Yucca Mountain Site Characterization Project

DISPOSAL CRITICALITY ANALYSIS METHODOLOGY TOPICAL REPORT

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DISCLAIMER

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ABSTRACT

This report describes the risk-informed methodology to be used for performing postclosure criticality analyses for waste forms in the proposed repository at Yucca Mountain, Nevada. The risk-informed 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 various models contained in the methodology and presents the validation process for these models. The criticality-related criteria for determining the suitability of waste packages for emplacement in the repository are described. Two appendices contain sample evaluations that illustrate the methodology presented in the report, while details of the experimental data used to validate the models, sources of information to establish the probabilities of events, and calculational data are provided in references.

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, though a limited validation over parameter range potentially applicable to the repository is presented. 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 to 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 proposed Yucca Mountain repository to demonstrate the acceptability of proposed systems for limiting the potential for postclosure criticality.

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1.0 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 proposed repository at Yucca Mountain, Nevada, or its references.

In addition to this chapter, which presents the background, objective, scope, and general overview of the methodology, the report is divided into five 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 criticality. The expected dose increment is the product of the probability of criticality multiplied by the consequence of the criticality (dose increment). Chapter 3.0 describes how these two components of risk are individually estimated and then combined to give the risk estimate.

Chapter 4.0 describes specific models used to illustrate the methodology: neutronic models, models to define configurations with potential for criticality, models for estimating the likelihood (or probability) of these configurations, and models to project the consequence of a criticality. The validation process and limited validation of these models are also presented. In addition, the total system performance models used in estimating the dose increment at the accessible environment are discussed.

Chapter 5.0 summarizes the methodology presented and provides conclusions regarding the purpose, potential uses, and limitations of its use. Chapter 6.0 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. Example applications of the methodology described in the report are provided in Appendix C and Appendix D. Appendix C provides an example application for commercial SNF, and Appendix D provides an example application for DOE SNF.

[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 naval SNF); immobilized plutonium; and vitrified HLW glass. Present information is that HLW will not contain sufficient amounts of fissile material to pose a criticality risk, even in the absence of any criticality control material. Therefore, the only foreseen application of this criticality analysis methodology to HLW will be to demonstrate this fact for a few worst case configurations of moderator and geometry.

1.1 BACKGROUND

The methodology presented in 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 postclosure criticality in the repository. This section describes the various features, processes, and events that can affect criticality; the blend of deterministic and probabilistic analysis methods; and the need for a risk-informed methodology.

Limiting the potential for 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 60, 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 system for emplacing and monitoring the waste package, including openings and backfill materials, but excluding shafts, boreholes, and 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. For example, the current waste package design is actually two separate shells, outer and inner, that degrade through different corrosion mechanisms (general and pitting corrosion, respectively). These separate shells act as redundant barriers to protect the fissile material from water (moderator) contact. 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.

The methodology described in this report addresses the design features of the EBS as it is 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, criticality potential 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 are used in establishing the risk to the health and safety of the public from the release of radioactive material. As described in Section 1.5, decisions concerning the acceptability of measures to limit the potential for criticality are based on design criteria that are, in part, performance-based (related to risk). Therefore, decisions concerning design features to minimize criticality potential are based on risk, in conjunction with other information. Hence, the methodology may be referred to as risk-informed.

Because of the planned near-term development of the License Application for the repository, it is important to submit the new criticality analysis methodology described in this topical report to the NRC for review now. However, the risk-informed methodology presented in this report is not clearly consistent with the existing NRC criticality regulation in 10 CFR 60. The NRC staff has developed a draft, site-specific regulation for Yucca Mountain, which, if eventually issued, would be known as 10 CFR 63. The risk-informed methodology presented in this topical report is consistent with the new draft regulation. This topical report is being submitted on the assumption that the new draft regulations, or something similar, will be issued. Issues with the regulations are discussed in further detail in Chapter 2.0 of this report.

1.2 OBJECTIVE

The fundamental objective of this topical report is to present the planned risk-informed disposal criticality analysis methodology to the NRC to seek acceptance that the principles of the methodology and the planned approach to validating the methodology are sound.

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, though a limited validation over a parameter range potentially applicable to the repository is presented for approval. If the NRC accepts the methodology as described in this section, the methodology will be fully validated for repository design applications to which it will be applied in the License Application and its references.

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. 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 1-1 (discussed in Section 1.5) 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 Section 3.4: the calculated k_{eff} for 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 *Probability* criterion discussed in Section 3.5: a criticality frequency of 10^{-4} per year for the entire repository will not be exceeded in any of 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 4.

   3. The *Criticality Consequence* criterion discussed in Section 3.6: the expected radionuclide increase from any criticality event will be less than 10 percent of the radiologically significant radionuclide inventory (curies present at time of criticality) that is available for release and transport to the accessible environment. This criterion is intended to ensure that the average radionuclide increment form any single criticality is much less than the uncertainty of the performance assessment dose estimation, and is also 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 4.

   4. The Repository *Performance Objectives* criterion discussed in Section 3.7: 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 presented in Section 3.1, and summarized in Figures 3-1a, 3-1b, 3-2a, and 3-2b, comprehensively identifies degradation scenarios based on features, events, and processes associated with the proposed 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 Sections 3.2 and 3.3 is acceptable in general for developing a comprehensive set of potential postclosure configurations for disposal criticality analysis.

D. The portion of the methodology for performing criticality evaluations of postclosure configurations and using critical limits discussed in Section 3.4 is acceptable in general for disposal criticality analysis.

E. The portion of the methodology for estimating the probability of postclosure critical configurations and using multivariate regressions discussed in Section 3.5 is acceptable in general for disposal criticality analysis.

F. The portion of the methodology for estimating consequence of postclosure criticality events discussed in Section 3.6 is acceptable in general for disposal criticality analysis.

G. The neutronic model validation process described in Subsection 4.1.3 is acceptable in general for model validation. Specifically:

1. The process presented in Subsection 4.1.3.2 for calculating the CL values and the process presented in Subsection 4.1.3.3 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. Acceptance of the full range of CL values and their applicability for postclosure repository conditions will be sought as part of the License Application. Acceptance of a CL for a specific range is part of the model validation requested in item M.1 below.

2. The proposed requirements presented in Subsection 4.1.3.1.4 define the validation process for the isotopic model for waste packages containing commercial SNF.

H. The validation process for the degradation analysis portion of the methodology presented in Section 4.2 for calculating the chemical composition of fuel and waste-package component degradation products is acceptable in general for model validation. Specifically:

1. Validation of the flow-through mode (internal to the waste package) is provided by hand calculation to verify that the computer code that correctly adjusts the solute amounts downward from one output to the next input (rollover).

2. Validation of the open system mode (external to the waste package) is provided by the conservatism available in, and the application of, the methodology.

I. The validation process for the probability calculation and configuration generator models described in Subsection 4.3.4 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 4.4.3 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 4.1.3.1.4 for modeling burnup of commercial SNF for design applications are sufficient, if met, to ensure adequate conservatism in the isotopic model for burnup credit.

L. The principal isotopes selected to model burnup in intact commercial SNF, presented in Table 3-1 in Subsection 3.4.3, are acceptable for disposal criticality analysis. The process for selecting isotopes from the list of principal isotopes for degraded commercial SNF presented in Subsection 3.4.3 is also acceptable for disposal criticality analysis.

M. The following models are acceptable as described below. The validation of these models is for a range of the currently expected postclosure repository conditions for the proposed repository at Yucca Mountain, Nevada. The postclosure repository conditions are dependant upon the waste form, waste package design, engineered barrier design, data from material tests, data from natural systems tests, and Performance Assessment models of postclosure time dependent repository conditions. At the time this report is being released, all the waste forms are not fully defined, the final waste package and engineered barrier designs have not been finalized, data is still being collected from the material tests and natural systems, and the Performance Assessment models of postclosure repository conditions are still being refined. Thus, the conditions that will be presented for License Application are not fully defined, and the formal validation of these models for License Application will be provided or referenced in the License Application.

1. The neutronic models described in Subsection 4.1.1 and 4.1.2, including the SAS2H sequence of the SCALE 4.3 (CSCI:30011 V4.3, CRWMS M&O 1997g; Oak Ridge National Laboratory [ORNL] 1995) code system using the 44-energy group cross-section library and the MCNP 4B2 (CSCI:30033 V4B2LV, CRWMS M&O 1998t. ORNL 1997) computer code using the referenced cross section libraries, are acceptable for evaluating criticality potential for the range of neutronic parameters presented in Subsection 4.1.3.4.1. The applicability of these models to specific waste package conditions in the repository will be demonstrated or referenced in the License Application using the validation process referred to in item G above.

2. The degradation model (the geochemistry code EQ3/6) described in Subsection 4.2.2 is acceptable for the range of environmental conditions currently expected in the repository. The bounding cases have been identified for the current range of environmental parameters and may be modified for the environmental parameters most suitable for License Application.

3. The configuration generator models described in Section 4.3 (equations representing physical and chemical release, transport, and accumulation processes), are acceptable for the range of environmental conditions currently expected in the repository. The bounding cases have been identified for the current range of environmental parameters and may be modified for the environmental parameters most suitable for the License Application.

4. The steady-state consequence models (equations representing physical material and heat balance processes) described in Section 4.4 are acceptable for the range of environmental conditions expected in the repository, for both internal and external

criticality. The portion of the methodology for consequence evaluation of transient criticalities is acceptable for both internal and external criticality for the range of environmental parameters expected in the repository. The bounding cases have been identified for the current range of environmental parameters and may be modified for the environmental parameters most suitable for the License Application.

With the exception of the determination of isotopic inventories, the methodology described above will be used for degraded naval fuel. There are a number of exceptions with this methodology, which may exist for intact naval fuel. There are a number of exceptions with this methodology, which may exist for intact naval fuel. These include: a) the use of a different CL criterion and the use of a deterministic approach; b) the possibility of not calculating consequences if a sufficiently conservative criticality criterion is imposed; c) different codes and cross sections used to calculate the range of applicability and isotopic inventories; d) the specific codes, benchmarks, and radiochemical samples and data applicable to validation of methods for naval fuel; and e) a principal isotope list applicable to naval fuel. Differences will be described in the naval fuel addendum.

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 public). 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) over time.

The methodology presented in Chapter 3.0 of this report 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. Specific models are presented in Chapter 4.0 of this report. These include neutronic models, models to define configurations with potential for criticality, models for estimating the likelihood of these configurations, models to project the consequence of criticality, and TSPA models used for estimating dose increment at the accessible environment. Because of its classified nature, models unique to naval SNF will be described in a separate submittal, which is scheduled for release in September 1999.

Experimental data for neutronic model validation are referenced, and a validation process is described in Subsection 4.1.3. Proposed requirements are presented in Subsection 4.1.3.1.4 that define the validation process for the isotopic model for waste packages containing commercial SNF. The validation process for the isotopic model for waste forms containing naval SNF shall be presented in a separate addendum. The fabrication design values (or HLW technical specification concentration limits for fissile isotopes) will be used for isotopic concentrations of fissionable materials for other waste forms. The process presented in Subsection 4.1.3.2 for

[2] Discussions of naval fuel in this report refer primarily to fully 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 will be discussed in a classified addendum, which is scheduled for release in September 1999.

calculating CL values will be used in fully validating the criticality model. The criticality model validation also includes examining the range of neutronic parameters represented by the experimental data. Trending analyses are performed for these parameters, and the range of applicability of the experimental database is established as discussed in Subsection 4.1.3.3. The criticality model validation process consists of calculating the CL values and establishing the range of applicability of the CL data. The range of applicability criterion discussed in Subsection 3.4.4 will be developed and applied to criticality evaluations for the repository to ensure that the design criteria for k_{eff} (CL) are covered by the experimental database. If the criticality evaluations are outside of this range, either the range of applicability must be extended (e.g., by extrapolation) with an additional conservative k_{eff} margin applied or the experimental database must be expanded as described in Subsection 4.1.3.3.3. Acceptance for the neutronic model validation process and acceptance for the establishment of the CL design criterion are sought in this report. In addition, acceptance of the models themselves over a limited range of neutronic parameters expected to represent repository conditions is sought in this report, as discussed in Subsection 4.1.3.4.1. Full validation of the models over the actual expected postclosure repository conditions awaits additional information that is not yet available. Therefore, this validation will be provided in the License Application or its references.

Three additional model types are considered in this report: degradation models, probability calculation models (including the configuration generator code), and criticality consequence models. All three types involve the use of equations describing physical and chemical processes. Their validation has been illustrated for the input parameter set specified in Appendix C. The comparison with benchmark experiments or hand checked calculations is illustrated in Subsections 4.2.4 and 4.3.4. The relation of the benchmark environmental parameters to the Yucca Mountain parameters is discussed in Subsection 4.2.4.2. In addition, those degradation models which deal with environmental parameters will be validated separately as part of the performance assessment process.

Additional design criteria are presented in this report. These include the probability criterion (discussed in Section 3.5), the criticality consequence criterion (discussed in Section 3.6), and criterion based on the repository performance objectives (discussed in Section 3.7). Specific values are recommended for the probability criterion and the criticality consequence criterion, and acceptance of these values is sought in this report. The criterion based on the repository performance objectives addresses the effect of potential criticalities on dose at the accessible environment. Regulatory standards for dose at the accessible environment have not been finalized at the time of this report. The requirements of existing regulations at the time of the License Application will be addressed using this criterion.

Example applications of the methodology for commercial light water reactor (LWR) SNF and for an aluminum-clad, DOE-owned SNF are provided for illustrative purposes in Appendices C and D, respectively.

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 1998a) controls. The report was initially prepared in accordance with the Civilian Radioactive Waste Management System (CRWMS) Management and Operating Contractor (M&O) Quality Administrative Procedures (QAPs). 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, waste isolation, and physical protection of materials and facility in the QAP-2-3 evaluation titled *Classification of the Preliminary MGDS Repository Design* (CRWMS M&O 1997h). The final topical report was prepared in accordance with Yucca Mountain Site Characterization Project Procedure YAP-5.8Q, *Technical Document Preparation*, and was reviewed in accordance with the OCRWM Procedure QAP 6.2, *Document Review*.

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 information presented in this report is not design information that can be used to support procurement, fabrication, or construction.

This report has no interfaces outside the OCRWM program. This topical report does have interfaces on common topics being developed in different areas of OCRWM, namely burnup credit. This report also references information presented in the *Topical Report on Actinide-Only Burnup Credit for PWR Spent Nuclear Fuel Packages* (DOE 1997). Some of the data and part of the methodology described in DOE 1997 are referenced as appropriate in describing the disposal criticality analysis methodology.

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.

1.5 OVERVIEW OF THE METHODOLOGY

The potential for nuclear criticality is determined by the composition of the waste and its geometry (i.e., waste form configuration, including presence of moderator, reflecting structural material, and neutron absorbers). The initial emplaced configuration of the waste form is a dry waste package, placed in a mined passageway (or drift) inside the repository. As discussed in Section 1.1, waste packages will be designed to preclude nuclear criticality from occurring in sealed, undamaged packages. Criticality evaluations will be performed in support of each waste package and engineer barrier design to demonstrate that the initial emplaced waste package and waste form configuration will remain subcritical for as long as the waste package remains intact. The methodology described in this report will be used to support confirmation that even with waste-package failure, followed by degradation of the materials inside, the addition of moderator material, and the loss of neutron absorber material, consistent with design predictions, the repository will provide adequate protection of the health and safety of the public against postclosure criticality.

Figure 1-1 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/engineered barrier system (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. The Master Scenario List, as discussed in Section 3.1, 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

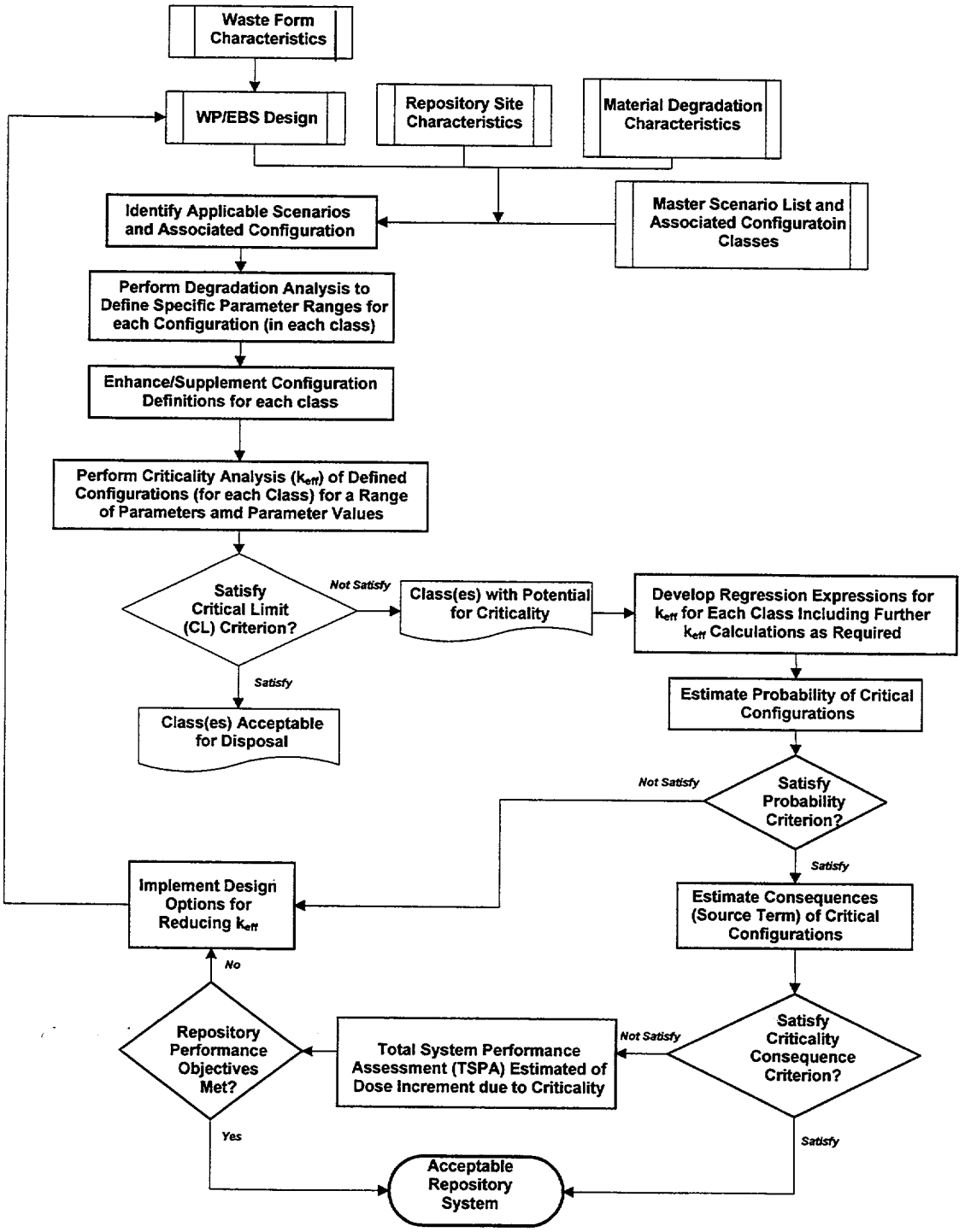


Figure 1-1. Overview of Disposal Criticality Analysis Methodology

criticality for the TSPA Viability Assessment (VA) abstraction/testing effort (CRWMS M&O 1998c, 1998d).

