calculating the concentrations of components in solution inside the waste package and waste-package component degradation products is acceptable in general for model validation. Specifically:

1. Validation of the models for geochemical degradation of waste package components (leading to potentially critical configurations within the waste package) is by benchmark comparisons with a set of experiments covering both fixed volume and flow-through conditions.

2. Validation of the models for external accumulation of fissionable material (leading to potentially critical configurations external to the waste package) is by benchmark comparison with precipitation of minerals in laboratory experiments having chemical conditions representative of the repository.

I. The validation process for the probability calculation and configuration generator models described in Subsection 3.6.4 is acceptable in general for model validation. Specifically,

the computer code that implements the Monte Carlo probability calculation portion of the methodology is validated by comparison with the hand calculation of combinations of probabilities of individual events taken from distributions similar to those used for the Monte Carlo selection process.

J. The validation process for the criticality consequence models presented in Subsection 3.7.3 is acceptable in general for model validation. Specifically:

1. The range of parameters, permitting selection of the most conservative, demonstrates the acceptability of the criticality consequence models for internal and external criticality and for transient as well as steady-state criticality.

2. Verification of the individual models implementing the basic physical processes by hand calculation, where appropriate.

K. The proposed requirements presented in Subsection 3.5.3.1.2 for modeling burnup of commercial SNF for design applications are sufficient, if met, 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 validation reports, which will be referenced in the License Application. NRC acceptance of the confirmation of the conservatism in the application model for postclosure repository conditions will be sought in the License Application.

L. The principal isotopes selected to model burnup in intact commercial SNF, presented in Table 3-3 in Subsection 3.5.2.1.1, are acceptable for disposal criticality analysis provided that:

1. The bias in k_{eff} associated with predicting the isotopic concentrations is established in the validation reports as described in Subsection 3.5.3.1.

2. Deviations from the predicted concentrations because of radionuclide migration from intact fuel assemblies through pinholes and cracks in the cladding are addressed in the geochemical analysis.

The k_{eff} values from criticality evaluations of intact commercial SNF with pinholes and cracks 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. The applicability of the principal isotopes for intact commercial SNF will be demonstrated in validation reports, which will be referenced in the License Application.

M. The process for selecting isotopes from the list of principal isotopes for degraded commercial SNF presented in Subsection 3.5.2.1.4 is also 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 validation reports, which will be referenced in the License Application. NRC acceptance of the application of the selected isotopes to postclosure repository conditions will be sought in the License Application.

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APPENDIX A

ACRONYMS AND ABBREVIATIONS

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APPENDIX A

ACRONYMS AND ABBREVIATIONS

ANS	American Nuclear Society
ANSI	American National Standards Institute, Inc.
B-SS	Borated Stainless Steel
BWR	Boiling Water Reactor
°C	Degrees Celsius
CDF	Cumulative Distribution Function, for a probability distribution
CFR	Code of Federal Regulations
CGC	Configuration Generator Code
CL	Critical Limit
CR	Contract Report
CRC	Commercial Reactor Critical
CRWMS	Civilian Radioactive Waste Management System
df	Variable in an equation, number of degrees of freedom
DFTL	Distribution Free Tolerance Limit
DOE	U.S. Department of Energy
EBS	Engineered Barrier System or Segment
EPA	U.S. Environmental Protection Agency
FEP	Features, Events, and Processes
FF	Far-field
FM	Fissionable Materials
FR	Federal Register
FWF	Fissionable Waste Form
GWd/mtU	Gigawatt-Day per Metric Ton of Uranium
HLW	High-level Waste
IP	In-package
J-13	The designation of a well on Yucca Mountain
k_{eff}	Effective neutron multiplication factor
LCE	Laboratory Critical Experiment
LLNL	Lawrence Livermore National Laboratory
LUTB	Lower Uniform Tolerance Band
LWR	Light Water Reactor

M&O	Management and Operating Contractor
MGR	Monitored Geologic Repository
MOX	Mixed Oxide
mSv	milli-Seiverts
mtU	Metric Tons of Uranium
NDTL	Normal Distribution Tolerance Limits
NF	Near-field
NRC	U.S. Nuclear Regulatory Commission
NUREG	Designator for an NRC Document
OCRWM	Office of Civilian Radioactive Waste Management
OIC	Other Internal Components of the waste package (not SNF)
P	Variable in an equation, proportion of the population covered
PA	Performance Assessment
pdf	Probability Density Function
PMR	Process Model Report
PRA	Probabilistic Risk Assessment
PWR	Pressurized Water Reactor
QA	Quality Assurance
QARD	Quality Assurance Requirements and Description
RCA	Radiochemical Assay
REV	Revision of a document
ROA	Range of Applicability
ROP	Range of Parameters
SER	Safety Evaluation Report
SNF	Spent Nuclear Fuel
SZ	Saturated-Zone
TDSS	Assumption identifier, Technical Data Subsurface
TSbv	Topopah Springs basal vitrophyre
TSPA	Total System Performance Assessment
UCRL	University of California Research Laboratory
UZ	Unsaturated-Zone
VA	Viability Assessment
WP	Waste Package
WF	Waste Form
wt%	Weight Percent
YMP	Yucca Mountain Site Characterization Project

Symbols

β	Bias or the reciprocal of the time duration over which there is a significant probability of criticality occurrence
Δ	Change in
df	Number of degrees of freedom
Eh	Negative of the common logarithm of the electron chemical activity of electron in solution, multiplied by 2.303RT/F, where R is the molal 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
T	A random variable in the probability density function
τ	Time, primarily as variable of integration ($d\tau$)
W	(Wilkes-Shapiro) normality test for data sets of fewer than 50 observations

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APPENDIX B

GLOSSARY

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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 (10 CFR 60.2).

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.

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

Aperture is the opening (distance) between fracture walls.

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 is any material or structure that prevents or substantially delays movement of water or radionuclides (10 CFR 60.2).

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. Burnup credit is one of the licensing issues which will be addressed in the Topical Reports submitted to the U.S. Nuclear Regulatory Commission. For geologic disposal, burnup credit (if accepted by the NRC) will account for the

reduction in reactivity associated with 29 isotopes (Principal Isotopes) from commercial light water reactor spent nuclear fuel. This credit applies specifically to the ceramic form of commercial spent nuclear form.

Canister is 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 HLW, 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 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^{-6} that are suspended in a solvent. Colloids that are transported in groundwater can be filtered out of the water in small pore spaces or very 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 is the confinement of radioactive waste within a designated boundary (10 CFR 60.2).

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.

Cumulative distribution function (CDF) is a function that gives the probability that a random variable (representing some physical parameter) is less than the value of the argument of the function.

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 is the isolation of radioactive wastes from the accessible environment (10 CFR 60.2). Disposal means the emplacement in a repository of high-level radioactive waste, spent nuclear fuel, or other highly radioactive material with no foreseeable intent of recovery, whether or not such emplacement permits the recovery of such waste (10 CFR 961.11) Nuclear Waste Policy Amendment (NWPA 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 (EBS) is the waste packages and the underground facility (10 CFR 60.2).

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

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

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

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

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

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

High-level radioactive waste (HLW) means (1) the highly radioactive material resulting from the reprocessing of spent nuclear fuel, including liquid waste produced directly in reprocessing and any solid material derived from such liquid waste that contains fission products in sufficient concentrations; and (2) other highly radioactive material that the U.S. Nuclear Regulatory Commission, consistent with existing law, determines by rule requires permanent isolation. The CRWMS will only accept solidified HLW. For the purposes of this document, HLW is vitrified borosilicate glass cast in a stainless steel canister (NWPA Section 2[12] 1987) (10 CFR 72.3) (10 CFR 960.2) (10 CFR 961.11).

Hydration is the adding of 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.

Intact fuel. See Spent nuclear fuel.

Invert is the level bottom placed in the drifts.

Isolation is inhibiting the transport of radioactive material so that amounts and concentrations of this material entering the accessible environment will be kept within prescribed limits (10 CFR 60.2).

J-13 is the designation of a well on Yucca Mountain from which water has been taken. The water is assumed to be 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).