The decision points represent design criteria that are applied to ensure sufficient measures are implemented to limit the potential for criticality. Although not explicitly shown in this diagram, the design process includes the examination of the significant contributing factors to the risk of criticality with the intent of implementing feasible and practical design enhancements to minimize overall criticality risk.

The process represents a logical, step-by-step approach. Moving through Figure 1-1, the process examines how the emplaced material may degrade by examining the characteristics of the repository site and the types of likely conditions and anticipated interactions that could take place, and then build scenarios that result in degraded configurations. The possible degraded configurations are grouped into classes and each class is defined by a single scenario or set of related scenarios. The composition and geometry of the configurations in each class vary as a function of specific parameters. These parameters may include the amounts of fissionable material, neutron absorber material, corrosion products, and moderator, and may also stipulate the time of occurrence. Subsequent criticality evaluations focus on the range of values of these configuration parameters.

After the applicable scenarios and configuration classes are identified, degradation analyses are performed to define appropriate 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.

The configurations in each class are then evaluated for criticality potential. These evaluations are performed at various parameter values for the range of parameters comprising each configuration class. The criterion for judging the potential for criticality is provided by the critical limit. The CL is the value of k_{eff} at which the configuration is considered potentially critical. CL values are obtained by analysis of experimental systems with a range of neutronic parameters that are representative of those analyzed for the repository. The process for calculating the CL is described in Subsection 4.1.3.2.

For configuration classes showing potential for criticality, multivariate regressions are developed in which k_{eff} values are expressed as a function of configuration parameter values for each of these classes. The regression expressions cover the range of these parameter values for which the peak k_{eff} may exceed the CL. The standard error of regression is established during the development of the regression expressions and is added to the predicted k_{eff} values for comparison with the CL criterion. The portion of the methodology for criticality evaluations (including the CL criterion) and the development of multivariate regressions for k_{eff} are discussed in Section 3.4.

The probability of exceeding the CL criterion is estimated for each 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 per package probability criterion. If this criterion is exceeded, additional design options for reducing k_{eff} are implemented. The portion of the methodology for estimating the probability of critical configurations is presented in Section 3.5.

For postclosure, additional design guidelines beyond the probability criterion are followed. When the probability criterion is satisfied, a criticality consequence evaluation is performed. The purpose of this evaluation is to estimate changes in the radionuclide inventory that may impact the TSPA. Changes are measured against a criterion for increase in the radionuclide inventory (the criticality consequence criterion). If this criterion is satisfied, the design criteria are satisfied and the system is acceptable for disposal. If this criterion is not satisfied, the estimated additional source term is provided as input to the TSPA. The TSPA estimates the dose increment due to the criticality 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 (repository performance objective) is not satisfied, additional design options for reducing k_{eff} are implemented. Otherwise, the design criteria are satisfied, and the system is acceptable for disposal.

The portion of the methodology for estimating the consequence of a criticality is discussed in Section 3.6. A discussion of estimating criticality risk (by TSPA) is presented in Section 3.7.

2.0 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. This methodology will be used to demonstrate compliance with NRC regulatory criticality requirements for disposal of fissionable material. Application of the methodology will address any applicable NRC design criteria and will also provide input to total system performance assessments that will determine if the repository will meet its overall performance objectives.

The topical report is being submitted in accordance with the *Topical Report Review Plan* (NRC 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. However, the criteria developed in conjunction with the methodology presented in this topical report are not fully consistent with the existing regulations for disposal criticality. New regulations applicable to Yucca Mountain are expected to be issued in the near future,[3] and the methodology presented in this topical report will support demonstration of compliance with the risk-informed regulations likely to be implemented by NRC. Should the methodology not clearly support compliance with the new regulations as eventually issued, the U.S. Department of Energy (DOE) will work with the NRC to identify an appropriate course of action for postclosure criticality analysis. Issues regarding 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 criticality during postclosure.

2.1 APPLICABLE NRC REGULATIONS

The future direction of the U.S. Environmental Protection Agency (EPA) and NRC regulations applicable to a geologic repository is uncertain, but new EPA standards and NRC regulations for Yucca Mountain are expected to be implemented. The discussion that follows, therefore, focuses on the existing regulations, followed by a discussion on potential near-term revisions to the regulations. Section 2.2 includes discussion of how the methodology presented in this report is related to the existing and potential regulations.

2.1.1 Existing Regulations

Two types of requirements currently within 10 CFR 60 apply directly to disposal criticality: design criteria and performance objectives. The repository and waste-package designs must

[3] The NRC staff has developed a draft, site-specific regulation for Yucca Mountain, which, if eventually issued, would be at 10 CFR 63. As of this writing, the NRC has not issued the draft for public comment. However, the draft has been made available for public information.

meet a design criterion applicable to postclosure criticality. In addition, it must be demonstrated that potential criticality events during the postclosure phase do not prevent the repository and waste package from meeting the subsystem and overall performance objectives in effect when the License Application is submitted.

The existing regulatory design criterion applicable to disposal criticality control is 10 CFR 60.131(h), which states:

> All systems for processing, transporting, handling, storage, retrieval, emplacement, and isolation of radioactive waste shall be designed to ensure that nuclear criticality is not possible unless at least two unlikely, independent, and concurrent or sequential changes have occurred in the conditions essential to nuclear criticality safety. Each system must be designed for criticality safety assuming occurrence of design basis events. The calculated effective multiplication factor (k_{eff}) must be sufficiently below unity to show at least a 5 percent margin, after allowance for the bias in the method of calculation and the uncertainty in the experiments used to validate the method of calculation.

This regulation currently applies to both preclosure and postclosure criticality. As discussed in Section 2.2, this regulation has been the subject of discussions between the NRC and the DOE because DOE believes there is inadequate consideration for risk-informed issues in the rule's wording. The risk-informed, performance-based analysis methodology presented in this topical report is not fully consistent with 10 CFR 60.131(h), which is worded deterministically. The topical report is being submitted in anticipation of new regulations the NRC plans to issue for the repository (61 FR 64260). As previously noted, a draft of the new regulations has been made available for public information.

To address the existing regulations, criticality must also be considered as part of demonstrating compliance with the repository and waste-package performance objectives of 10 CFR 60.112 and 10 CFR 60.113. The overall performance objective of 10 CFR 60.112 is:

> The geologic setting shall be selected and the engineered barrier system and the shafts, boreholes, and their seals shall be designed to assure that releases of radioactive materials to the accessible environment following permanent closure conform to such generally applicable environmental standards for radioactivity as may have been established by the EPA with respect to both anticipated processes and events and unanticipated processes and events.

It is assumed that an overall performance objective, similar to this one, will be implemented in new regulations applicable to Yucca Mountain. To demonstrate compliance with it, a TSPA will be performed. This assessment will consider a variety of inputs, such as site characteristics, repository design, radioactive material source term, and postulated events and processes. Models will be used to determine the ability of the site, the repository, and the waste package to collectively comply with applicable environmental standards for radiation exposure. The probability of criticality events and consequences of those events (potential perturbations to the repository source term and to the repository thermal pulse) will be determined using the methodology presented in this report. These probabilities and consequences will be considered

in the total system performance assessment (TSPA).[4] No EPA requirements currently apply to a high-level waste facility licensed in accordance with the Nuclear Waste Policy Act of 1982 as amended, because the previous standards of 40 CFR 191 were remanded and then reissued as not applicable to Yucca Mountain. New standards are being developed by the EPA.

The performance objectives for particular barriers of 10 CFR 60.113 (often referred to as "subsystem performance objectives"), though lengthy, may be paraphrased as (a) containment of waste within the waste packages will be substantially complete for up to 1000 years, and (b) release rate of any radionuclide following the containment period shall be very small (less than one part in 100,000 of the amount of that radionuclide present at 1000 years after repository closure). A criticality event would change the mix of radionuclides present due to the production of relatively short-lived radionuclides that would not otherwise be present in measurable quantities thousands of years after spent nuclear fuel and high-level waste are emplaced in a repository. Because the release-rate performance objective is stated in terms of the fraction of the amount of a given radionuclide present 1000 years after the repository closes, introducing more of that radionuclide at a later time due to a criticality could pose a concern and would need to be evaluated to address 10 CFR 60.113. The methodology provided in this report will be used to support the determination of whether and how disposal criticality affects the ability of the repository and waste package to meet these subsystem performance objectives, if they are in effect at the time the License Application is submitted. However, revisions to the regulations are likely to eliminate subsystem performance objectives, as discussed in Subsection 2.1.2.

It should be noted that, for the License Application, the framework within which the DOE will ensure compliance with regulatory requirements is contained in the Office of Civilian Radioactive Waste Management (OCRWM) technical document hierarchy. This hierarchy includes the *Civilian Radioactive Waste Management System Management and Operating Contractor Requirements Document* (DOE 1998b), the *Mined Geologic Disposal System Requirements Document* (YMP 1998), and the applicable system description documents.

2.1.2 Potential Changes to the Regulations

In August 1995, in accordance with Congressional direction, the National Academy of Sciences (NAS) made recommendations to the EPA for use in developing new performance standards for Yucca Mountain (National Research Council 1995). The Energy Policy Act of 1992 requires that the EPA issue, within a year of receipt of the NAS report, new environmental protection standards to replace the remanded ones of 40 CFR 191. The same act also requires the NRC to revise its regulations to implement the new EPA standard.

As stated earlier, the new standards and regulations are still being formulated. However, the NRC has recognized (61 FR 64257-64270) the need to address uncertainties in the applicability of the existing disposal criticality regulation to the postclosure period. The NRC commissioners have directed (NRC Memorandum, J.C. Hoyle to L.J. Callan, subject Staff Requirements - SECY-97-300 - Proposed Strategy for Development of Regulations Governing Disposal of High-Level Radioactive Wastes in a Proposed Repository at Yucca Mountain, Nevada, March 6, 1998. TIC 238418) the NRC staff to develop a new, site-specific regulation

[4] Performance of a design that complies with 10 CFR 60.131(h) would not be expected to be impacted by criticality because (absent two unlikely events) the applicant would need to show that criticality would not occur to address 10 CFR 60.131(h). Nevertheless, a comprehensive TSPA would assign a probability to the occurrence of criticality and determine the associated risk as one of many factors to be considered.

whose performance standard is "generally consistent" with the NAS report. The NAS report supports using risk-based analysis in repository regulation, and DOE has asked the NRC (Letter, R.A. Milner to Secretary, NRC Docketing and Service Branch, Transmitting DOE comments regarding NRC-proposed revisions to 10 CFR 60 Regulations for Design Basis Events, June 16, 1995. HQO:19950619.0002; Letter, S.J. Brocoum to J.J. Holonich, Submitting the Annotated Outline for the planned Disposal Criticality Analysis Topical Report, August 18, 1995. MOV.19950914.0001; and Letter, S.J. Brocoum to M.J. Bell, Providing DOE acknowledgment of receipt of NRC comments on the Annotated Outline for the Disposal Criticality Analysis Topical Report, April 12, 1996. MOL.19960826.0110) to revise the regulation to incorporate risk analysis as the appropriate approach to postclosure criticality analysis. For these reasons, it is anticipated that the new regulation will incorporate risk-informed, performance-based analysis. This point is discussed further in Section 2.2. The methodology discussed in this topical report is based on risk-informed, performance-based analysis. This methodology is believed to be fully consistent with the draft Yucca Mountain regulations developed by the NRC staff and recently made available for public information.

The NAS Report also states that subsystem performance objectives may not support optimizing repository performance in protecting the health and safety of the public. This situation could occur because a design developed to satisfy subsystem performance objectives may not be the best approach to optimizing overall repository performance. Should subsystem performance objectives be deleted as a result of this conclusion (as seems likely, based on the new draft regulations), the focus of criticality analyses would be on the predicted consequences of a postulated criticality event for the repository's overall performance.

The new regulations are likely to be based on providing reasonable assurance that doses to the public will be limited to acceptable levels (and therefore will be based on limiting risk to the public) rather than directly based on limiting release of radionuclides from the engineered barrier system. The approach taken to criticality analysis that is described in this report is considered likely to be compatible with the new regulations.

Because the form of the new standards and regulations is not definitively known, the methodology presented will focus on supporting compliance with DOE's interim standards (Letter, W.E. Barnes to L.D. Foust; subject: Interim Postclosure Requirement and Goal, July 14, 1997. MOL.19971006.0152) which the DOE believes will be similar to the new standards and regulations. Because the topical report presents a methodology, the exact values of the standards (or differences between the values in the DOE standard and the final regulations and standards) are not considered relevant to the acceptability of the topical report. Should 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 probabilistic risk 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. The specific requirement is that systems for the isolation of radioactive waste, "...shall be designed to ensure that nuclear criticality is not possible unless at least two unlikely, independent, and concurrent or sequential changes have occurred...". In the closed and isolated repository, where all changes are directly influenced by the environment and manifested primarily through groundwater flow, most changes that occur concurrently or sequentially will not be independent. Several scenarios could, under given conditions, produce a criticality. However, all scenarios examined thus far consist of two, or more, extremely unlikely changes, and only a few such changes are concurrent or sequential, with none, likely, being independent. Without being able to use exceptions for unlikely changes, the requirement, 10 CFR 60.131(h), is reduced to the deterministic, "criticality is not possible."

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 notable 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.

Notwithstanding the deterministic wording in 10 CFR 60.131(h), other regulations in 10 CFR 60 implicitly recognize the uncertainties inherent in the extended period of performance for a geologic repository. The regulation 10 CFR 60.101(a)(2), which discusses the "reasonable assurance" concept, may be interpreted to allow the applicant to demonstrate that the probability of a criticality occurring is so small as to provide "reasonable assurance" that it will not occur. However, such an interpretation has not been formally made or tested in any licensing proceeding.

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 staff's draft site-specific regulations for Yucca Mountain. 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 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 NAS 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 recent 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. TIC 238419).

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.

The Project recognizes 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 may be sufficient for intact navy spent fuel, which is a uniquely robust waste form. The methodology for this analysis will be described in an addendum to this topical report.

2.2.2 Defense in Depth Against Postclosure Criticality

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. In order 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 avoid 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 in the basket materials. Similarly, use of two separate waste-package shell materials to impede entry of water into the waste package is an example of the use of redundant barriers. (Discussion of how these features perform as barriers to criticality is provided in Appendix C.) 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. 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), has 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, Section 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 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, 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 a core melt. 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 and critical limit. 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* (NRC 1997) has been used for guidance on how to extend a defined range of applicability for the establishment of an upper subcritical limit and 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 subcritical limits. Its guidance for establishing bias by correlating the results of criticality experiments with results obtained for these same systems by the method being validated has been used in the development of the disposal criticality analysis methodology, as has its guidance for using 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 subcritical limit (referred to in the standard as "Criteria to Establish Subcriticality"). The approach for establishing subcriticality prescribed in Section 5.1 of this standard is the approach recommended in NUREG/CR-6361 (Lichtenwalter et al. 1997).

- 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 Guides

Two NRC Regulatory Guides were also used in developing the methodology: Regulatory Guide 3.4, *Nuclear Criticality Safety in Operations with Fissionable Materials at Fuels and Materials Activities* (NRC 1986a), and Regulatory Guide 3.58, *Criticality Safety for Handling, Storing, and Transporting LWR Fuel at Fuels and Materials Facilities* (NRC 1986b). These Regulatory Guides are used as follows:

- Regulatory Guide 3.4 (NRC 1986a) endorses using ANSI/ANS-8.1 for general storage and transport of fissionable materials. Aspects of the postclosure criticality analysis methodology consistent with ANSI/ANS-8.1 are described in Subsection 2.3.2, and these aspects therefore are consistent with Regulatory Guide 3.4 to the same extent. As called for in the Regulatory Guide, validation of the calculational methodology is provided in Chapter 4.0 of this report and in its references.

- Regulatory Guide 3.58 (NRC 1986b) endorses ANSI/ANS-8.17 for storage and transportation of light water reactor spent fuel. However, it takes exception to using exposure history as an acceptable way to verify burnup in support of taking burnup credit. This method is one of two that is presented in the standard.

The Regulatory Guide states that credit for fuel burnup may be taken only when the amount of burnup is confirmed by reactivity measurements that are appropriate for each type of fuel assembly in the environment in which it is to be stored. As noted in the previous subsection, the methodology presented in this report is consistent with ANSI/ANS-8.17. The DOE's *Topical Report on Actinide-Only Burnup Credit for PWR Spent Nuclear Fuel Packages* (DOE 1997) includes verification of exposure history and flux measurements as possible approaches to verifying burnup. This methodology therefore differs from Regulatory Guide 3.58 (NRC 1986b) in that reactivity measurements of each spent fuel bundle or waste package are not planned. Reactivity may be indirectly determined by measuring flux, inferring burnup from the flux, and inferring reactivity from burnup. However, it has not been determined whether such measurements are needed for all spent fuel bundles, for suitable samples, or are not needed. Reactivity of bundles not subjected to flux measurements will be inferred from burnup as discussed in this topical report. With the exception of the reactivity measurements, the planned implementation of the methodology presented in this report is consistent with Regulatory Guide 3.58 (NRC 1986b) to the same extent it is consistent with ANSI/ANS-8.17, as discussed in Subsection 2.3.2.

3.0 METHODOLOGY

This chapter presents the methodology for performing criticality analyses for waste forms for long-term disposal in the proposed repository at Yucca Mountain. This methodology applies only 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 uncertainties change. Acceptance of the principles of the risk-informed approach discussed in this chapter is sought in this report. In addition, specific aspects of the methodology for which U.S. Nuclear Regulatory Commission (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. The specific aspects noted in Chapter 3.0 are items A, B, C, D, E, and F from the full list in Section 1.2.

The analyses performed are described in the following sections of this chapter. Section 3.1 describes how degradation scenarios are built from features, events, and processes. 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. Sections 3.2 and 3.3 discuss the steps of the methodology to specify the configuration parameters, starting from the configuration classes, with the non-equilibrium geochemistry code, EQ3/6, described in Subsection 4.2.2 as being a principal evaluation tool. The portion of the methodology for evaluating criticality (k_{eff}) once the configuration has been completely specified is described in Section 3.4.

The last three sections are concerned with probability 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 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 3.5 gives the portion of the methodology for estimating the probability of the potentially critical configuration; this portion of the methodology is described with respect to probability distributions of the scenario-related parameters discussed in Section 3.1 and the configuration-related parameters discussed in Sections 3.2 and 3.3. The portion of the methodology for estimating the consequences of criticality is explained in Section 3.6. This consequence portion of the methodology is illustrated for commercial SNF in Appendix C. Section 3.7 describes the methodology for combining probability and consequence estimates, which is part of the general total system performance assessment (TSPA) portion of the methodology, including the modeling of radionuclide transport to develop an estimate of incremental dose at the accessible environment.

3.1 STANDARD CRITICALITY SCENARIOS

Degradation scenarios comprise a combination of features, events, and processes (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 effect on the emplaced material. Examples of events would be the sudden collapse of a basket due to the corrosion of structural members 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-Viability Assessment (VA) abstraction/testing effort (CRWMS M&O 1998c). 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 1998d). This scenario definition process is believed to have produced a set that is 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 1998c; 1998d), by the expert participants in the workshop constitutes validation of the scenario definition process. This report is seeking acceptance that the Master Scenario List, discussed in this section and summarized in Figures 3-1a, 3-1b, 3-2a, and 3-2b, comprehensively identifies degradation scenarios based on features, events, and processes associated with Yucca Mountain that may affect criticality.

The scenarios are conveniently 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).