Methodology as used in this document methodology refers to the systematic procedures 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. For purposes of the disposal criticality analysis methodology, near-field is the volume inside an emplacement drift, excluding the interior of the waste package.

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 is final backfilling of the underground facility and the sealing of shafts and boreholes (10 CFR 60.2). **Note:** A decision on backfilling the emplacement drifts has not been finalized at this time.

Plume, for this document, is the envelope of groundwater paths 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 in the configuration generator code to represent any localized combination of water solution and solid material that can be subject to analysis by a geochemistry code (e.g., EQ3/6 or PHREEQC).

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 (pdf) 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 is HLW and other radioactive materials other than HLW that are received for emplacement in a geologic repository (10 CFR 60.2).

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 (NWPA 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 path.

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. (Specifically in this

document, SNF includes (1) intact, non-defective fuel assemblies; (2) failed fuel assemblies in canisters; (3) fuel assemblies in canisters; (4) consolidated fuel rods in canisters; (5) non-fuel assembly hardware inserted in PWR fuel assemblies, including, but not limited to, control rod assemblies, burnable poison assemblies, thimble plug assemblies, neutron source assemblies, instrumentation assemblies; (6) fuel channels attached to boiling water reactor fuel assemblies; and (7) non-fuel assembly hardware and structural parts of assemblies resulting from consolidation in canisters.) (NWPA Section 2(23)) (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).
>
> **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 ranges from intact fragments of partially degraded waste forms/fuel to elements in solution to 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 is stable or maintained over a long period of time as nearly time-independent.

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 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 is the underground structure, including openings and backfill materials, but excluding shafts, boreholes, and their seals (10 CFR 60.2).

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 is the radioactive waste materials and any encapsulating or stabilizing matrix (10 CFR 60.2). 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 60.2).

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

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

Crosswalk for SER Open Item in Revision 01 of the Topical Report

Open Item	Location in Topical Report Revision 01
#1. The staff believes that burnups of spent fuel assemblies must be verified through measurements before their loading into the waste packages for the purpose of burnup credit verification.	Section 2.3.2 (8th paragraph) and 2.3.3 (2nd paragraph), p. 2-9 (This item is planned to be addressed in a Preclosure Report)
#2. The consequence criteria for transient and external criticalities are not addressed in the TR. The DOE must specify if it intends to perform full consequence analyses for transient and external criticality events and include them in TSPA or use some type of criteria for the purpose of criticality control design selection.	The Consequence Criteria has been removed from the methodology. This is shown in Figure 3-1 and discussed in Sections 3.1 (9th paragraph), p.3-4. No screening is performed based on consequences, all criticality consequences are considered in the TSPA evaluation, as discussed in Section 3.8.
#3. The DOE needs to provide modeling approach for igneous-activity induced criticality.	Section 3.3.4, p. 3-18 and p. 3-19
#4. The DOE must include the effects of radionuclide migration from an intact fuel assembly though pin-holes and cracks in the cladding.	Section 3.5.1.1 (4th paragraph) p. 3-31; Section 3.5.2.1.1 (3rd & 4th paragraph) p. 3-35; Section 3.5.2.1.4 (2nd & 3rd paragraph) p. 3-38
#5. The DOE must include a criticality margin when comparing k_{eff} values from regression analyses to CL values.	Section 2.3.2 (8th paragraph) pp. 2-8 & 2-9 and Figure 3-5 in Section 3.5.1.3
#6. The DOE must present an approach for developing the criticality margin	Section 3.5.3.2.3 (1st paragraph) p. 3-48 Other sections where is is addressed include: Section 3.5.1.2 (3rd paragraph) p. 3-32, Section 3.5.2.1.3 (4th paragraph) p. 3-38, Section 3.5.3.2 (4th & 5th paragraph) p. 3-45, and Section 3.5.3.2.5 (5th paragraph) p. 3-50
#7. The DOE must demonstrate the adequacy of using one-dimensional calculations to capture three-dimensional neutron spectrum effect in their point-depletion calculation or use two/three dimensional calculations for determining the neutron spectra during the depletion cycles to be used in the depletion analyses.	Section 3.5.2.1.2 (4th & 5th paragraph) p. 3-36 . Section 3.5.3.1.1 (5th – 7th paragraph) p. 3-42 and p. 3-43
#8. The DOE needs to use the cross section data corresponding to the temperature for the waste package or critical benchmarks.	Section 3.5.2.2 (3rd paragraph) p. 3-39
#9. The DOE must include the cross dependency of configuration parameters for k_{eff} regression equations.	Section 3.5.3.2.7 (5th paragraph) p 3-55, Section 3.5.3.3 (2nd paragraph) p. 3-58, Section 3.6.1 (7th paragraph) p. 3-61
#10. The DOE must provide the technical basis for the correction factors developed for boron remaining in the solution.	Section 3.4.1.1 (1st list, item 6) p. 3-21
#11. The DOE is required to develop an acceptable methodology for establishing uncertainties for isotopic depletion model.	Section 3.5.3.1.1 (2nd & 3rd paragraph) p. 3-42
#12. The DOE needs to establishing the bias and the associated uncertainty on the analysis or model keeping track of isotopic inventory loss -through cracks or pin-holes from intact spent fuel assemblies.	Section 3.5.3.1.1 (2nd & 4th paragraph) p. 3-41
#13. The DOE should address the types of criticality uncertainties and biases, which is based on ANSI/ANS-8.17, presented by the staff in this SER.	Sections 3.5.3.2.5-3.5.3.2.10, pp. 3-50 – 3-58