The internal degradation scenarios are summarized in Figures 3-1a and 3-1b; the external scenarios, in Figures 3-2a and 3-1b. It should be noted that each of these figures is given in two parts (a, b) to avoid the need for fold-outs. In the sequence of Figures 3-1a and 3-1b, 3-2a and 3-2b, the first three have outgoing connectors represented by triangles, and all have incoming connectors represented by circles. In Figures 3-1a and 3-1b, the outgoing connectors labeled E, F, and I are connected to incoming connectors in Figure 3-2a. All the other outgoing connectors (with the alphabetic designations A, B, and C) are reconnected to incoming connectors (represented by circles) in Figures 3-1a and 3-1b, 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 3.1.1 below. 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. Of course, many of the configurations can be reached by indirect scenarios routed through the triangle and circle connectors described in the previous paragraph.

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

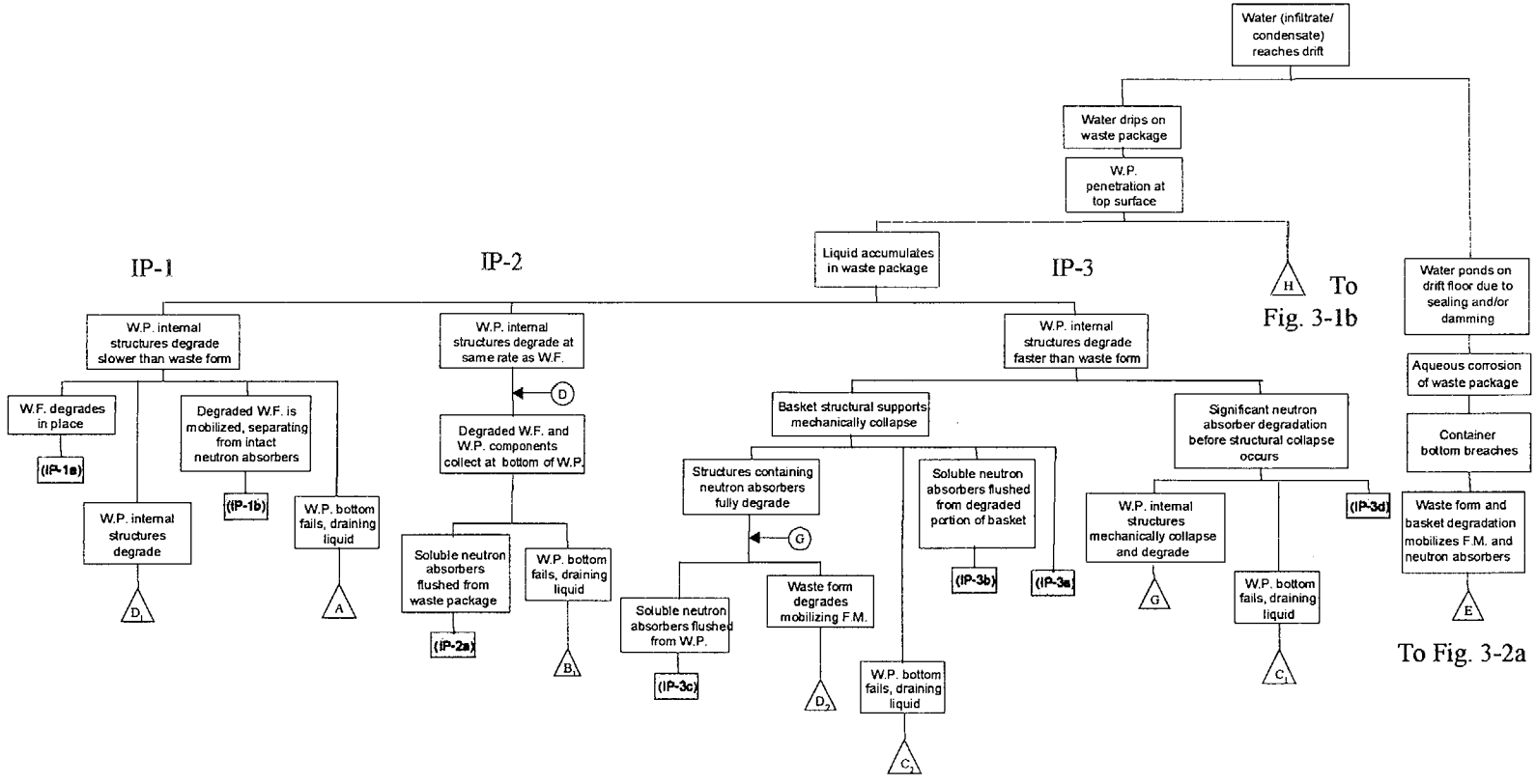
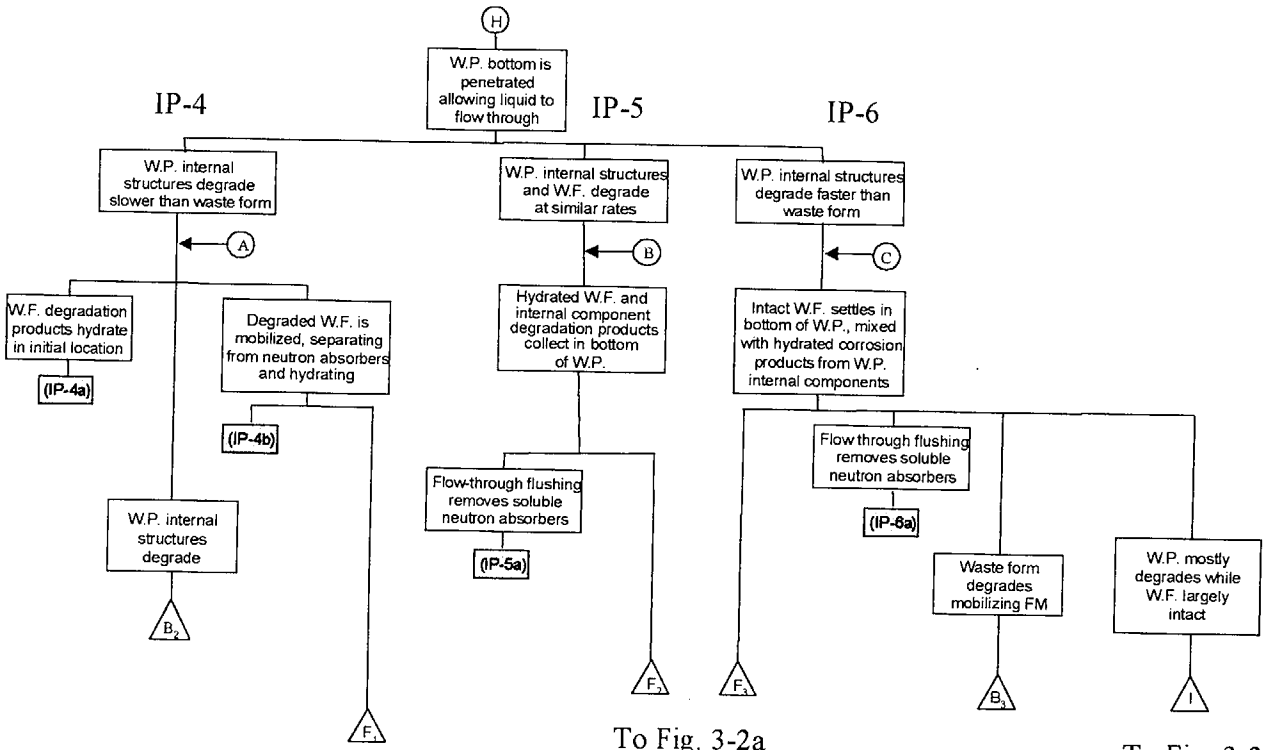


Figure 3-1a. Internal Criticality Master Scenarios, Part 1

From Fig. 3-1a



Note: hydrated degradation products may include hydrated metal oxides, metal hydroxides, and clayey materials

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

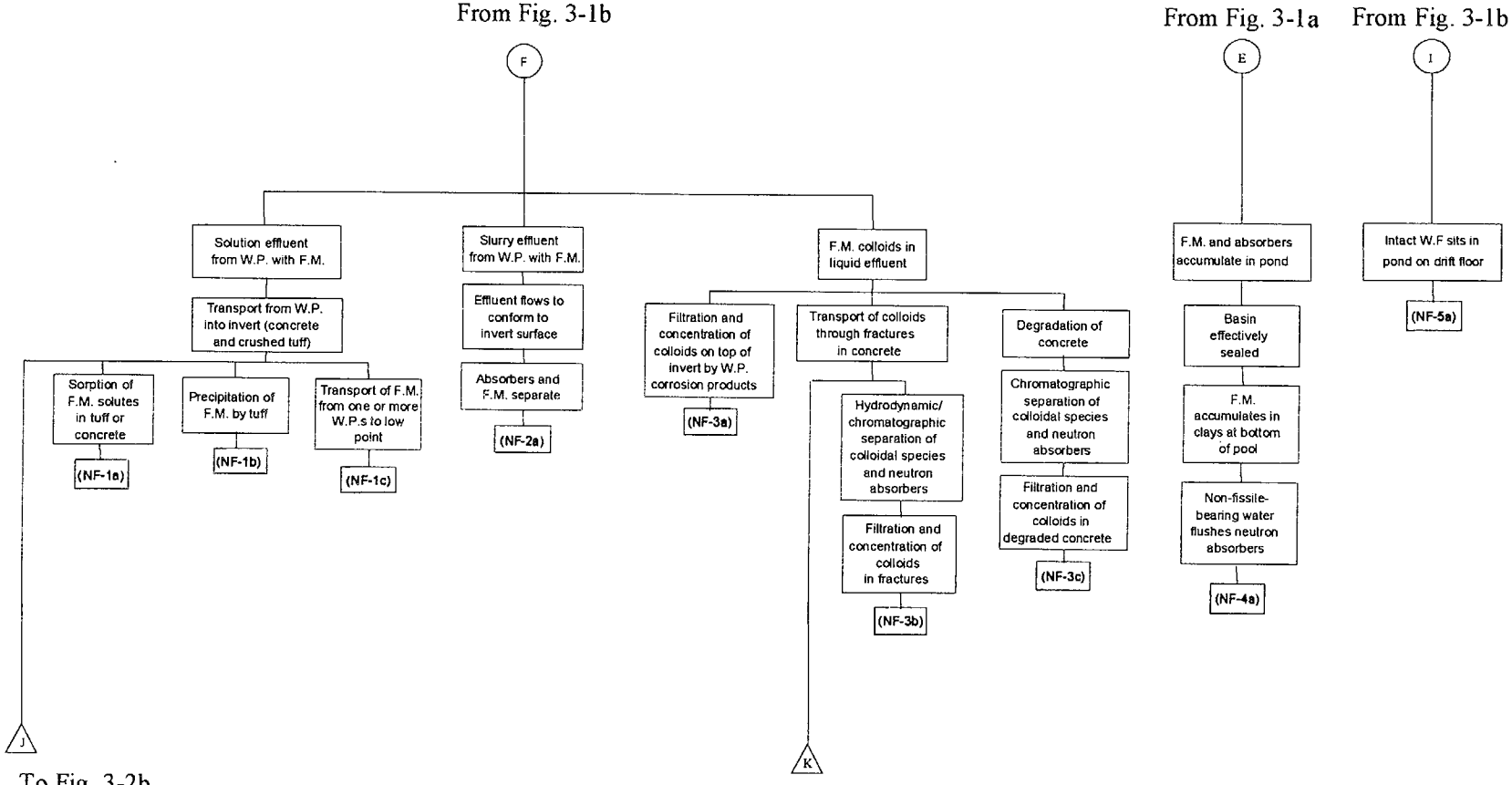


Figure 3-2a. External Criticality Master Scenarios, Part 1

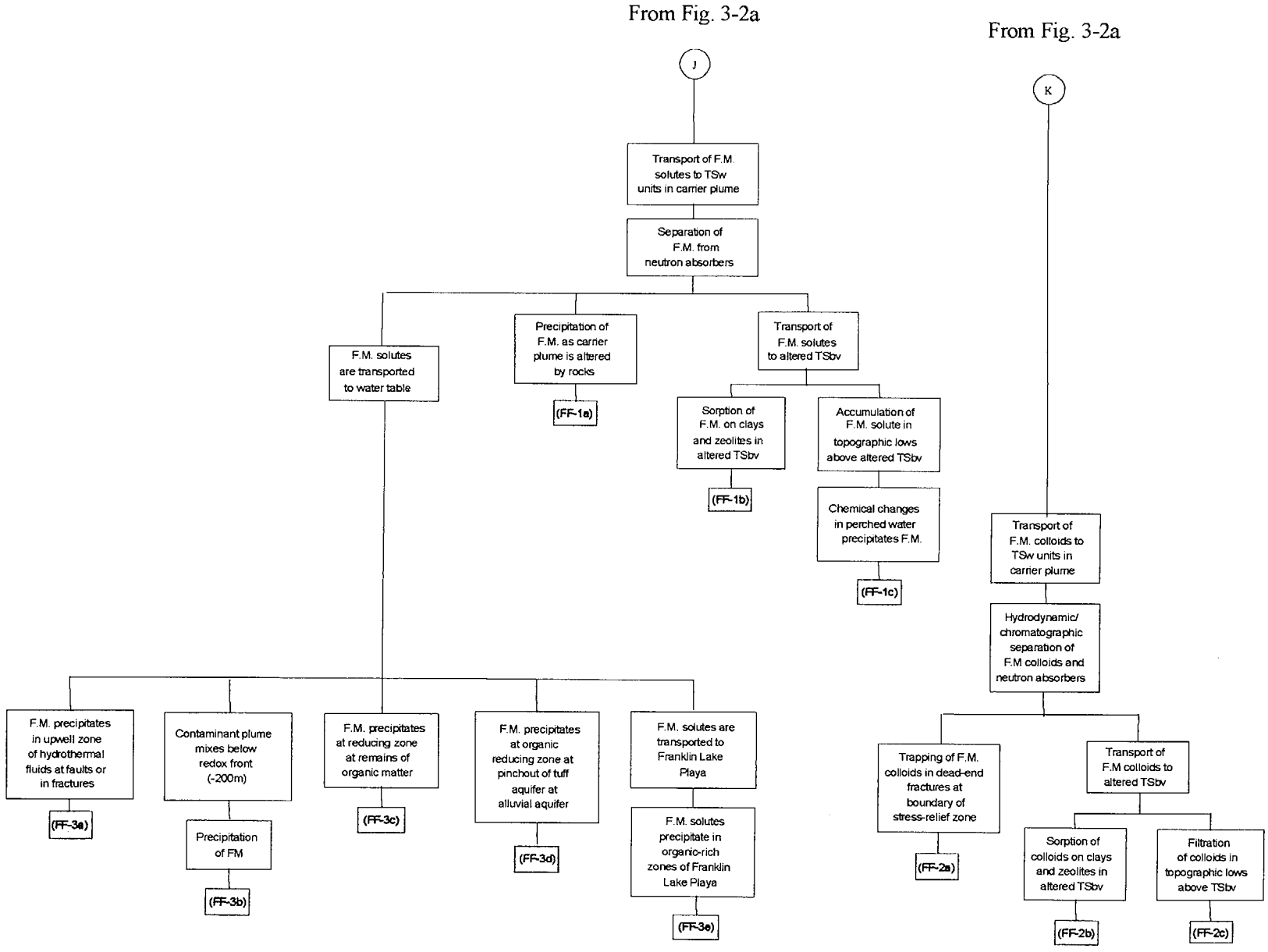


Figure 3-2b. External Criticality Master Scenarios, Part 2

The top-level discriminator among the possible internal criticality scenarios (Figure 3-1a) 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 3.1.1 and 3.1.2. Quantification of the parameters represented by the boxes in Figures 3-1a and 3-1b and 3-2a and 3-2b for individual waste forms will be developed for the License Application. The examples in the appendices are intended to facilitate the evaluation and acceptance of the methodology given here.

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 3-1a and 3-1b and in circles in Figures 3-2a and 3-2b. 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 3.3.

The configuration classes are shown as the shaded boxes at the end of each scenario chain in Figures 3-1a and 3-1b and 3-2a and 3-2b. 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.

The requirement for moderator (either 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 fissile material, and will identify any possible fast criticality as part of this process.

3.1.1 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 more reactive geometry, (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.

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 3-1) 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 3.2.

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 mobile, or readily available, moderator. 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 3.2 for more detail).

Degradation scenario groups IP-1 through IP-3 (Figure 3-1a) 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 identifies the scenarios that lead to them. These class definitions encompass all of the configurations shown in Figures 3-1a and 3-1b. The more likely of these configuration classes have already been the subject of preliminary investigation, and the results are presented in Appendices C and D, or are referenced therein. 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), and the results are summarized in Appendix C. This example uses the current 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 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 basket or 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 1998e).

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 fissile 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 3-2a and 3-2b.

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 1998e).

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 WF. This can happen with the highly enriched research reactor SNF (CRWMS M&O 1998e).

3.1.2 External Scenarios

The scenarios leading to near-field configuration classes begin with the source term consisting of the fissile material transported out of the waste package, represented generically by the incoming connectors E and F at the top of Figure 3-2a. The only exception is the scenario leading to configuration class NF-5a (from the incoming connector I), which has the fissile 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 particulates) that can be transported into or over the invert (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 3-2a.

The external criticality configurations 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) located in the unsaturated zone (rock above the water table so that all the porespace is not filled with water) either beneath the repository, at a narrowing of the tuff aquifer, or at the surface outfall of the saturated zone flow (FF-3c, 3d, 3e, respectively). Although the probability of the existence of such a reducing zone at Yucca Mountain is extremely low (CRWMS M&O 1996c), it is important because it has the potential for accumulating a higher mass of fissionable material than any of the other external configuration classes.

2. Accumulation, by sorption, onto clay or zeolite (FF-1b).

3. Precipitation of fissionable material in fractures and other void space of the near-field, either from 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, configuration NF-4a, 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. Since there is no mechanism for completely sealing the fractures in the bottom of the drift, an in-drift pond would be expected to occur only within a short time (weeks or less) following a high infiltration episode. The detailed analyses for the License Application will determine the range of leakage rates from such an in-drift pond.

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 the configurations FF-2a, 2b, 2c, 3b, 3c, for final accumulation in dead-end fractures, clay or zeolite, topographic lows, open fractures, and degraded concrete, respectively.

6. Accumulation at the low point of the emplacement drift (or any connecting drift), 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 (uranium) by precipitation, in the saturated zone, at the contact between the waste-package plume and a hypothetical up welling fluid or a redox front (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.

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

3.2 DETERMINING INTERNAL CONFIGURATIONS

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. 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. The validation of this portion of the methodology and the validation of the models used are discussed in Subsections 4.2.4 and 4.3.4. For each combination of waste form and waste package being evaluated, the corresponding configuration class, introduced in Section 3.1, must be further specified with the appropriate range of configuration parameters. For internal configurations this is a two step process. The first step involves performing a geochemistry analysis for each configuration class to identify the chemical composition of the corrosion products remaining in the waste package. The second step is the determination of the physical properties of the remaining corrosion products. The result of this process is a specific and detailed range of configurations that must be considered as part of the parametric criticality evaluation of each class of configurations as discussed in Subsection 3.4.4.

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 continuing analyses for the License Application will utilize 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, that will cover the officially approved range, specified by the appropriate project documents (currently the *Controlled Design Assumptions Document* (CRWMS M&O 1998h)).

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.

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

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

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

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

The 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 undegraded).

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

3.3 DETERMINING EXTERNAL CONFIGURATIONS

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 portion of the 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 very conservative approximations to compensate for the much greater uncertainty. This validation process is described in Subsection 4.2.4.

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, by combining the geochemical and physical flow analyses of Section 3.2. The essential subsequent steps are:

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

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

3. Determination of mineral precipitates from reactions of the waste package plume with the host rock fracture walls, using EQ3/6. The calculation must account for both fissile 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. 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 for this purpose; the validation of EQ3/6 in the repository environment is discussed in Subsection 4.2.4.

For those configurations found to have criticality potential (according to the portion of the methodology given in Section 3.4, below), 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 3.5.

3.4 CRITICALITY EVALUATION OF CONFIGURATIONS

The portion of the methodology for evaluating the potential for nuclear criticality in the Yucca Mountain repository is summarized in this section. First, the computer codes used for the neutronic evaluations are presented. This is followed by a discussion of the portion of the methodology for establishing burnup credit for commercial SNF (including the selection of principal isotopes). The section concludes with an overview of the portion of the methodology for evaluating criticality potential. The portion of the methodology presented in this section is part of the overall risk-informed approach for criticality analysis. As noted in Chapter 1.0, acceptance of the portion of the methodology for performing criticality evaluations of postclosure configurations as discussed in this section is sought in this report. Specific aspects of the portion of the methodology for which NRC acceptance is sought are noted throughout this section. The full list of items for which acceptance is being sought are listed in Section 1.2

The potential for nuclear criticality is determined by material composition and geometry of this material (i.e., waste form configuration). For a commercial SNF assembly and for a naval SNF assembly, the initial material composition (i.e., composition at time of emplacement in a repository) is governed primarily by the operating history of the assembly in a nuclear reactor. For other waste forms, no credit is taken for previous operating history. One component of the methodology addresses the effects of reactor operating history on the initial material composition of commercial SNF. During the long disposal time period, the material

composition and geometry will change from their initial condition based on isotopic decay and material degradation processes. Thus, the potential for nuclear criticality will change during the disposal time period. The criticality analysis methodology is applicable for evaluating the criticality potential of fissionable material configurations throughout the postclosure period of regulatory concern. The flow of the criticality analysis process is presented in Figure 3-3. This figure is referenced throughout the discussion in Section 3.4.

3.4.1 Computer Codes

Criticality analyses for disposal are performed using a combination of computer codes to calculate the material (isotopic) composition of commercial SNF and the effective neutron multiplication factor (k_{eff}) of waste form geometric configurations. Criticality is defined by the value of k_{eff} (k_{eff} = 1.0 for criticality). However, as discussed in Subsection 3.4.4, a configuration is considered potentially critical when the calculated value of k_{eff} is less than unity because allowances are made for the bias and uncertainty in the calculation model, as well as other potential margin. Isotopic concentrations for commercial SNF are obtained from computer codes contained in the SAS2H sequence of SCALE (ORNL 1995). Isotopic concentrations for naval SNF will be described in a separate addendum. For other waste forms, the fabrication design values are used for the isotopic concentrations of fissionable material. Neutron multiplication factors (k_{eff}) are calculated with the MCNP (ORNL 1997) code, which uses the isotopic compositions of the materials (including those from the degradation analysis described in Sections 3.2 and 3.3), and a system of nuclear data libraries, plus a detailed model of the geometry, to calculate the k_{eff} of the system. Subsections 4.1.1 and 4.1.2 describe the code systems and their associated nuclear data libraries. A validation process for the neutronic models that uses these codes is described and illustrated in Subsection 4.1.3. Acceptance of the validation process is sought in this report. The applicability of the neutronic models to specific waste package conditions in the repository will be demonstrated and referenced in the License Application using this validation process. Validation of the neutronic model for the range of neutronic parameters presented in Subsection 4.1.3.4.1 is sought in this report.

In the future, it is possible upgraded versions or other computer code systems will be selected to perform analyses for the License Application. If these upgraded or different computer codes are to be used, they will be validated in accordance with the same processes presented in this topical report.

3.4.2 Material Composition of Commercial SNF

The portion of the methodology for predicting SNF composition at any postclosure time starts with calculating the isotopic concentrations of fissionable and neutron absorbing isotopes to be used for criticality evaluations (Figure 3-3). These calculations (for commercial SNF) are based on conservative model input parameters (discussed in Chapter 4.0), fuel-assembly burnup data (which are verified with measurements), disposal time period, and fuel-assembly design data.

Taking credit for the reduced reactivity associated with the net depletion of fissionable isotopes and the creation of neutron-absorbing isotopes during the period since nuclear fuel was first inserted into a commercial reactor is referred to as burnup credit. This period includes both 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.

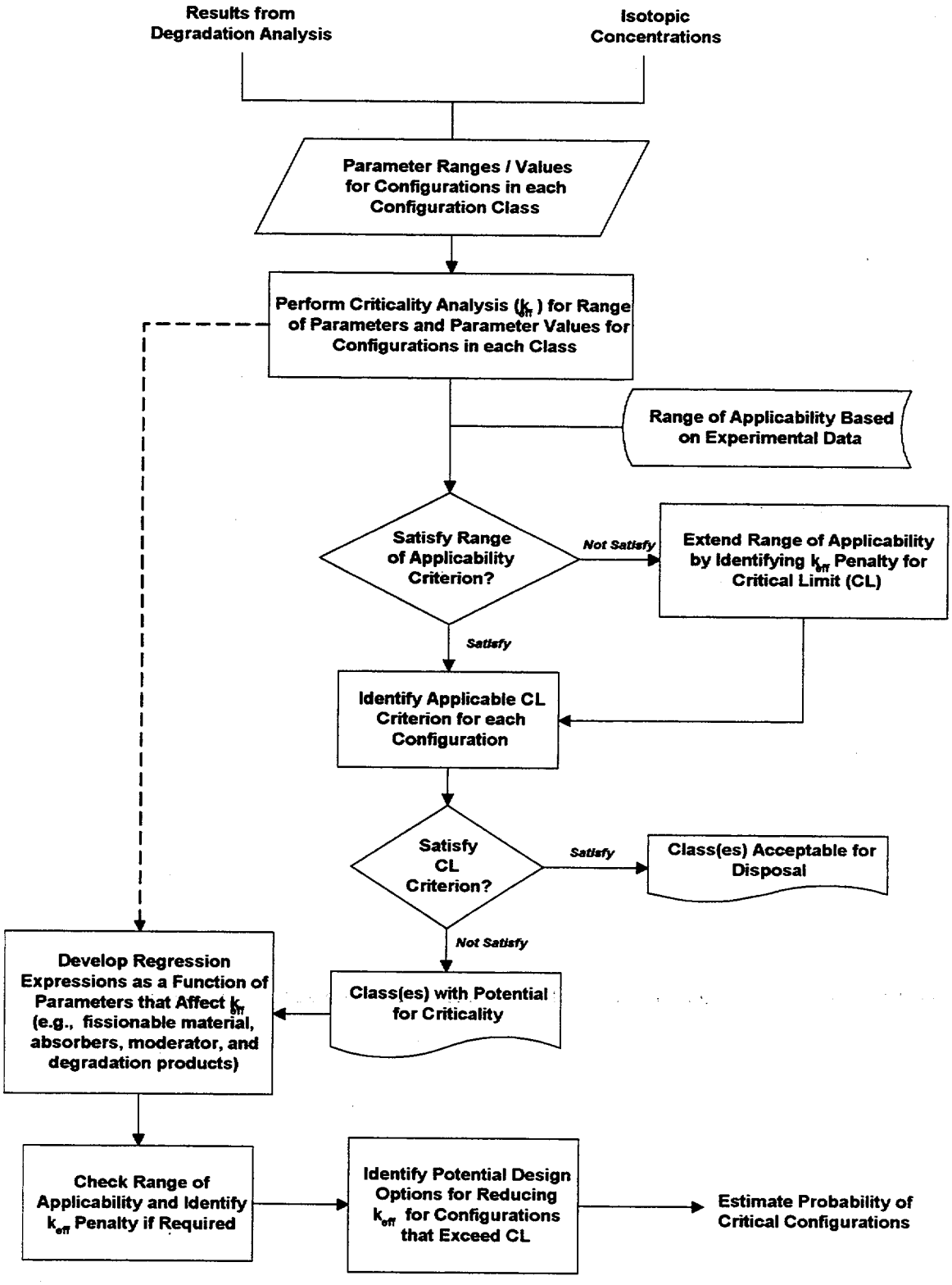


Figure 3-3. Criticality Analysis Methodology

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. Burnup credit accounts for the reduced reactivity potential of a fuel assembly associated with this power production mode and varies with the fuel burnup, cooling time, and the initial enrichment of fissile material in the fuel.

Local conditions in the reactor core during burnup that affect the neutron spectrum, and therefore the isotopic composition of the fuel at discharge from the reactor, must be quantified if burnup credit is to be appropriately applied. These conditions include variations in reactor power density (and associated moderator and fuel temperature variations), addition of neutron-absorbing materials (e.g., soluble boron, control rods, control blades, and burnable poison rods), and alteration of the amount of moderator material (e.g., void fractions and moderator displacement by non-fuel rods). Investigations of some of these conditions are discussed in DeHart (1995). The disposal criticality analysis methodology examines local variations in these conditions in reactor cores when the fuel is irradiated to produce commercial SNF. The treatment of these local variations by the methodology is discussed as part of the model validation process in Subsection 4.1.3.

When the methodology is applied to the waste package/engineered barrier system (WP/EBS) design, conservative values will be used for modeling reactor conditions for burnup calculations. Proposed requirements for modeling burnup of commercial SNF for design applications are presented in Subsection 4.1.3.1.4. As noted in Section 1.2, this report is requesting NRC acceptance of these requirements as being appropriate to ensure adequate conservatism in the isotopic model for burnup credit. If NRC acceptance is granted, these requirements will be followed for isotopic model validation for repository applications. The isotopic model for burnup credit will be demonstrated, during model validation, to produce conservative k_{eff} values for commercial SNF throughout the postclosure period of regulatory concern. Acceptance of the isotopic model validation will be sought as part of the License Application.

3.4.3 Principal Isotopes for Commercial SNF Burnup Credit

The criticality analysis methodology uses a subset of the isotopes present in commercial SNF. The process of establishing the isotopes to be included is based on the nuclear, physical, and chemical properties of commercial SNF isotopes. The nuclear properties considered are cross-sections and half-lives of the isotopes; the physical properties, concentration (amount present in the SNF) and state (solid, liquid, or gas); and the chemical properties (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 3-1 lists these isotopes. Analyses supporting the selection of these isotopes are presented in *Principal Isotope Selection Report* (CRWMS M&O 1998f). The conservatism in the use of the principal isotopes for criticality analyses with spent nuclear fuel is addressed in *Summary Report of Commercial Reactor Critical Analyses Performed for Disposal Criticality Analysis Methodology* (CRWMS M&O 1998k).

Table 3-1. Principal Isotopes for Commercial SNF Burnup Credits

^{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 listed in Table 3-1 are sufficient and adequately justified to model intact commercial SNF in support of seeking burnup credit. The relative importance to criticality potential of individual isotopes will vary as a function of disposal time and the condition of the SNF. The proposed process for selecting isotopes from this list for degraded SNF conditions relies upon the degradation analyses geochemical models presented in Section 4.2.

Acceptance is sought for the process of using detailed geochemical models to account for the presence of elements, and then using the statistical method presented in Subsection 4.1.1.2, to account for the uncertainty in long-term decay of individual isotopes. The isotope's effect on criticality potential will be analyzed and acceptance of the specific isotopes, from those listed in Table 3-1, will be sought along with the isotopic model validation for the specific postclosure repository conditions as part of the License Application.

3.4.4 Criticality Evaluations

Waste form configurations are identified for evaluating criticality potential as described in Sections 3.2 and 3.3. The configuration classes are identified and degradation analyses are performed to define specific parameter ranges and parameter values for configurations in each class. As shown in Figure 3-3, parametric criticality evaluations are performed for configurations in each class, using the criticality model described in Subsection 4.1.2. For these evaluations, a critical limit (CL) is placed on the calculated value of k_{eff} for the configurations 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 method bias and uncertainty are obtained from analyzing experimental systems with a range of neutronic parameters that are representative of those used in the parametric criticality evaluations. The process for establishing CL values (and hence the CL criterion) is discussed in Subsection 4.1.3.2. The experimental data for estimating the method bias and uncertainty are used in establishing the range of applicability of the CL. The range of applicability is defined by the range of the parameters covered by the experimental database and the trending analysis performed for this data. A description of the process for defining the range of applicability of the experimental database used for this report is provided in Subsection 4.1.3.3.1. The results of trending analyses performed for the experimental data are illustrated in Subsection 4.1.3.4. The criticality model validation process consists of calculating the CL values and establishing the range of applicability of the CL data. Acceptance of this validation process and the CL criterion is sought in this report. The acceptance of specific CL values, and the accompanying range of applicability of these values for specific waste package conditions in the repository will be sought as part of the License Application.

The material composition and geometry (i.e., configurations of fissionable and other materials) may vary significantly during the time period of regulatory concern. Thus, different sets of experimental data are used in the validation process to represent different ranges of degraded waste form configurations that may occur during the disposal time period. The range of applicability criterion will be developed from the experimental database and documented as part of the License Application. As indicated in Figure 3-3, parametric criticality evaluations are compared with the range of applicability criterion. These comparisons establish the configurations covered by the experimental database. The process of satisfying the range of applicability criterion also identifies the applicable CL criterion for the configuration. If the criterion is not satisfied, the range of applicability may be extended by extrapolating the trended CL data and identifying a conservative k_{eff} margin to be applied. Although not shown in Figure 3.3, another option is to enlarge the range of the experimental database by adding additional experiments. If this option is chosen, new trending analyses are made, and the range of applicability criterion and the CL criterion would be revised to reflect the new experimental data. The approach for extending the range of applicability is described in Subsection 4.1.3.3.3.

Values of k_{eff} from the parametric criticality evaluations are compared with the CL criterion. This comparison separates the configuration classes based on their potential for criticality. For configurations where the peak k_{eff} may exceed the CL criterion over some portion of the parameter range of a configuration class, multivariate regressions for k_{eff} are developed as a function of parameters that significantly affect criticality. These parameters include the amounts of fissionable material (e.g., based on burnup, enrichment, and cooling time for commercial SNF), absorber material, moderator material, and degradation products. The multivariate regressions are developed from MCNP calculations for representative configurations and values of these parameters. The standard error of regression is established during the development of the regression expressions and is added to the predicted k_{eff} values for comparison with the CL criterion. The regression expressions provide a convenient method for identifying the range of parameter values where k_{eff} may exceed the CL. Potential design options can then be implemented for reducing k_{eff} of configurations that exceed the CL. The regression expressions also facilitate developing loading curves (e.g., for commercial SNF, identifying acceptable enrichment versus burnup ranges for assemblies loaded in waste packages). The process for developing the multivariate regressions for k_{eff} will be documented as part of the License Application.

The range of parameters and parameter values covered by the regressions must be checked against the range of applicability criterion and a conservative k_{eff} margin applied if the trended CL data must be extrapolated. For those configurations showing potential for criticality, an estimate of the likelihood (probability) of the configuration is made. The regression expressions also facilitate probability calculations. The portion of the methodology for estimating the probability of occurrence of potential critical configurations is described in the following section.

3.5 ESTIMATING PROBABILITY OF CRITICAL CONFIGURATIONS

This section describes the general portion of the methodology for estimating the probability of occurrence of criticality in the fissionable material contained in a waste package emplaced in the repository. Acceptance is sought for this portion of the methodology for estimating the probability of occurrence for potentially critical configurations. Further details of the models used in this portion of the methodology are given in Section 4.3, and the application of this methodology to two specific types of waste forms and waste packages is illustrated through

examples in Appendices C and D. Acceptance is also sought for the use of the multivariate regression model as a significant component this portion of the methodology.

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. The calculated probability per waste package is compared with the waste package probability criterion, which is derived from the repository probability criterion, which is defined as an expected number of criticalities of 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 fissile 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 (CRWMS M&O 1998h) to obtain a derived waste package probability criterion of approximately 10^{-4} expected criticalities, per waste package in 10,000 years.

This derived probability criterion is not proposed for regulatory purposes, and will only be used to guide decision processes internal to waste package design. A more refined analysis for applying the probability criterion to the individual waste packages may be developed for the license application.

The first step in estimating criticality probability is to identify the configuration classes that are critical, which, in turn are developed from the master scenarios. Probability will be estimated for all configuration classes that have a k_{eff} exceeding the critical limit 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 that can occur. For waste forms that have a wide range of

characteristics (e.g., burnup and enrichment, which vary significantly over the family of commercial SNF), this screening uses a multivariate regression for k_{eff} as a function of waste form parameters and configuration parameters. Such a regression function is developed from a set of MCNP calculations for representative values of these parameters. An illustration of the regression development and application is given in Appendix C. 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 (Monte Carlo trials, 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.

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). And there are those 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 borated stainless steel remaining in the waste package. Definitions of these concepts are given with the discussions of the probabilistic model in Section 4.3.

The distributions developed for scenario-related parameters involve the physical and chemical analyses identified in Sections 3.2 and 3.3 and using the models and computer codes for these models, as described in Chapter 4.0. 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. 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. Some of the configuration-related parameters are specified deterministically by the Configuration Generator Code (described in Subsection 4.3.4), which, in turn, uses inputs from

detailed chemical process codes, such as EQ3/6 (described in Section 4.2). 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 example given in Appendix C evaluates the increase in probability of a criticality caused by the misloading of assemblies having a high criticality potential into a waste package designed with only minimal criticality controls. This example is given for illustrative purposes only, because misloading is a recognized risk in nuclear power plant operation; it is expected that operation plans developed for License Application will reduce the probability of misload to a level so low as to be of little or no concern.

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 ESTIMATING CONSEQUENCE OF CRITICALITY EVENT

This section describes the portion of the methodology for estimating the consequence of potentially critical events internal and external to the waste package. Acceptance is sought for this portion of the methodology for estimating the consequences of potential criticality events with the criticality consequence models. When the k_{eff} of the configuration analyzed exceeds the CL and the probability of occurrence of that configuration exceeds the waste package probability criterion, currently derived in Section 3.5 as approximately 10^{-4} per waste package in 10,000 years, a consequence analysis is performed.

The consequence analysis determines the impact of a potential criticality event on the radionuclide inventory and on the thermal effect (based on the energy yield) within the repository. Probabilities of criticality events and the results of the consequence analyses provide input for a PA to demonstrate that the repository performance objectives are met.

It should be noted that, since the CL may be significantly less than 1.0 (reduced by the bias and uncertainty, and any additional quantified margin), criticality consequences will generally be estimated for configurations with a k_{eff} significantly less than 1.0 (to allow for bias and uncertainty).

3.6.1 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 specific types of criticality events that might occur in, or near, the Yucca Mountain repository, it is useful to summarize those aspects of criticality that strongly influence the nature of the consequence; slow versus fast reactivity insertion rate, steady-state versus transient, and under-moderated versus over-moderated.

Slow versus fast reactivity insertion rate. Typical potential reactor criticality accidents could involve reactivity insertion times of 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 such as an earthquake or a rockfall (CRWMS M&O 1997a).

Steady-state versus transient. A steady-state criticality produces energy at a constant rate, and that energy is immediately converted to heat. Criticality transients that can occur in the repository will be sufficiently slow that significant kinetic energy released will not occur. In order to produce a sufficiently rapid transient that a significant kinetic energy is released to move masses of material, the assembly would have to (1) be confined either externally or by inertia, (2) experience a rapid increase in k_{eff}, in a time short compared to the interval between source neutron emissions, and (3) have a reactivity sufficiently above critical that the rate of increase of neutron density and power generated (they are proportional) is greater than doubling every 1/1000 second.