Enclosure 2

Crosswalk for SER Open Item in Revision 01 of the Topical Report

Open Item	Location in Topical Report Revision 01
#14. The DOE must include a multi-parameter approach in its bias trending analysis.	Section 3.5.3.2.7., (6th paragraph) p.3-55.
#15. The DOE is required to include the isotopic bias and uncertainties as part of delta k_c if not included as isotopic correction factors.	Section 3.5.3.2.10 (Eqn 3-7) p. 3-58
#16. DOE must present a model validation methodology or work scope for external criticality models.	Section 3.5.3.2 (2nd paragraph) p. 3-44
#17. The DOE should subject the method used for extending the trend to the procedures defined in ANSI/ANS-8.1-1998, C4(a) and C4(b).	Section 3.5.3.2.3 (3rd paragraph) p. 3-49
#18. The DOE must verify the regression equation or look-up table for all ranges of configuration and waste form parameters affecting k_{eff}.	Section 3.5.3.3 (all) p. 3-58 and p. 3-59
#19. The DOE is required to include all uncertainties and variabilities introduced by the regression equation or the look-up table.	Section 3.5.3.3 (all) p. 3-58 and p. 3-59
#20. In developing the methodology for steady-state criticality consequences, the DOE must consider other types of moderators, especially with respect to external criticality.	Section 3.7.2 (2nd paragraph) p. 3-76
#21. The DOE must also consider the loss of soluble neutron absorbing isotopes through pinholes and cracks in the spent fuel cladding, and its effect on steady-state criticality consequence.	3.7.3.1 (5th paragraph) p. 3-85
#22. The DOE must also include other types of steady-state criticality consequences, especially with respect to internal criticality, in its consequence analysis approach.	Section 3.7.1 (1st paragraph) p. 3-73, Section 3.7.1.1 (4th paragraph) p. 3-74, Section 3.7.1.2 (3rd paragraph) p. 3-75, and Section 3.7.2 (2nd & 3rd paragraph) p. 3-76
#23. The DOE needs to develop, and present for acceptance, the modeling approach for an external steady-state criticality consequence.	Section 3.7.2.3 (all) p. 3-81
#24. The DOE must develop and present request for approval of a methodology for transient criticality consequence.	Section 3.7.3 (all) p. 3-84
#25. The DOE needs to develop and present, for NRC acceptance, the modeling approach for transient criticality consequence.	Section 3.7.3.2 (3rd paragraph) p. 3-86
#26. The DOE needs to develop a validation approach for the power model for steady-state criticality consequence.	Section 3.7.2.1 (1st paragraph) p. 3-77, Section 3.7.2.3 (2nd paragraph) p. 3-81, and Section 3.7.3.1 (2nd paragraph) p. 3-84
#27. The DOE is required to develop a validation approach for a transient criticality consequence model.	Section 3.7.3.2 p. 3-86
#28. The DOE should describe the interface between Figure 1-1 of the RAI responses and the TSPA criticality risk analysis.	Section 3.8.1 p. 3-91 and Section 3.8.2 p. 3-93

Crosswalk for RAI Actions Items for Inclusion in Topical Report Revision 01

RAI Action Items	Location in Topical Report Revision 01
1-1 The last two sentences in the footnote at the bottom of page 1-1 will be removed in a revision of the Topical Report	Chapter 1 (Footnote), p. 1-1 Sentences were removed from footnote in Rev. 1 of the Topical Report.
1-2 DOE plans to add the feed of all criticality consequence results to the overall TSPA when the Topical Report is revised. DOE plans to address multiple, or common mode, criticalities	Section 3.1, p. 3-2 The feed of all criticality consequence results to the overall TSPA is provided in Figure 3-1 of Rev. 1 of the Topical Report. Section 2.2.2, Section 3.6.2 (item 3), and Section 3.7.2.1
1-3 Revise item G, Section 1.2 of the Topical Report for clarification.	Section 1.2, p. 1-4 and 1-5 Item G, Section 1.2 was revised to include validation approach for the isotopic, criticality, and regression models.
1-4 None – Discussion of range of configurations	Section 3.5.1.1 (4th paragraph) p. 3-31;
1-5 Examples and waste-form specific items will either be removed or more clearly labeled in the revision to the Topical Report.	Clarifications were made throughout Rev. 1 of the Topical Report so that the scope in Section 1.3 is consistent with the remainder of the report.
1-6 RAI requested clarification of a statement in Section 1.4 of the Topical Report with respect to Quality Assurance.	Section 1.4 p. 1-7 and 1-8
1-7 Remove reference to the "Topical Report on Actinide-Only Burnup Credit for PWR Spent Nuclear Fuel Packages (DOE 1997).	Reference removed in Rev. 1 of the Topical Report.
1-8 The box in Figure 1-1 discussed in this RAI will be modified to read: "Perform Criticality Analysis (k_{eff}) of Defined Configurations (for each Class) Over the Range of Parameters and Parameter Values."	The changes specified were made to Figure 3-1 (Note: Section 1.5 OVERVIEW OF METHODOLOGY was moved to Section 3.1 in Rev. 1 of the Topical Report– thus, Figure 1-1 from Rev. 0 becomes Figure 3-1 in Rev. 1)
2-1 Replace references to Regulatory Guides 3.4 and 3.58 with reference to Regulatory Guide 3.71	Section 2.3.3 (1st paragraph) p 2-9
3-1 Will add section on seismic and volcanic disruptive events	Section 3.3.3, p. 3-16 and Section 3.3.4, p. 3-18
3-2 None	NA
3-3 None	NA
3-4 Reword item to clarify.	Sections 3.3.2, Item 1, p. 3-15
3-5 Provide consideration of all reactions	Sections 3.3.2, Item 3, p. 3-15
3-6 Provide effect of fracture sealing on the probability of ponding in the drift	Sections 3.3.2, Item 4, p. 3-15
3-7 Provide consideration of all reactions	Sections 3.3.2, Item 3, p. 3-15
3-8 Section will be modified	Sections 3.3.2, Item 5 (this is reorganized from the way discussed in the RAI response)
3-9 None - Current text contains the discussion	Tables 3-1 and 3-2, Section 3.4.1.3 p. 3-24 and 3-25
3-10 Address validity of fresh fuel assumption in the internal criticality evaluation for waste forms other than commercial or naval SNF.	Sections 3.5.1.1 (1st paragraph), 3.5.2.1 (2nd paragraph), and 3.5.3.1 (1st paragraph).
3-11 Address validity of fresh fuel assumption in the external criticality evaluation for waste forms other than commercial or naval SNF.	See status for RAI 3-10 – internal and external not differentiated in these subsections of the Topical Report.
3-12 The assumption that neutron-induced breeding of isotopes in the repository will not generate significant amounts of fissionable isotopes	DOE still considers this an application issue, not a methodology issue and plans to provide a complete evaluation of this assumption as support