Under-moderated versus over-moderated. For thermally critical configurations, there is an optimum moderator concentration (which yields the smallest possible critical mass); 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 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. 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.

3.6.2 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) estimate of total radionuclide increase for the same initial conditions. Both types are illustrated by example for commercial SNF in Appendix C.

The steady-state analysis starts with the already identified potentially critical configurations and estimates the power and duration of a steady-state criticality. The power level is determined by the reactivity feedback (the influence of temperature 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 drip rate into the waste package, for internal criticality, or 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 with ORIGEN-S, to estimate the increment in radionuclide inventory caused by the criticality event.

The transient analysis uses codes that model both the neutronics and the response of the physical system to any heat or pressure pulse caused by the criticality event. Such codes will be demonstrated to be appropriate as part of the License Application process. The example given in Appendix C shows only insignificant energy and pressure pulses. Although some theoretical analyses have identified larger, disruptive consequences, the required accumulation and geometry of fissionable mass is expected to be beyond anything physically possible in the repository, which will be demonstrated as part of the License Application.

3.6.3 Criticality Consequence Criterion

The criticality consequence criterion is that for each radiologically significant nuclide, the expected value of the radionuclide increment from any single criticality event be less than 10 percent of the radionuclide inventory (curies present at time of criticality) that is available for release and transport to the accessible environment. (Available for release means that the waste packages that have breached barriers and the waste form that have degraded sufficiently to expose the radionuclides to dissolving water.) The average time of breach is estimated from the Performance Assessment corrosion model for the waste package barriers. The value of this criticality consequence criterion was chosen to be one order of magnitude less than the uncertainty of a typical input parameter to the TSPA estimate of dose (CRWMS M&O 1998j). If the calculation of the radionuclide increment due to a possible criticality in a specific waste form in a specific waste package is greater than this criterion, then the ultimate consequence, the increment on the dose at the accessible environment, will be calculated according to the methodology of the TSPA. The impact of this dose increment on the performance objectives of the repository will be assessed as discussed in Section 3.7.

This criticality consequence criterion can be multiplied by the repository probability criterion (an expected number of criticalities less than 1 in 10,000 years given in Section 3.5) to give an intermediate risk criterion of less than 10 percent increment in radionuclide inventory in 10,000 years. Changes in the value of this intermediate risk are directly reflected in the overall repository risk, dose at the accessible environment (Section 3.7). Therefore, intermediate risk may be a good surrogate for dose at the accessible environment, to get rapid design guidance feedback without lengthy TSPA calculations. It should be noted that the consequence criterion is intended for design guidance only. All the probability-consequence products will be included in the full TSPA dose used to demonstrate licensing compliance for the final waste package design.

3.7 ESTIMATING CRITICALITY RISK

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. 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 appropriate regulatory agency) at a later date.

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 input, the increased radionuclide inventory and thermal effects estimated by the criticality consequence model.

Appendix C illustrates the process for estimating total dose to the affected population as a function of time.

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 criticality-induced inventory, 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 portion of the methodology which has been briefly described in Subsection 3.6.2, and is described further in Section 4.4. 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 concentration 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 glass, 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 also can 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.

4.0 MODEL DESCRIPTION

Chapter 3.0 described the methodology for performing criticality analyses for the repository. This methodology is based on using models to perform neutronic calculations, developing degraded internal and external configurations of fissionable materials, estimating the likelihood (or probability) of occurrence of critical configurations, and assessing both the consequences of potential criticality events and repository performance. Chapter 4.0 describes each of these models and discusses their validation. Specific aspects of these models, for which NRC acceptance is sought, are noted throughout this chapter. The full list of items for which acceptance is being sought are listed in Section 1.2. The specific aspects noted in Chapter 4.0 are items G through M from the full list in Section 1.2.

The models are described and discussed in the following sections of this chapter. The neutronic models are presented in Section 4.1. The isotopics model is presented in Subsection 4.1.1 and the criticality model in Subsection 4.1.2. The validation process for which NRC acceptance is sought for the neutronic models, and the limited validation, are presented in Subsection 4.1.3. The degradation models are presented in Section 4.2, the corrosion models in Subsection 4.2.1, and the geochemistry models (internal and external) in Subsections 4.2.2 and 4.2.3. The validation process for, and validation of, the degradation models are presented in Subsection 4.2.4. Section 4.3 presents the probability calculation models that determine the likelihood of potential criticality events, the validation process for the model, and the validation of the model for a specific case. The criticality consequence models are presented in Section 4.4. A brief description of the total system performance models and process that will be used to evaluate the impact of any potential criticality event(s) on the repository performance is presented in Section 4.5.

4.1 NEUTRONIC MODELS

This section describes two types of neutronic models used in assessing the criticality potential of waste forms during the postclosure period of the geologic repository. The first model uses the SAS2H (ORNL 1995) computer code to calculate the isotopic composition of SNF from commercial light water reactors. The isotopic compositions model for naval SNF will be discussed in a separate addendum. The isotopic compositions for other waste forms are assumed to be fabrication design values (for HLW the technical specifications concentration limits for fissile isotopes will be used). However, it must be confirmed that this composition is conservative 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). Isotopic decay during disposal is modeled for all waste forms as a function of time. The second model uses the MCNP (ORNL 1997) computer code to analyze configurations of fissionable material for potential criticality events. This model is intended to apply to all waste forms except intact naval fuel. The range of applicability for the models (to the proposed repository at Yucca Mountain), which will be established during the validation process, is also discussed in this section. The experimental data and supporting analyses for illustrating the validation process are described in CRWMS M&O 1997b, 1998k, 1998m, and 1998n. Acceptance of the validation process for both of these models is sought in this report. Acceptance of the limited validation of these models for commercial SNF in the range of neutronic parameters presented in Subsection 4.1.3.4.1 is also sought in this report. The applicability of these models for specific waste package conditions in the repository will be demonstrated and referenced in the License Application using the validation process described in later subsections of this chapter.

4.1.1 Isotopic Models

The isotopic model is used to calculate the concentrations of the fissionable and absorbing isotopes for criticality evaluations in a two-step process. First, the values to be used as the initial isotopic concentrations for the waste forms are calculated. For commercial SNF, these concentrations are the values when the fuel is discharged from the reactor. Proposed requirements are provided in Subsection 4.1.3.1.4 for ensuring conservative values are used for generating design basis values to be used in waste-package design. The naval SNF isotopic model will be used to obtain isotopic concentrations for naval waste forms. For other waste forms, the concentrations are assumed to be the waste form fabrication design values. The second step considers isotopic decay. The period for decay extends from the time when the initial depleted (or undepleted, depending on the waste form) concentration was established to the time for which the criticality evaluation is performed. The isotopic model used in each step is described in the following two sections.

The isotopic model will be validated using two types of commercial SNF data: criticality data and radiochemical assay data. The proposed requirements presented in Subsection 4.1.3.1.4 define the validation process and will be followed in the isotopic model validation for commercial SNF. Acceptance for the isotopic model validation process is sought in this report. Additionally, acceptance of this model (as described in this section) for the limited range of neutronic parameters presented in Subsection 4.1.3.4.1 is sought. Full validation of the isotopic model using this process will be performed to support the License Application.

4.1.1.1 Initial Isotopic Concentrations

This section addresses the model for predicting the isotopic concentrations of commercial SNF when it is discharged from the reactor. The concentrations calculated with this model, for the 29 principal isotopes defined in Subsection 3.4.3, are used for burnup credit (i.e., isotopic concentrations of discharged fuel) for intact SNF configurations inside the waste packages. Isotopic concentrations of the fission products (15 of the principal isotopes) are not included for degraded SNF configurations outside the waste package because the material separation, transport, and deposition processes for fission products differ from those of the actinides.

The neutronic model for calculating isotopic concentrations of commercial SNF uses the SAS2H sequence of the SCALE-4.3 computer code with the 44-energy group cross-section library (CSCI:30011 V4.3, CRWMS M&O 1997g). SAS2H is the control module for the analytical sequence. The functional modules (or codes) within the sequence are BONAMI, NITAWL-II, XSDRNPM, COUPLE, and ORIGEN-S. SAS2H converts user input data into the forms required by the functional modules. BONAMI and NITAWL-II perform problem-dependent resonance weighting of neutron cross-sections. XSDRNPM is a one-dimensional, discrete-ordinates code that produces a weighted cross-section library and spectral data. COUPLE uses this data to update an ORIGEN-S data library for selected nuclides. ORIGEN-S is a point-depletion and decay code that calculates the time-dependent isotopic concentrations using a matrix, exponential-expansion technique. For short-lived nuclides, a form of the Bateman equation is used to ensure better accuracy. ORIGEN-S computes the isotopic concentrations (actinides and fission products) for all specified operating histories. These histories include both power operation and shutdown intervals while the fuel was in the reactor. ORIGEN-S uses a point model; therefore, spatial effects are not explicitly modeled. However, fuel geometry and spectral effects are incorporated in the model (within the limits of the process) through the one-dimensional spatial and the 44-energy group spectral weighting of data by

XSDRNPM. ORIGEN-S is also used in calculating radioactive decay and the buildup of daughter isotopes after the fuel has been withdrawn from the reactor core.

A fuel assembly is modeled with SAS2H in one-dimensional cylindrical geometry. This modeling is a two-step process. First, XSDRNPM models the fuel as an infinite lattice of rods incorporating resonance self-shielding data from BONAMI and NITAWL-II. Second, cell-spectrum-weighted cross-sections from XSDRNPM are applied to the fuel zone in a larger cell model representing part or all of a fuel assembly within an infinite lattice. Material and volume ratios for the various regions or zones depicted by the larger cell model must be appropriate for the physical system being represented. Weighted cross-section and spectra data from this model are used by COUPLE to update the ORIGEN-S data library. ORIGEN-S performs point-depletion calculations to provide updated isotopic concentrations that are fed back into the one-dimensional model. The first step is then repeated and new weighted cross-section and spectra data are obtained for the next depletion calculation. Updating of the ORIGEN-S library for depletion time steps is performed to appropriately represent changes (with depletion) in the neutron energy spectrum within the fuel assembly. Once all of the ORIGEN-S working cross-section libraries are developed, a final ORIGEN-S calculation is performed using all of the previously created libraries to determine the depleted isotopic concentrations. A more detailed discussion of the SAS2H model for light-water-reactor (LWR) fuel is presented in CRWMS M&O 1998k.

4.1.1.2 Postclosure Isotopic Concentrations

This section discusses the method for addressing isotopic decay for the postclosure time period. The evaluation starts with the initial isotopic concentrations described in the previous section. Then ORIGEN-S uses the initial concentrations and the decay time of interest to calculate postclosure isotopic concentrations. The effects of uncertainties in the half-life and branching fractions used in predicting postclosure isotopic concentrations will be evaluated by a statistical method (using Monte Carlo). This approach is used to model the entire system of isotopic decay with all of the parent-daughter relationships. The effects of the uncertainties are quantified in this analysis in terms of the resulting isotopic distribution and its effect on reactivity.

This method for propagating uncertainties with a Monte Carlo analysis is based on performing many ORIGEN-S 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 ORIGEN-S calculations (i.e., including all isotopes) are used in a criticality calculation to predict the k_{eff} (criticality potential) for that set of isotopic concentrations. Uncertainties in the k_{eff} resulting from uncertainties in the half-life and branching fractions are established as a function of enrichment, burnup (for commercial SNF), and decay time. As will be noted later in Section 4.1.3.1.4, this method for treating isotopic decay will be applied repeatedly to a range of sets of initial postclosure isotopic concentrations to determine the largest values for uncertainty in k_{eff}. When a sufficient number of calculations are performed, a distribution of k_{eff} values is obtained about a mean value. The mean value for k_{eff} for each of these sets will also be compared with the k_{eff} value from a single criticality calculation for each set. The isotopic concentrations for each of these calculations will be based on a single set of ORIGEN-S calculations performed with nominal half-life and branching fraction values. Based on these comparisons, any potential bias in the k_{eff} associated with this method for evaluating uncertainties is estimated from the difference between the mean k_{eff} values and the k_{eff} values at nominal conditions.

This method for propagating uncertainties with a Monte Carlo analysis is repeated for a range of decay times. For commercial SNF, the process is also repeated for representative ranges of enrichment and burnup. The bias and uncertainty in k_{eff} are combined for each calculation, and the results are used to define bounding values. The bounding bias and uncertainty values are added to the predicted k_{eff} values for configurations of SNF in the repository for comparison with the critical limit criterion.

4.1.2 Criticality Model

The criticality model is used to calculate the k_{eff} of a wide range of fissionable material configurations during the disposal time period. A CL criterion is used for judging the predicted k_{eff} values. Although criticality occurs when k_{eff} of the configuration is equal to unity, allowances are made for the bias and uncertainty in the calculation model, as well as other potential margins. The CL is the calculated value of k_{eff} at which the configuration is considered potentially critical. CL values are established during the criticality model validation process. This section describes the computer code used in the criticality model and briefly discusses the solution method and material cross-section data used. More detailed descriptions of the computer code and criticality model are provided in ORNL (1997) and CRWMS M&O (1998k).

The neutronic model for predicting the potential for criticality uses the MCNP 4B computer code to calculate k_{eff} (or chain reaction potential) of systems with fissionable material (CSCI:30033 V4B2:V. CRWMS M&O 1998t). MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron transport, and has the capability to calculate k_{eff} for systems containing fissionable material. 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, as applied to neutrons in an MCNP criticality calculation, is based on following a number of individual neutrons through their transport, including interactions such as scattering, fission and absorption, and including leakage. The fission process is regarded as the birth event that separates generations of neutrons. A generation is the lifetime of a neutron from birth by fission, to loss by either 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., effective neutron multiplication factor, k_{eff}).

Using appropriate material cross-section data in an MCNP criticality calculation is essential to obtaining credible results. The cross-sections for the various neutron interactions establish the flow of the criticality calculation at each interaction site. Nuclear cross-section data are obtained by MCNP from several source evaluations (data libraries) (CRWMS M&O 1998m). The neutron cross-sections in the libraries are not collapsed into energy groups; instead, cross-sections are provided at energies ranging from very low energies through 20 MeV in sufficient detail that the original evaluation can be accurately reproduced by linear-linear interpolation. A description of the MCNP cross-section data used for the validation analyses in this report is given in CRWMS M&O (1998m).

MCNP also allows explicit geometrical modeling of material configurations. The composition of the waste forms used by MCNP for evaluating criticality potential are obtained from the isotopic model described in Subsection 4.1.1. The composition of naval SNF used for evaluating criticality potential are obtained from the naval isotopic model. The MCNP code will not be used in modeling criticality for intact naval fuel.

4.1.3 Neutronic Model Validation

This section describes the validation process for the isotopic and criticality models. This process also includes validating the computer codes and cross-section libraries used in these models. Acceptance of the validation process is sought in this report. The criticality model will be validated against critical experiments that are representative of potential critical configurations of fissionable materials in the repository. The isotopic model for commercial SNF will be validated using two types of commercial SNF data: criticality data and radiochemical assay data. Limited validation of these models (using the SAS2H sequence of SCALE 4.3 and the MCNP 4B computer code systems) for commercial SNF is provided in this report. A complete validation of the criticality and isotopic models for repository applications will be performed to support the License Application.

Benchmark calculations of measured data are one part of the validation process. This section first describes the criticality and radiochemical assay databases and benchmark calculations performed using this data. It then presents proposed requirements that will be used to ensure adequate conservatism in the isotopic model for burnup credit. This is followed by the process for establishing critical limits and the process for establishing the range of applicability of the CLs. Finally, the section concludes with a discussion of benchmark results and an illustration of trending analyses. These results are intended to support the acceptance of the neutronic models and the limited validation of this model for commercial SNF.

In the future, it is possible upgraded versions or other computer code systems will be selected to perform analyses for the License Application. If these upgraded or different computer codes are to be used, they will be validated in accordance with the same processes presented in this topical report.

4.1.3.1 Benchmark Calculations

Three types of experimental data will be used in validating the neutronic model. These are laboratory critical experiments (LCEs), commercial reactor criticals (CRCs), and radiochemical assays. The CRCs and LCEs are used in this report to illustrate the method for estimating bias and uncertainty for the criticality model and to support acceptance of the validation process portion of the methodology over a limited range of parameters expected to be representative of repository conditions. 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 using the methods presented in Subsection 4.1.3.2. This portion of the methodology will be used in the License Application and its references to calculate this bias and uncertainty for specific postclosure repository conditions. In addition, CRC data are used in this report to benchmark the isotopic model for intact initial configurations of commercial SNF. The radiochemical assays will be used for confirming the adequacy of the isotopic model for commercial SNF. Proposed requirements are also provided for ensuring that appropriate conservatism is applied in the isotopic model for burnup credit.

4.1.3.1.1 Laboratory Critical Experiments

Laboratory critical experiments (LCEs) will be used to benchmark the criticality model (as part of the validation) for a range of fissionable materials, enrichments of fissile isotopes, moderator materials, and absorber materials. Both bare and reflected experiments are represented. A total of 338 LCEs were analyzed for this report. These experiments can be divided into four sets: (1) Homogeneous Thermal systems, (2) Homogeneous Fast systems, (3) Thermal Arrays, and

(4) Thermal Lattices (arrays of fuel rods). The first three sets of experiments are used for benchmarking high-enriched SNF and are also used for low-enriched applications, such as certain degraded states of commercial SNF. The lattice configurations set is used to benchmark a range of moderator (water) configurations and a variety of neutron absorber configurations for commercial SNF.

These LCE sets are further divided into categories according to enrichment and fissionable material. These categories are summarized below, where the number of experiments for each category is shown in brackets. The fissile isotope for the uranium criticals (i.e., ^{233}U or ^{235}U) is shown, where applicable.

Homogeneous Thermal systems [209]
1. Mixed plutonium and natural uranium [34]
2. Plutonium [73]
3. High-enriched uranium (^{235}U) [81]
4. Low-enriched uranium (^{235}U) [15]
5. High-enriched uranium (^{233}U) [6]

Homogeneous Fast systems [10]
1. High-enriched uranium (^{233}U) [10]

Thermal Arrays [51]
1. High-enriched uranium (^{235}U) [22]
2. Intermediate-enriched uranium (^{235}U) [29]

Thermal Lattices (arrays of fuel rods) [68]
1. Low-enriched mixed oxide [13]
2. Low-enriched uranium oxide (^{235}U) [55]

For the application in this report, intermediate-enriched uranium is defined as having uranium concentrations greater than 10 wt. percent but less than 80 wt. percent of ^{233}U or ^{235}U. Low- and high-enriched uranium are outside this range.

4.1.3.1.2 Commercial Reactor Criticals

The CRCs represent commercial SNF in known critical configurations. Although the CRC evaluations provide excellent criticality benchmarks for SNF in a reactor, they do not provide benchmarks for isotopic concentration of individual isotopes. However, the integral contribution of these isotopic concentrations to criticality is provided by the CRC benchmark calculations. Thus, CRC evaluations address both isotopic model validation and criticality model validation with a single class of experiments but do not provide complete validation of both models. Evaluations of both LCEs and radiochemical assays will be performed to supplement the CRC evaluations and complete the neutronic models validation for repository applications.

This report includes data for 45 CRC statepoints (measured critical conditions at zero-power) that were analyzed (CRWMS M&O 1998k), consisting of data from two Babcock & Wilcox- and two Westinghouse-designed pressurized water reactors (PWRs). The CRC data are used to benchmark both the isotopic and the criticality models for intact initial configurations of commercial SNF. This data is believed to accurately represent the composition and geometry of much of the commercial SNF to be loaded into the waste packages. The CRC database covers annual, 18-month, and 2-year fuel cycles; initial ^{235}U enrichments ranging from 1.93 to

4.17 wt. percent; soluble boron concentrations ranging from less than 400 ppmB to over 2300 ppmB; radial zone loaded fuel; and a variety of burnable poison designs. The CRC database also covers statepoints for beginning-of-life (BOL) with all fresh fuel, beginning-of-cycle (BOC) with a mixture of fresh and burned fuel, and middle-of-cycle (MOC) to end-of-cycle (EOC) with all burned fuel. Validation of the neutronic models using the 45 statepoint data is described in Subsection 4.1.3.4.1.

The CRC database is being expanded to include additional PWR data (including data from Combustion Engineering reactors) with enrichments ranging from 1.6 wt. percent to 4.97 wt. percent and fuel-assembly data with axial blanket fuel. In addition, CRC data from boiling water reactors (BWRs) are being analyzed and added to the database. The expanded database will be used to complete the criticality model validation for commercial SNF for License Application.

For the CRC evaluations, the material composition of the SNF for each criticality statepoint is obtained from SAS2H. For the data presented in this report, the change in material composition with burnup is modeled with 16 to 18 axial zones for each fuel assembly based on fuel-assembly design and core-operations data. Local thermal-hydraulic feedback effects during core operations are modeled based on core follow calculations. The number of axial zones for the SAS2H model is chosen to agree with the core follow calculations (CRWMS M&O 1998k). Thus, detailed core history data are provided as input to SAS2H.

The core follow calculations were performed with the CASMO/NEMO code system (Babcock and Wilcox 1993; Edenius and Forssen 1989). The NEMO computer code (NEMO 7.8, June 1996) uses neutron cross section data provided by CASMO (CASMO-3, version 4.4), and this methodology has been accepted by the NRC for use in reactor physics calculations for reload licensing. Babcock and Wilcox (1993) is a topical report for NEMO, and also includes the Safety Evaluation Report (SER).

The analysis of the CRC benchmarks follows the process described in Subsection 4.1.3.2. These analyses are used to illustrate the process for estimating the bias and uncertainties and establishing the critical limit. Subsection 4.1.3.4.1 presents the range of neutronic parameters for the CRC evaluations. The results of the CRC analyses are presented in Subsection 4.1.3.4. Comparisons of k_{eff}, the regression of k_{eff}, and the critical limit for commercial SNF are provided in Figure 4-6. This analysis of the CRC data, including estimating the bias and uncertainties and establishing the CL (Figure 4-6), is believed to validate the neutronic model for commercial SNF for the range of neutronic parameters represented by the CRC evaluations. Acceptance of this limited validation of the neutronic models using the SAS2H sequence of SCALE 4.3 and the MCNP 4B computer code system is sought in this report. Acceptance for the validation of the neutronic model for specific waste package conditions in the repository will be sought as part of the License Application.

4.1.3.1.3 Radiochemical Assays

Radiochemical assay data from 7 PWRS and 3 BWRs were analyzed for this report (CRWMS M&O 1997b; Hermann and DeHart 1998), including 84 samples, 54 samples of which were from PWRs and 30 from BWRs. The initial ^{235}U enrichments for the data ranged from 2.45 wt. percent to 3.87 wt. percent. The burnups for the data ranged from less than 7 GWd/mtU to 46.5 GWd/mtU. Radiochemical assay data will be used in conjunction with CRC data to validate the isotopic model. Additional experimental measurements of commercial SNF samples are being conducted, which will be used for the isotopic model validation to support the License Application.

The benchmark analyses reported in CRWMS M&O 1997b and Hermann and DeHart 1998 (and supporting calculation documents) provide comparisons of calculated and measured isotopic concentrations. These comparisons provide one means for evaluating the isotopic model. However, the isotopic concentrations are influenced by the operating history of the fuel and the accompanying local neutron spectra effects. Since detailed operating history data is generally unattainable, assumptions must be made relative to the operating history. For design application, it must be demonstrated that the assumptions made for modeling the burnup of commercial SNF yield conservative values of k_{eff} for all applications of the burnup data. Proposed requirements are presented in Subsection 4.1.3.1.4 for ensuring that the assumptions made for modeling burnup yield conservative k_{eff} results.

Two types of data are used to address variations in the quantities and distributions of the isotopic concentrations in commercial SNF. The CRC data described in the previous section address the integral contribution of isotopic concentrations to criticality. Radiochemical assay data provide measured concentrations for individual isotopes. The assay samples are typically from individual fuel pellets from discharged fuel assemblies. As discussed in the following section, the measured isotopic data will be used in an evaluation process to ensure appropriate conservatisms are incorporated in the isotopic model for design applications.

4.1.3.1.4 Requirements for Isotopic Model Validation

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. Full acceptance of the isotopic model validation, which includes demonstrating that the requirements are met, will be sought as part of the License Application.

The first requirement addresses how reactor operating histories and conditions affect the isotopic concentrations in commercial SNF assemblies discharged from reactors. The representation of the axial burnup profiles, commonly referred to as "end-effects" (DOE 1997), in calculating the isotopic concentrations is also considered. The quantities and distributions of the isotopic concentrations are governed by the operating history of the reactor, including accompanying local neutron spectral effects. The isotopic concentrations used for the CRC statepoint analyses referenced in this report are based on core-operations data. 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 CRC statepoint analyses. 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 statepoint analyses, 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 isotopic model validation process, the sufficiency of the fuel assembly database used in satisfying the first requirement will be demonstrated.

A. Reactor operating histories and conditions must be selected together with axial 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. These bounding reactor parameters will be used to predict isotopic concentrations that, when compared to best estimate isotopic predictions of the measured radiochemical assay data or the measured radiochemical data itself, must produce values for k_{eff} that are conservative.

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 axial burnup profiles, commonly referred to as "end-effect" (DOE 1997), in calculating the isotopic concentrations is also considered. The quantities and distributions of the isotopic concentrations are governed by the operating history of the reactor, including accompanying local neutron spectral effects. The isotopic concentrations used for the CRC statepoint analyses referenced in this report are based on core-operations data. 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 CRC statepoint analyses. 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 statepoint analyses, 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 isotopic model validation 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 validating 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. The criticality calculations will assume an infinite array of the small sample of fuel rod where the assay data was obtained. Both calculations will consider those isotopes that were measured, plus moderator and cladding material. Following this procedure, the isotopic model must be shown to be conservative with respect to k_{eff} based on analysis of the entire range of radiochemical assay data described in Subsection 4.1.3.1.3 and CRWMS M&O (1997b).

The third requirement addresses changes to the initial isotopic concentration values, as a function of time, for postclosure. As described in Subsection 4.1.1.2, 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 4.1.1.2, 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) are conservative with respect to criticality. Therefore, the proposed requirements define the isotopic model validation process. Acceptance of this validation process is sought in this report.

4.1.3.2 Determination of Critical Limits

An essential element of validating a method for calculating criticality multiplication factors, k_{eff}, is estimating biases and associated uncertainties and incorporating these into critical limits (CL). The CL is the calculated value of k_{eff} at which the configuration is considered potentially critical, as characterized by statistical tolerance limits and other potential margin. A CL is associated with a specific type of waste form as represented by a particular set of benchmark criticality experiments.

Two basic methods for determining CLs are described here. One of these basic methods can be performed using either of two techniques. The elements of the process are shown in Figure 4-1.

As defined above, a CL includes biases and uncertainties that are calculated using the estimated values of k_{eff} for a particular set of benchmark criticality experiments, and other potential margin. For purposes of the discussion in Section 4.1.3.2, 4.1.3.3, and 4.1.3.4, only the statistical bias and uncertainty part of the CL is considered, except where specifically stated.

The regression or "trending" method (Subsection 4.1.3.2.1) uses linear regression techniques with an associated lower uniform tolerance band (LUTB) to establish an estimate of CL. This trend is investigated using appropriate benchmark criticality experiments for the waste material of interest. Trending in this context is simple linear regression of k_{eff} on the predictor variable that exhibits the strongest correlation coefficient with k_{eff}, with a statistically significant slope. Statistical significance is defined by the test of the hypothesis that the slope is zero. Here the predictor variable 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. These types of parameters are called neutronic parameters or just parameters in Subsection 4.1.3.2, Subsection 4.1.3.3, and Subsection 4.1.3.4.

Statistical significance of a linear trend is defined by the test of the hypothesis that the slope of the line is zero. This level of significance may be arbitrarily chosen, although there is a rational method for choosing a significance level. One must also choose a confidence level, also referred to as a statistical tolerance limit, to be used when calculating a CL. The choice of the level of significance for the hypothesis test and the choice of a confidence level are independent.

There are no specific rules for choosing a level of statistical significance. The level of significance commonly used is 0.05, although 0.1, 0.01, and 0.001 are used. For the trending method a level of significance of 0.05 was used for this topical when testing the hypothesis that the slope is zero, because it is commonly used. This topical does not seek approval for any particular values for level of significance. Approval of this value will be sought in License Application or its references.

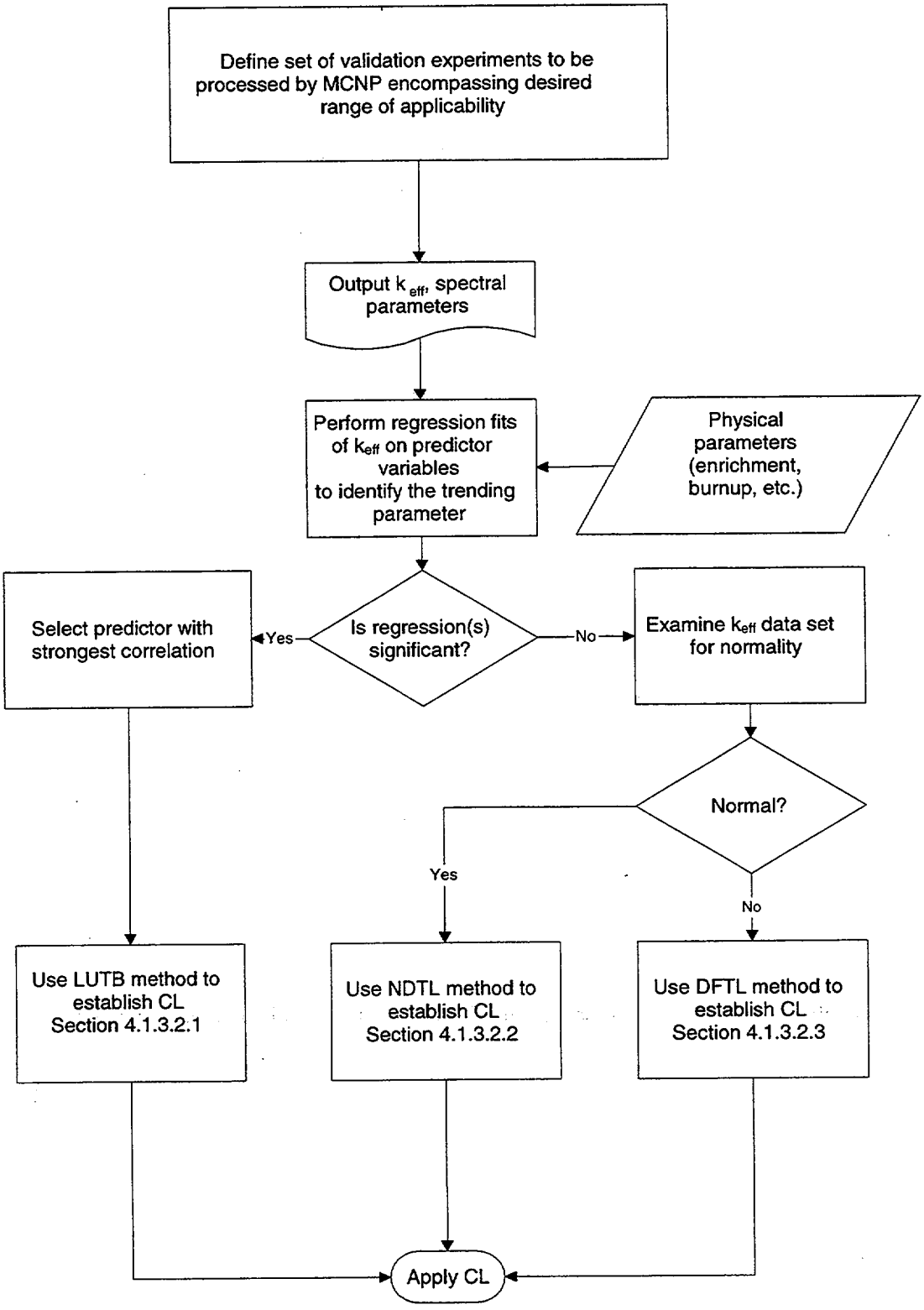


Figure 4-1. Process for Estimating a Critical Limit

The confidence level, characterized with two defining values, confidence limit and proportion of the population covered (or protected), is an estimation problem rather than a test of a hypothesis. The population is the number of calculated values of k_{eff} for a specific waste form, and waste package. For example a confidence limit of 95 percent with 99.5 percent of the population of the benchmark data set covered (95/99.5 percent) is predominantly used here. This applies to the trending and non-trending situations described in this section and illustrated in Section 4.1.3.4. The value of 0.95 (95 percent) for the confidence limit is common. The value of 0.995 (99.5 percent) for the population proportion is used here to maintain consistency with NUREG/CR 6361, *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages* (Lichtenwalter et al. 1997, p. 160). Other values could be used. The confidence level may be limited by the number of benchmark data points used. This is illustrated in Subsection 4.1.3.4.2. This topical report does not seek approval for any particular values for confidence limit or population coverage. Approval for these values will be sought in License Application or its references.

If there is no regression relationship, then statistical tolerance limit methods are used. These are described as non-trending situations. There are two tolerance limit methods described below, each specific to the description of the examination of k_{eff} values of the benchmark set with respect to the hypotheses of normality. Subsection 4.1.3.2.2 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 is the Normal Distribution Tolerance Limit, or NDTL. Subsection 4.1.3.2.3 describes the distribution-free tolerance limit (DFTL) technique.

In application, each of these methods must accommodate the concept described as the "no positive bias" rule, described in Lichenwalter et al. (1997, p. 160). This rule excludes benefits for cases in which the best estimate of the bias supplemented with associated uncertainties produce estimates of the multiplication factor greater than 1.0.

The range of a particular parameter for determining an estimate of CL becomes the range of applicability (ROA) of the parameter that characterizes the critical experiments used for benchmarking. Parameters other than those used for trending are also applied to characterize a system and the benchmark experiments. The range of these parameters, over the critical experiments used for benchmarking, also serve to define the ROA of the benchmarks. Since the benchmarks chosen to determine the range of these parameters do not always exactly represent the desired system, the ROA must be extended. The ROA and extension of the ROA are presented in the succeeding sections, as is a discussion of some results of trending over the ROA of the CRCs.

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

$$k_S + \Delta k_S \leq CL \qquad \text{Eq. 4-1}$$

where,

k_S = the calculated multiplication factor of a system to be considered subcritical,
Δk_S = the uncertainty in the value of k_S.

The CL is defined as,

$$CL = k_C(x) - \Delta k_C(x) - \Delta k_m \qquad \text{Eq. 4-2}$$

where,

$x =$ a neutronic parameter 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 the data set if there is no trend.

$\Delta k_C(x) =$ 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.

$\Delta k_m =$ additional quantified margin that would reduce the CL.

The statistical description of the scatter quantifies the variation of the data set and the contribution of the variability of the MCNP 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 of a parameter. Because both $\Delta k_C(x)$ and $k_C(x)$ can vary with this parameter, the CL is typically expressed as a function of this parameter, within an appropriate range of applicability derived from the parameter bounds.

Lichtenwalter et al. (1997, p. 158) defines an upper subcritical limit (USL) with an equation similar to equation 4-2. The difference between the definition of CL and USL is the definition of Δk_m. The Δk_m for a USL is defined as additional margin to ensure subcriticality and is often assigned an arbitrary administrative value of 0.05. The Δk_m for a CL does not contain an administrative margin. However, additional quantified margin is provided to ensure that sufficient conservatism is applied to prevent a criticality. Examples of additional quantified margin that will reduce the CL are: 1) the effect on k_{eff} associated with the long-term decay of radionuclides in the waste form and 2) the effect on k_{eff} associated with extending the range of applicability of the CL beyond the experimental database. The margin associated with the long-term decay of radionuclides is imposed by the third requirement for isotopic model validation discussed in Subsection 4.1.3.1.4. The margin associated with extending the CL beyond the range of applicability of the experimental database is discussed in Subsection 4.1.3.3.3.

The isotopic model provides additional conservatism. For commercial SNF, the first two requirements discussed in Subsection 4.1.3.1.4 are imposed to ensure that the assumptions made relative to the burnup characteristic of the SNF will produce isotopic concentrations, that when used for criticality evaluations, are conservative with respect to k_{eff}.

Additional conservatism is also imposed for commercial SNF by using the 29 principal isotope set discussed in Subsection 3.4.3. In addition, some types of DOE SNF will not use burnup credit. However, the conservatism in the isotopic model for all waste forms will be demonstrated for License Application.

If a calculational bias, β, is defined as $\beta = k_C - 1$, then 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 < 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. This positive bias adjustment sets $k_C = 1.0$ when k_C exceeds 1.0. This additional margin provides further assurance of subcriticality and represents additional conservatism (Lichtenwalter et al. 1997, p. 160).

The following sections present the three methods for the estimating a CL for nuclear systems or waste packages in a repository summarized above. One method addresses trending k_{eff} versus a neutronic parameter; the other two methods will be used if statistically significant trends cannot be identified using the first method for a set of benchmark experiments. Acceptance is sought for the following methods for estimating bias and uncertainty, and establishing the CL. Acceptance of specific CL values will be sought as part of the License Application.

4.1.3.2.1 Lower Uniform Tolerance Band

The first method for estimating a CL uses a tolerance band approach referred to as a single-sided, uniform width, closed interval, approach in *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages*, Lichtenwalter et al. (1997, pp. 160-162), and referred to in this report as a LUTB approach. This approach applies statistical techniques to estimate a lower tolerance band. 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 CL provided significant trends can be identified.

The purpose of this method is to estimate a uniform tolerance band over a specified closed interval for a linear least-squares model. The parameter chosen to trend the CL is the one that exhibits the best correlation. A detailed description of the LUTB method is given in Lichtenwalter et al. (1997, pp. 160-162); Bowden and Graybill (1966); and Johnson (1968, pp. 207-209). A description of the method for application to the methodology of this report is in CRWMS M&O (1998n, p. 73), which more fully describes the methods discussed here, and discusses in detail how the parameter that best correlates with the uncertainty is chosen. Provisions are made in the model 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 next two methods for estimating of a CL when trending is not used.

Figure 4-2 shows an illustration of the LUTB CL. The Y-axis is the value of k_{eff} and the X-axis is the value of a trending parameter, x. The plotted points represent a hypothetical set of k_{eff} values for the benchmark experiments. This is the data set used for the generation of the k – Regression, which is shown in Figure 4-2.