Crosswalk for RAI Actions Items for Inclusion in Topical Report Revision 01

RAI Action Items	Location in Topical Report Revision 01
will be documented to support License Application.	documentation for License Application.
3-13 DOE will seek acceptance of the method for selecting and verifying the principal isotopes to be used for burnup credit in a revision to the Topical Report.	Rev. 1 of the Topical Report presents two provisions for acceptability of the principal isotopes (Section 1.2, items L1 and L2, p. 1-6). Further discussion of these provisions is provided in Section 3.5.3.1 p. 3-41.
3-14 DOE will not seek acceptance for isotopic validation in the Topical Report but in validation reports. Acceptance of the validation process will be sought in Rev. 1 of the Topical Report, including isotopic availability as a function of time and degradation processes.	Rev. 1 of the Topical Report seeks acceptance of the validation process (Section 1.2, item G1, p. 1-5), which is described in Section 3.5.3.1 p. 3-41.
3-15 DOE will seek acceptance of the method for selecting and verifying the principal isotopes to be used for burnup credit in a revision to the Topical Report.	Rev. 1 of the Topical Report presents two provisions for acceptability of the principal isotopes (Section 1.2, items L1 and L2, p. 1-6). Further discussion of these provisions is provided in Section 3.5.3.1 p. 3-41.
3-16 Will replace paragraphs to clarify	Since the Topical Report has been re-organized, the revision is in Section 3.6.1 p. 3-59, not in the section originally promised.
3-17 None – Location of related discussion is provided	Section 3.7.2.1 (1st paragraph) p. 3-77 and Section 3.7.2.3 (2nd paragraph) p. 3-81
3-18 None – Location of related discussion is provided	With re-organization of the Topical Report, axial dependence is now discussed in Section 3.5.2.1.2 p. 3-35.
3-19 None	NA
3-20 The Topical Report will be modified so that there is no indication that there is any diminution of the transient criticality effort using RELAP5 [with respect to ensuring that the entire possible range of insertion rates is considered]	Section 3.7.2.2 p.3-79
3-21 None	NA
3-22 Will be modified to include references.	Section 3.7.1.1 p. 3-73 and 3-74
3-23 Incorporation into the Topical Report of specific references to consequences other than increased radionuclide inventory, particularly the potential enhancement of corrosion rate from long-term elevated temperature.	Section 3.7.1.2 (3rd and 4th paragraphs) Section 3.7.2.1 (4th paragraph)
4-1 None - Questions were answered concerning the use of Monte Carlo method to propagate half-life and branching fraction uncertainties to a bounding Δk_{eff} value for future disposal times.	NA
4-2 The effect of temperature limitations in MCNP (i.e., cross-section data) will be analyzed as part of the waste-form-specific validation reports. The critical limit development will consider the effects of temperature-related uncertainties.	Section 3.5.2.2 p. 3-38, paragraph 3 of Rev. 1 of the Topical Report states that the choice of specific cross-section data will be evaluated during criticality model validation and documented in validation reports that will be referenced in the License Application.
4-3 None - Information was provided in the response to this RAI on the range of initial enrichments and burnup for new radiochemical assays that will be analyzed as part of the isotopic model validation for commercial SNF.	NA