The CL is the lower bound of a tolerance limit for the critical system. There is a confidence that a percentage of the experiments that are at, or above, the CL are critical systems. The CL should be parallel to the k – Regression, except when a positive bias is indicated by the regression. In such an instance, the CL becomes "flat" because taking credit for a positive bias is not allowed. When a positive bias occurs, the regression prediction of k_{eff} are set to 1.0. This circumstance is shown in Figure 4-2 where the solid black "Critical Limit" line flattens because the positive bias is ignored. The red line extension indicates the CL with a positive bias.

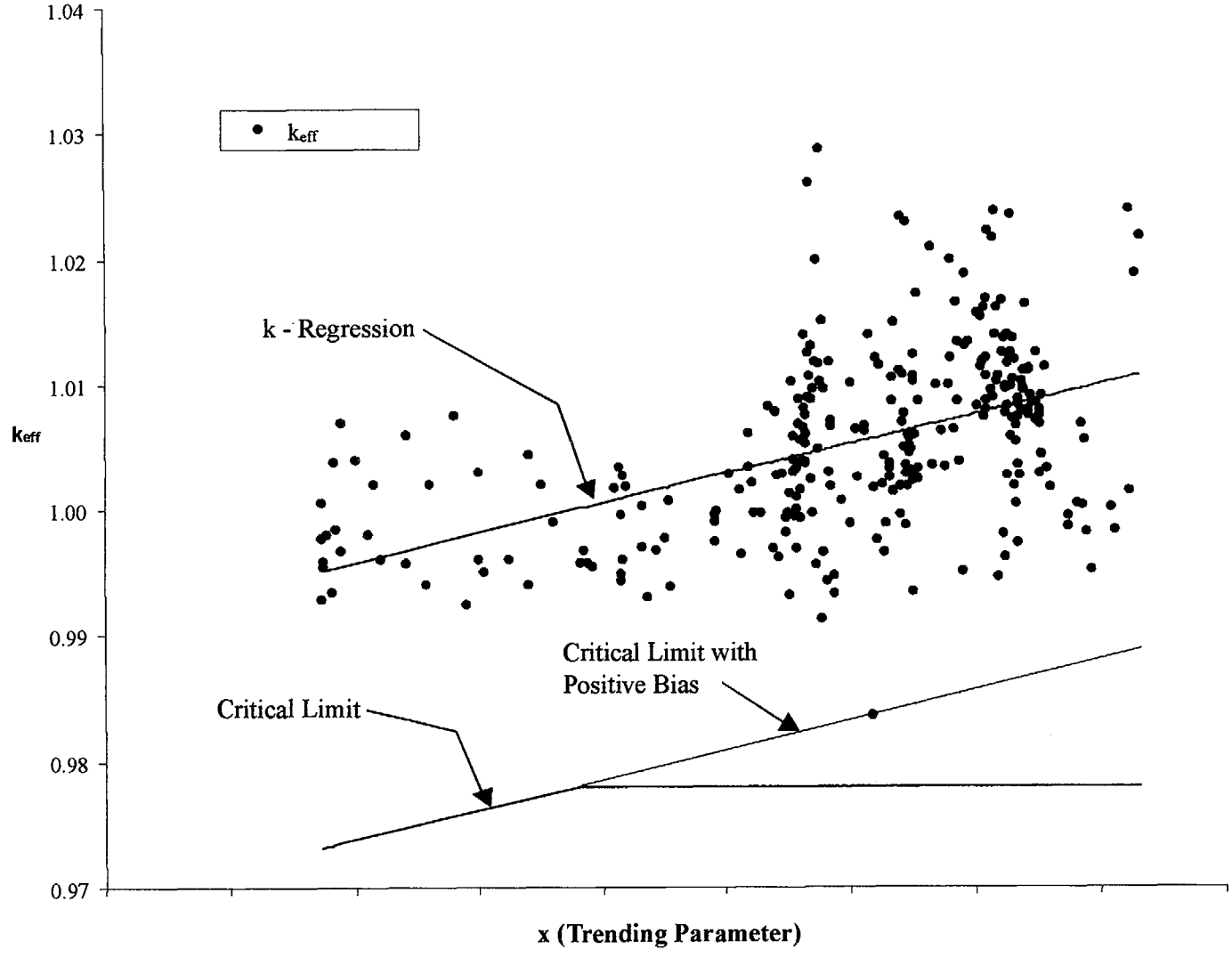


Figure 4-2. Illustration of Lower Uniform Tolerance Band Method

4.1.3.2.2 Normal Distribution Tolerance Limits

The NDTL method is one of two methods for estimating a CL for the repository in a non-trending situation. It is used for conditions in which the values of k_{eff} are sufficient in number and scope to determine if there is reasonable justification of normality of the k_{eff} values for the critical experiments. Given that the k_{eff} values produced by MCNP for the benchmark experiments can be shown to be normally distributed, then the CL can be calculated as

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

where: k_C is the average of the k_{eff} values, unless k_C is greater than unity (1.0), in which instance the appropriate value for k_C should be 1.0 to disallow positive uncertainty; $k(\gamma, P, df)$ is a multiplier defined in Owens (1963, pp. 399-402, Table 4.2) 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 S_P^2 is the sum of the inherent variance of the critical experiment data set plus the average of the MCNP variances for the critical experiment data set (Lichtenwalter et al. (1997, p. 159). A detailed explanation of this method is provided in CRWMS M&O 1998n, pp. 73-74).

There are several statistical techniques for testing the hypothesis that a random sample of data may be treated as originating from a normal distribution. Two such tests that can be applied for this hypothesis of normality are the **D´** test for data sets of 50 or more observations, and the **W** (Wilkes-Shapiro) test for fewer than 50 observations. These tests are described in ANSI N 15.15. Other tests for normality may be used in applications.

4.1.3.2.3 Distribution Free Tolerance Limit

The DFTL method, which is a variant of the previous method, also 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 requirements for applying distribution-free methods to establish a statistical tolerance limit are that the data be from a random sample from a continuous distribution. The methods are described in Natrella (1966, pp. 1-14, 1-15, 2-15); and Hogg and Craig (1965, 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 1966, 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 MCNP 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,

$$k_{eff1} < k_{eff2} < k_{eff3} < \ldots < k_{effN} \qquad \text{Eq. 4-4}$$

where 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

$$CL = k_{eff\,I} \qquad \text{Eq. 4-5}$$

provides the critical limit with the characteristics of confidence and population coverage available for the data set of interest.

4.1.3.3 Range of Applicability

This section presents the range of parameters that apply to the critical experiments used for benchmarks. Much of this section uses those parts of Lichtenwalter et al. (1997, pp. 157-180); ANSI/ANS-8.1; and Dyer and Parks (1997, pp. 11-17) that address validating the calculational method used to establish subcritical conditions outside of reactors.

Part of the range of applicability (ROA) of a benchmark data set is based on the range of parameter variation of the benchmark experiments that are used for estimating the CL. The other part is based on the range of fundamental parameters of the benchmark experiments. Lichtenwalter et al. (1997, p. 179) defines three classes of fundamental parameters or characteristics from which a fundamental parameter may be defined. The three classes are (1) materials of construction (including fissionable materials), (2) the geometry of construction, and (3) the inherent neutron energy spectrum affecting the fissionable material(s).

The next section describes the current range of neutronic parameters for the benchmark experiments. This is followed by Subsection 4.1.3.3.2, which relates the benchmark experiments to various waste forms. Extending the ROA is discussed in Subsection 4.1.3.3.3. After this, Subsection 4.1.3.4 provides some results where a CL is estimated within a defined ROA for commercial SNF.

4.1.3.3.1 Range of Neutronic Parameters

The process for validation of the calculational methods shown here is as follows:

A. Bias and uncertainties will be established through comparison with benchmark critical experiments that are applicable to the waste form and its associated waste package; a critical limit, previously described, will be estimated using the bias and uncertainties established.

B. The ROA for the bias and uncertainty, and the critical limit, will be based on the range of parameter variation in the experiments.

C. Any extension of the ROA beyond the experimental parameter field to the range of parameters in a particular waste package will be based on trends in the bias and uncertainty as a function of the parameters.

Guidelines for selecting the range of parameter variation in the experiments are given below.

Ideally, the set of benchmark experiments should match the waste form and package characteristics that most influence criticality. The characteristics of the waste package, including the waste form, and the benchmark experiments will be described by certain fundamental neutronic parameters. The following describes specific characteristics or parameters that should be considered.

A. The fissionable isotopes, the form (e.g., homogeneous, heterogeneous, metal, oxide, or fluoride), and isotopic composition of the fissionable material should match for the benchmark experiments and the applicable waste form. The fissionable isotopes used in the benchmark experiments should be as similar as possible, including enrichment and relative masses, and volumes as those materials in the waste form and waste package. Parameters such as enrichment and relative masses would be considered fundamental and should match for the benchmark and the applicable waste form.

B. The non-fissionable materials (stainless steel, boron, etc.) used in the benchmark experiments should be as similar as possible, including relative masses and volumes as those materials in the waste package design. Physical form and temperature of the materials should also be as similar as possible. The ratio of non-fissionable materials to fissionable materials should be similar.

The next set of parameters or characteristics relates to the geometry of the waste package, including the fissionable material contained therein. Potential fundamental parameters for geometry are more difficult to define than other parameters, but should in general cover the following characteristics:

A. The relative geometric position and quantity of the materials
B. The homogeneity or heterogeneity of the system
C. Shape of units and system(s)
D. Lattice pattern, spacing and interstitial materials in arrays, or reflector materials used

Comparison of the geometry of the waste package with the geometry of the benchmark experiments will be made to determine the most common characteristics of the two. A characteristic or a parameter derived from this characteristic is fundamental and will be defined with a range of applicability.

With regard to neutron energy spectrum, the neutron density versus energy should be considered by comparison of the following typical items from the benchmark experiments and the waste package environment:

A. Neutron leakage
B. Neutron absorption

C. Neutron fission or production
D. Neutron flux

The average energy of a neutron causing fission or absorption are commonly used parameters and would constitute fundamental parameters in this category.

Once fundamental parameters and a set of critical experiments have been established, calculated values of k_{eff} will be trended against a number of these parameters to determine the parameter that provides the best fit to the data from the benchmark critical experiments. This parameter will be used for extending the range of applicability, which will be necessary in almost all waste forms and their waste packages. If one parameter trends almost as good as another, the more conservative parameter should be used. The guidelines for extension of the range of applicability are in Subsection 4.1.3.3.3.

Acceptance of the process and guidelines for establishing a range of applicability given above is sought in this report. The applicability of this process and guidelines to specific waste package conditions in the repository will be demonstrated and referenced in the License Application using the validation process described in Subsections 4.1.3.2 and 4.1.3.3.

The following three figures are shown to illustrate the range and distribution of neutronic parameters that characterize the current benchmark critical experiment data set of 338 laboratory critical experiments (LCEs) and 45 commercial reactor critical experiments (CRCs). CRWMS M&O (1998n) presents a number of parameters for this benchmark data set. Three of those parameters are shown in this report.

Figure 4-3 shows the range and distribution of the average energy of a neutron causing fission (AENCF) parameter over the existing benchmark data set. The AENCF is used for the trending analysis of certain types of SNF, and is an index of the neutron spectrum of a system. As such, it is a fundamental parameter. This histogram plot shows the number of experiments within selected ranges of the parameter AENCF. Note that the scale on the abscissa of this figure changes.

Figure 4-4 shows the range and distribution of system ^{235}U enrichments included in the benchmark data set. Enrichment is a fundamental parameter for characterizing benchmark experiments. The system enrichment is the total weight of ^{235}U in each experiment divided by the total weight of uranium in each experiment. For the laboratory criticals the system enrichment is the enrichment of the fuel in the experiment or an average if several enrichments are used. For the commercial reactor criticals this number represents the average enrichment over the entire system. Here again the units on the abscissa change.

Figure 4-5 shows range and distribution of the core average burnup for the commercial reactor criticals in the benchmark data set. For this figure the units on the abscissa are constant. As shown later, k_{eff} for commercial SNF trends well with the average burnup of a commercial core.

The following is a summary of Subsection 4.1.3.3.1.

Fundamental parameters are those that relate to 1) material concentrations, 2) geometry, and 3) spectrum. Lichtenwalter et al. (1997, p. 163) further states that the fundamental parameter that gives the best correlation will be used to define a ROA.

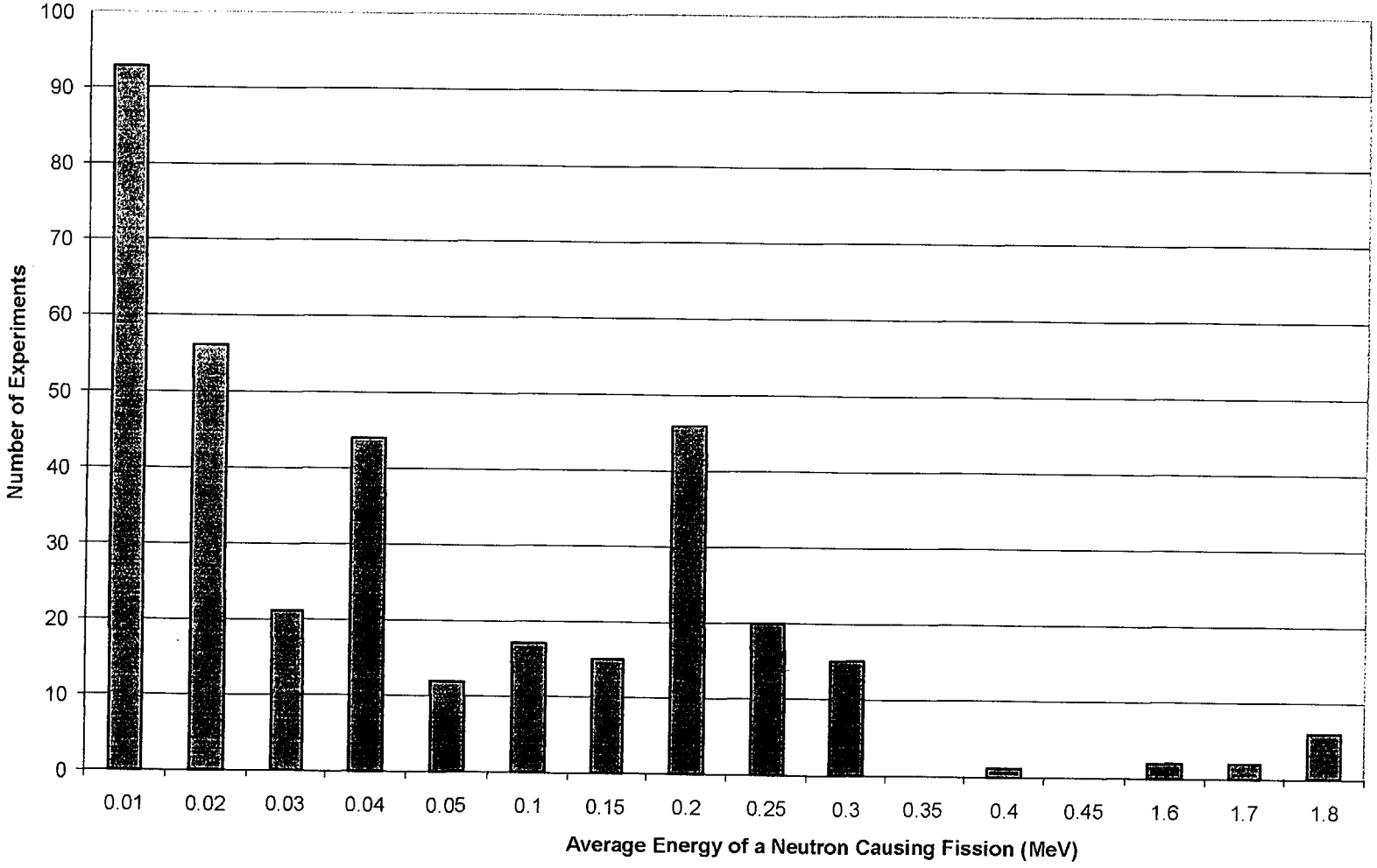


Figure 4-3. Range and Distribution of the Average Energy of a Neutron Causing Fission (AENCF) for the Benchmark Data Set

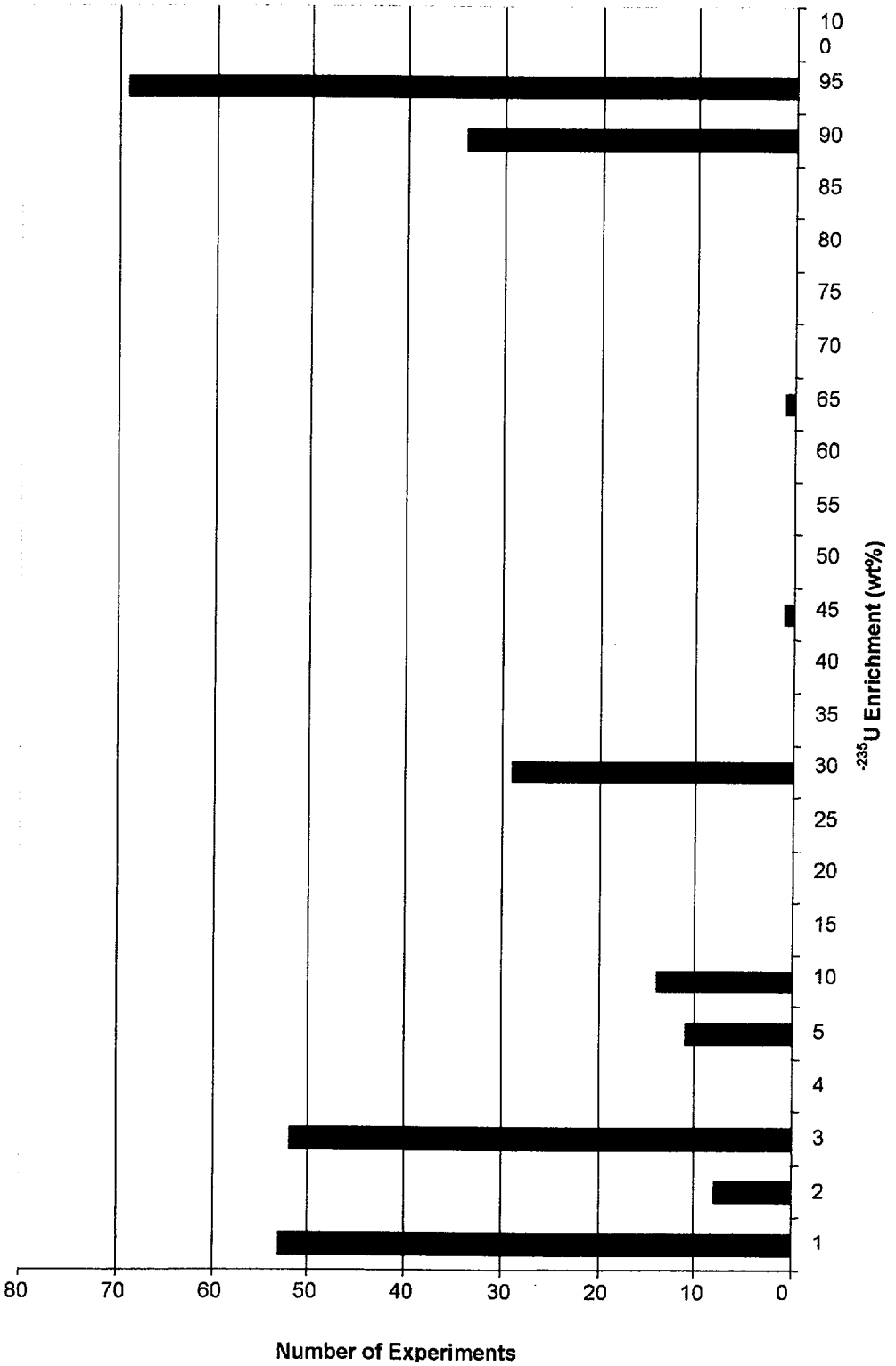


Figure 4-4. Range and Distribution of the Enrichment of ^{235}U for the Benchmark Data Set