Crosswalk for RAI Actions Items for Inclusion in Topical Report Revision 01

RAI Action Items	Location in Topical Report Revision 01
4-4 None - Information was provided in the response to this RAI concerning the requirements for confirmation of conservatism in the application model. This is discussed further in Subsection 3.5.3.1.2 of Rev. 1 of the Topical Report.	NA
4-5 DOE will develop a method during model validation to appropriately account for isotopic bias in the critical limit. The Topical Report will be revised as appropriate to clarify the concerns raised by this RAI.	Clarification is provided in Sections 3.5.3.1.1 p. 3-41 and 3.5.3.2.10 (equation 3-7) p. 3-58
4-6 None - Information was provided on the selection of k_{eff} adjustment over direct adjustment of individual isotopic inventory for capturing the isotopic decay and branching-ratio uncertainties. The method is further discussed in Subsection 3.5.2.1.3 of Rev. 1 of the Topical Report.	NA
4-7 None - Clarification and additional discussion was provided relative to incorporating information specified in the RAI into Figure 4-1 of Rev. 0 of the Topical Report (Figure 3-8 of Rev. 1). Additional discussion is provided in Subsection 3.5.3.2.6 of Rev. 1 of the Topical Report.	NA
4-8 None - The response to this RAI notes that DOE is not seeking acceptance for any particular value of level of significance in identifying linear trends with respect to the trending parameter. However, DOE is seeking acceptance of the methodology used to establish the level of significance. The rationale that will be applied to the choice of level of significance in the validation submittals is provided in the response.	NA
4-9 DOE will revise the Topical Report to clarify differences between ANSI/ANS-8.17 definition of subcritical margin and the definition in the Topical Report.	This is discussed in Rev. 1 of the Topical Report in Section 2.3.2 (8th paragraph) pp. 2-8 & 2-9, Section 3.5.1.3 (Figure 3-5), Section 3.5.1.2 (3rd paragraph) p. 3-32, Section 3.5.2.1.3 (4th paragraph) p. 3-38, Section 3.5.3.2 (4th & 5th paragraph) p. 3-45, Section 3.5.3.2.3 (1st paragraph) p. 3-48, and Section 3.5.3.2.5 (5th paragraph) p. 3-50.
4-10 None - Information was provided in response to this RAI on the use of linear regression for the illustration presented in Rev. 0 of the Topical Report. It was noted that justification of the appropriateness of a specific model for establishing a critical limit for a range of applicability would be provided in supporting documents for the License Application.	NA
4-11 None - Information was provided in response to this RAI relative to the methodology presented in Rev. 0 of the Topical Report concerning the use of a single predictor variable for the least-square fits in establishing critical limit values. Additional clarification of the methodology is provided in Subsections 3.5.3.2.6 and 3.5.3.2.7 of Rev. 1 of the Topical Report.	NA

Crosswalk for RAI Actions Items for Inclusion in Topical Report Revision 01

RAI Action Items	Location in Topical Report Revision 01
4-12 None - Information was provided relating to extending the range of applicability. This includes the use of parameters other than those used for trending. Further discussion is provided in Subsection 3.5.3.2.3 of Rev. 1 of the Topical Report.	NA
4-13 None - Clarification was provided on the intended use of NUREG/CR-6361 relative to Method 1 and 2. Additional discussion is provided in Subsection 3.5.3.2.7 of Rev. 1 of the Topical Report.	NA
4-14 None - Clarification was provided on the use of Normal Distribution Tolerance Limits (NDTL). Additional discussion is provided in Subsection 3.5.3.2.8 of Rev. 1 of the Topical Report.	NA
4-15 See action item for RAI 4-9.	See status for RAI 4-9.
4-16 None - Additional information and clarification relative to the use of the Distribution Free Tolerance Limit was provided in the RAI response.	NA
4-17 See action item for RAI 4-9.	See status for RAI 4-9.
4-18 None - An explanation of the "3 standard deviations (3Φ)" limit in a distribution-free mode was provided in the RAI response.	NA
4-19 DOE will use a systematic, comprehensive, and complete approach to identify the area and range of applicability with respect to criticality model validation for each configuration class and waste form. DOE will provide a basic description of the method to be used in a revision to the Topical Report. This method will then be applied to criticality model validation and documented in the criticality model validation reports for each waste form.	A basic description of the method is provided in Section 3.5.3.2 p. 3-44, Section 3.5.3.2.2 p. 3-47, and Section 3.5.3.2.3 p. 3-48 of Rev. 1 of the Topical Report.
4-20 DOE will remove from the Topical Report those parts that imply that the spectral parameter AENCF is a trending parameter or is fundamental for any waste form. This includes removal of Figure 4-3 from the Topical Report (Rev. 0).	This material was removed from Rev. 1 of the Topical Report.
4-21 None - A discussion of the rationale for switching from LUTB method to NDTL method for extending the range of applicability was provided in the response to this RAI.	NA
4-22 The term "(Δk_m) as defined in Subsection 4.1.3.2" will be removed from Subsection 4.1.3.3.3 of the revised Topical Report.	This term was removed from Section 3.5.3.2.3 p. 3-48 of Rev. 1 of the Topical Report. This subsection corresponds to Subsection 4.1.3.3.3 of Rev. 0 of the Topical Report.
4-23 Table 4-1 will be removed from the revised Topical Report.	Table was removed from Rev. 1 of the Topical Report.
4-24 DOE will remove from the revised Topical Report the request for approval of application of the methodology to commercial fuel in an intact form and those parts that imply AENCF is the chosen	This material is not contained in Rev. 1 of the Topical Report. This appears in Subsection 4.1.3.4.1 of Rev. 0 of the Topical Report.

Crosswalk for RAI Actions Items for Inclusion in Topical Report Revision 01

RAI Action Items	Location in Topical Report Revision 01
trending parameter or is fundamental for any waste form.	
4-25 DOE plans to revise the Topical Report to state that corrosion rates will be determined from an extensive corrosion testing program.	Section 3.4.1.2.1 (1st paragraph) p. 3-22
4-26 None	NA
4-27 None	NA
4-28 DOE plans to include information about PHREEQC in any revision to the Topical Report	Section 3.4.3.1 (entire subsection) p. 3-28
4-29 None	NA
4-30 DOE plans to revise the Topical Report to indicate that if a geochemistry evaluation shows very low pH, or other corrosion-enhancing condition, that geochemistry will be re-evaluated with appropriately enhanced corrosion rates reflecting the affected waste package components.	Section 3.4 (last paragraph) p. 3-19, Section 3.4.1.1 (2nd paragraph) p. 3-20, and Section 3.4.1.2.1 p. 3-22 note that ranges of corrosion rates will be considered, the ranges reflect the expected and enhanced corrosion rates.
4-31 The treatment of colloids	Section 3.3.2 (1st paragraph and items 5 and 8) p. 3-14, Section 3.4.3 (1st paragraph) p. 3-26
4-32 Modification to the discussion of geochemistry models	Section 3.4.1.2.2 p. 3-22, which is different from the section promised in the RAI response, because of the re-organization of the Topical Report.
4-33 Discussion of the geochemistry code applications for external accumulation	Section 3.4.3 p. 3-26 and Section 3.4.3.1 p. 3-28.
4-34 None	NA
4-35 None	NA
4-36 None	NA
4-37 The mention of solution characteristics other than pH	Section 3.6.3.2 p. 3-63, particularly in item A of the sub-section on External Criticality
4-38 Mention of avoidance of redundant sampling	Section 3.6.3.2, paragraph at the top of page 3-64.
4-39 This RAI is nearly identical with RAI 4-37	NA
4-40 The need to calculate both matrix and fracture flow	Section 3.6.3.2 (p. 3-68, item B), Section 3.6.3.3 (p. 3-70 III B&C), Section 3.8.2 (p. 3-96 1st paragraph)
4-41 None	NA
4-42 None	NA
4-43 None	NA
4-44 None	NA
4-45 The response to this RAI stated that the issue sub-to-super criticality reactivity insertion would be clarified in the revised Topical Report	This material is not contained in Rev. 1 of the Topical Report. The example to which this RAI refers has been eliminated, along with the rest of Appendix C, from the revised Topical Report, so there is no longer any place for such discussion. This issue will be thoroughly addressed in the validation reports for transient criticality, both internal and external.
4-46 The considerations required for the application of RELAP 5 to highly enriched SNF	Section 3.7.1.2 (4th paragraph) p. 3-75 and Section 3.7.2 (1st paragraph) p. 3-76
4-47 The ability of RELAP 5 to handle over-moderated conditions	Section 3.7.2.2, last paragraph of p. 3-79
4-48 None	NA
4-49 None	NA
4-50 None	NA
4-51 None	NA
4-52 None	NA

Crosswalk for RAI Actions Items for Inclusion in Topical Report Revision 01

RAI Action Items	Location in Topical Report Revision 01
4-53 The validation of transient criticality codes, particularly RELAP 5	Section 3.7.3.2 p. 3-86.
All C and D RAIs	NA. The examples have been eliminated from the Topical Report. The validation reports and application analyses will contain the information when they are complete.