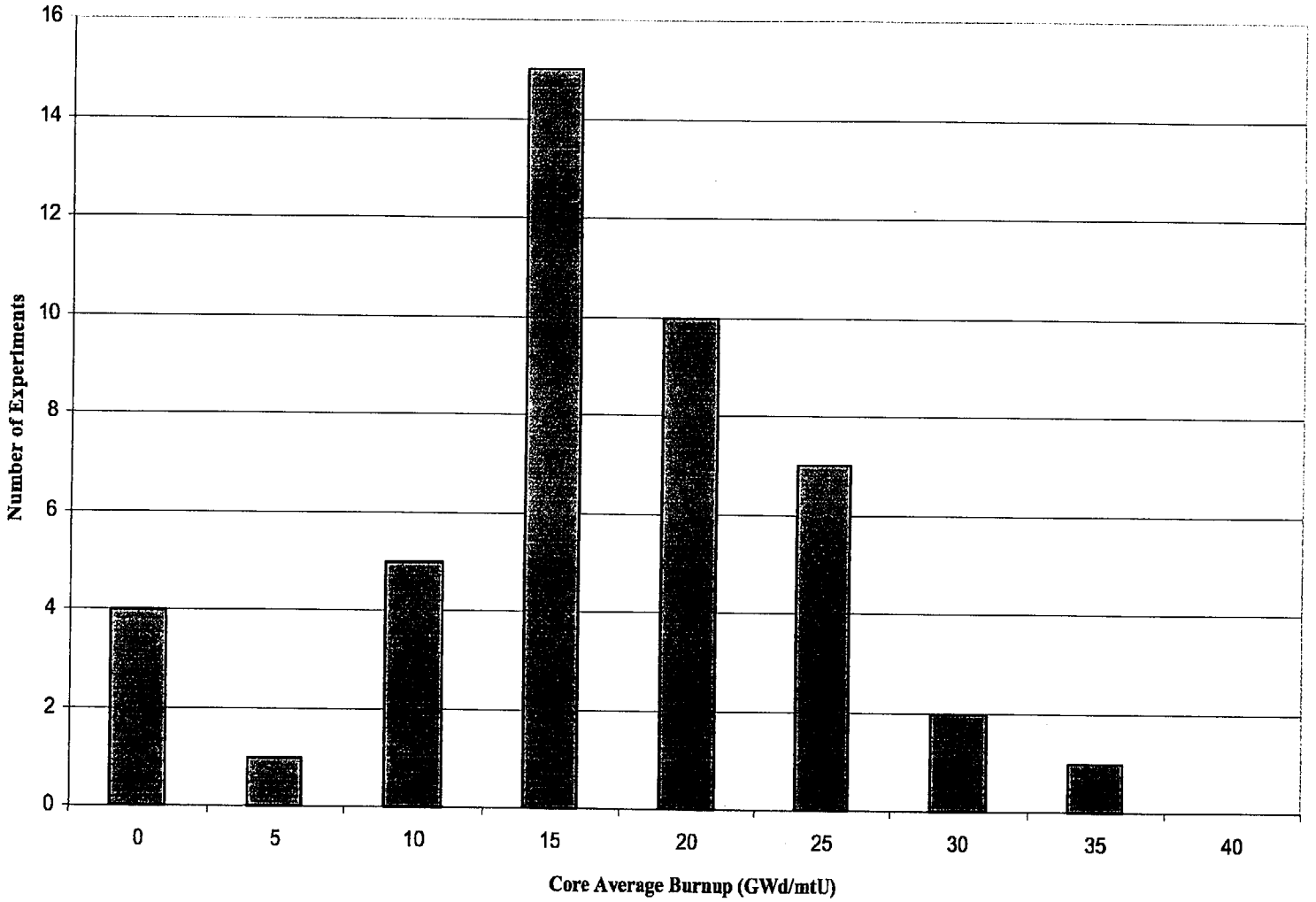


Figure 4-5. Range and Distribution of the Core Average Burnup for the Commercial Reactor Criticals in the Benchmark Data Set

Spectrum, for example, is a parameter that will change in a repository versus the benchmark parameters for commercial fuel. Other changes will be known after the final designs are established and possible degraded states are defined. Once these possible degraded states are defined, the ROA can be established.

Guidelines for selecting the Range of Applicability, once degraded states are defined, were given, and a process for validation of the calculational methods using the ROA were also given. The range and distribution of neutronic parameters are shown to illustrate the range and distribution of neutronic parameters that characterize the current benchmark critical experiment data set of 338 laboratory critical experiments (LCE's) and 45 (CRCs).

Acceptance of the process and guidelines for establishing a range of applicability given above is sought in this report. The applicability of this process and guidelines to specific waste package conditions in the repository will be demonstrated and referenced in the License Application using the validation process described above.

4.1.3.3.2 Application to Waste Forms

Subsection 4.1.3.2.1 defines methods for trending k_{eff} versus parameters such as burnup, which are discussed in Subsection 4.1.3.3.1. The use of these parameters is discussed here to illustrate how they are applied for a given fuel type or waste form. The conclusions stated are based on the results from using the current benchmark data to estimate trends. The bases for assertions made in this subsection are documented in CRWMS M&O (1998n, pp. 75-85). This section connects the benchmark data with some of the waste forms in the repository. The following section presents a process for extending the range of applicability. The process will be the same for all waste forms, but the extension and waste package obtained through use of the process will depend on the specific waste form.

The repository will contain various types of waste forms, the majority of which will be commercial SNF. The various types of commercial SNF (i.e., PWR and BWR fuel) will have separate and different waste packages. The different types of waste package and its waste form will be analyzed separately for criticality potential. As such, each combination will be characterized with a set of benchmark criticals that span the characteristics of the waste package and the waste form. In turn the waste form and waste packages must be evaluated for criticality potential while in an intact or degraded state. Each of these states will require a different set of benchmark critical experiments since the neutronic parameters will also change. For example, the geometric structure of degraded commercial SNF will be different from the intact state, therefore, this difference must be accommodated in the benchmark data set. The set of laboratory critical experiments classified as thermal lattices will be a part of the data set used as a benchmark for degraded commercial SNF.

For commercial PWR SNF in the intact form, CRC data (as discussed in Subsection 4.1.3.1.2) are being used as benchmark data to estimate critical limits for a limited range. Evaluation of additional CRC benchmark data will be performed to verify the trends shown in Subsection 4.1.3.4.1, and reported for the License Application. Burnup as a trending parameter for intact commercial SNF is presented in Subsection 4.1.3.4.1.

The trends for other types of waste forms in the intact or degraded state will be based on their own benchmark data sets. The set of laboratory critical experiments classified as homogeneous systems and thermal arrays 270 experiments, will be a part of the data set used as a benchmark for other types of waste. This set, with additions, will be used for estimating CL for all

waste forms in a degraded condition. CRWMS M&O (1998n) shows that this set of laboratory critical experiments correlates well with the parameter AENCF, previously defined. The AENCF parameter, or a similar characterization of the neutron energy spectrum, is likely to be used as a fundamental parameter for a number of waste forms.

For all fuel types, enrichment or the concentration of certain fissionable materials will be a fundamental parameter for validation, regardless of its use for trending. The enrichment data referenced in this report, and planned for future analysis, as discussed in Subsection 4.1.3.1.2 are considered collectively sufficient to benchmark the model for the entire range of enrichments that will be analyzed for commercial SNF; however, it is likely that some data will have to be added for other waste forms. Most of the waste form categories, and therefore their waste packages, will have a small range of enrichments limited by the nature of the waste form. For example, commercial SNF will most likely be less than 10 percent enriched; therefore, its range of applicability will be limited by the nature of the waste form.

4.1.3.3.3 Extension of the Range of Applicability

The range of parameters used for determining the CL for the k_{eff} values of the critical experiments that are applied to a waste form defines a range of applicability for those waste forms in a repository. The waste forms must also be characterized by fundamental parameters such as enrichment, isotopic content of the benchmark data set, and geometric form. If a fundamental parameter of a waste form is outside of the range of the same parameter in the benchmark data set, its acceptability must be justified by extending the range of applicability of the benchmark set.

The planned approach for performing an extension of the range of applicability is as follows:

A. Calculate the extent of the trended neutronic parameter for a particular waste form and its waste package.

B. Compare the extent of the trended neutronic parameter for a particular waste form with the range of applicability of this parameter as defined by the critical experiment data set.

C. Estimate the trend of k_{eff} versus the trended neutronic parameter and obtain an understanding of the reasons for this trend.

D. Extend the range of applicability by either,

   1. Including new data in the critical experiment data set that expands the data set such that the expanded range of applicability includes the data calculated in part A above, or

   2. Use the established trend to extend the ROA to include the data calculated in part A above, and add additional margin (Δk_m) as defined in Subsection 4.1.3.2. Note that the LUTB bound would be replaced by standard regression tolerance limit methods (Owens 1963, pp. 399-402) for values beyond the ROA for the trended parameter.

E. Parameters not used for trending also define the ROA. The ROA of non-trended parameters can only be extended by adding data to the benchmark set.

If this extension is made, a detailed justification of the need for an extension, along with a thorough description of the method and procedure used to estimate a new CL in this extended range will be documented in a validation report.

Acceptance of the process and guidelines for establishing a range of applicability given above is sought in this report. The applicability of this process and guidelines to specific waste package conditions in the repository will be demonstrated and referenced in the License Application using the validation process described above.

4.1.3.4 Discussion of Results

The following subsections present results showing CL for commercial SNF and illustrative results showing CL where the non-trending methods, described previously in Subsection 4.1.3.2, are used. Details of the analyses that produced these results are provided in CRWMS M&O 1998n (pp. 75-85).

CRWMS M&O (1998l) provides a summary description of the LCEs and the k_{eff} values calculated for each of these experiments, using the cross-section data described in Subsection 4.1.2 and its references. Table 4-1 summarizes the k_{eff} information for the LCE categories discussed in Subsection 4.1.3.1.1 and for the CRC benchmark set discussed in Subsection 4.1.3.1.2. The measured k_{eff} value was unity for all of these experiments in Table 4-1, hence they were true critical experiments. The data in Table 4-1 are not final. This table is used to illustrate data that is applied for establishing the CL presented in Subsections 4.1.3.4.1 and 4.1.3.4.2.

4.1.3.4.1 Trending Results for Commercial SNF

A linear regression on the average energy of a neutron causing fission (AENCF), and separately on burnup, was fit to the set of k_{eff} values of the 45 available Commercial Reactor Critical (CRC) statepoints. These statepoints are used as a set of benchmark data for commercial PWR SNF in the intact state. Evaluation of several statistics showed that burnup is highly correlated with AENCF and that burnup has the strongest correlation with the calculated k_{eff} values for the CRC benchmark data set. Therefore, the trended parameter (burnup) and its range define the ROA for commercial SNF in the intact state that may be used to extend the ROA of the benchmark data set.

Table 4-1. Summary Results of LCE and CRC k_{eff} Calculations

Type of System	Number	k-effective			
		Average	Max.	Min.	Standard Deviation
Homogeneous Thermal Systems	209				
Mixed Pu and Natural U	34	1.00431	1.01511	0.99318	0.00527
Plutonium	73	1.01172	1.02390	1.00169	0.00525
High Enriched ^{235}U	81	1.00504	1.02880	0.98345	0.00817
Low Enriched ^{235}U	15	1.00078	1.00425	0.99469	0.00267
High Enriched ^{233}U	6	0.99977	1.00153	0.99826	0.00124
Homogeneous Fast Systems	10				
High Enriched ^{233}U	10	0.99818	1.00705	0.99297	0.00447
Thermal Arrays	51				
High Enriched ^{235}U	22	1.00744	1.01399	0.99730	0.00395
Intermediate Enriched ^{235}U	29	0.99923	1.00780	0.99300	0.00374
Thermal Lattices	68				
Low Enriched Mixed Oxide	13	1.00277	1.00835	0.98750	0.00593
Low Enriched Uranium Oxide	55	0.99896	1.00827	0.98895	0.00432
Commercial Reactor Criticals	45	0.99220	1.00141	0.98541	0.00323

Figure 4-6 (CRWMS M&O 1998n, p. 79) compares the data (k_{eff}) calculated by the model for the CRC benchmark set, the regression of k_{eff}, and the critical limit for the commercial SNF. Note that the slope of the regression is negative; therefore, as burnup increases, the regression model estimates of k_{eff} decrease, which is an example of negative bias as described in Lichtenwalter et al. (1997, p. 160). The CL for the commercial SNF was calculated at a confidence level of 95 percent with 99.5 percent of the population of the benchmark data set covered (95/99.5 percent).

The ROA of core average burnup is from 0.0 to 33.1 GWd/mtU for commercial SNF in a reactor environment as is shown in Figure 4-6. The CL for this range is approximately from 0.988 to 0.979. This would establish burnup as the trending parameter for extending the range of applicability to include average burnup values outside the stated range. As mentioned before, this extension could be made by adding more experimental data or by increasing the margin (Δk_m) which would lower the CL for waste packages outside the stated range. Initial ^{235}U enrichments range from 1.93 to 4.17 wt. percent.

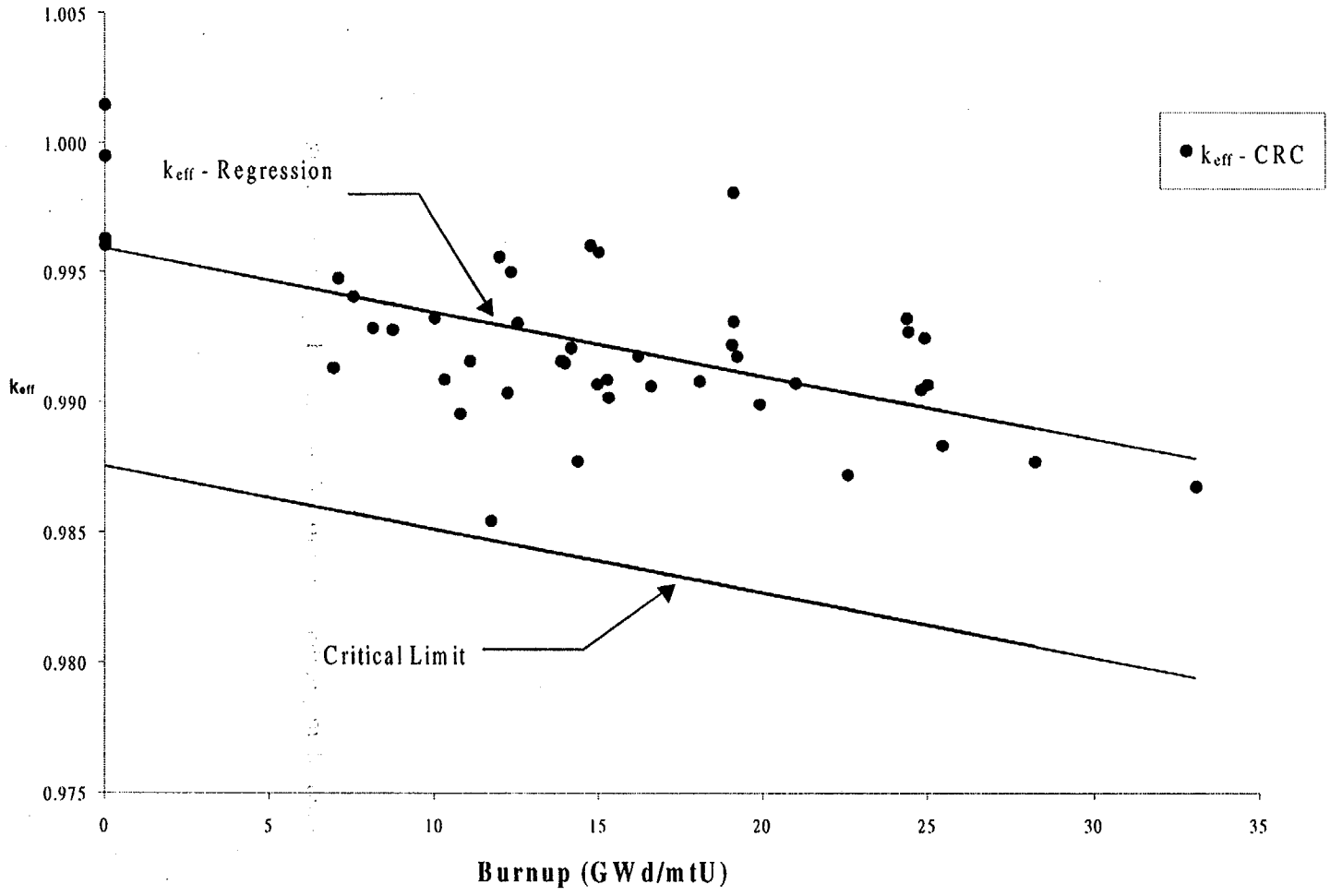


Figure 4-6. Comparison of k_{eff}, the Regression of k_{eff}, and the Critical Limit for Commercial SNF

As for the fundamental parameter of geometry, the benchmark data set and the waste characteristics are the same for the intact waste form. Therefore, the entire CRC data set is applicable to the intact waste form.

For commercial pressurized water reactor SNF in the degraded state the lattice geometry will change (i.e., the distance between fuel rods will change as the skeletal structure of the assemblies corrode). In this case the repository conditions and the benchmark conditions will not be identical. Therefore, the value of the average energy of a neutron causing fission will change. Thus, the ROA for degraded fuel will have to be extended to include this different geometry. The ROA of AENCF for intact commercial PWR SNF is from 0.234 to 0.266 MeV, since this is the range of AENCF covered by the 45 CRC experiments.

There are also other parameters that will change for a waste package in a repository versus the benchmark parameters. The importance of these parameters relative to their effect on criticality will have to be analyzed to establish their importance as a fundamental parameter with a defined ROA. The ROA depends on the final waste package, engineered barrier, and repository design, which will be established for the License Application.

The data shown above, with details on the data and the models given in the references, demonstrate validation of the criticality and isotopic models for commercial PWR SNF in waste package geometries, for the range of AENCF from 0.234 to 0.266 MeV. Acceptance of this limited validation is sought in this report. The existing CRC and LCE data, plus the provisions for extrapolation and augmentation described in Subsection 4.1.3.3.3, are considered sufficient to accommodate changes from the example design provided in Appendix C to the License Application design.

4.1.3.4.2 Results for Non-Trending Methods

The entire LCE data set (338 values of k_{eff}) was used (CRWMS M&O 1998n, p. 84) to obtain a CL for situations that exhibit no trend. Although a portion of the LCE data set exhibits a trend, the entire LCE data set is used only for illustrating the non-trending method. Therefore, these results do not apply to any specific waste package or its waste form. In the first example the normal distribution tolerance limit (NDTL) method was used to obtain a CL of 0.978. The set of 338 values tested to be normal, and this value was calculated at the 95/99.5 percent level. Therefore, these results do not apply to any specific waste package or its waste form.

In the second example of no trends, the 338 data points of the LCE set were used to obtain a CL of 0.979, using the distribution free tolerance limit (DFTL) method. This was done at the 95/99.1 percent level. To cover 99.5 percent of the population of calculated values of k_{eff} for a given waste form and waste package, approximately 600 critical experiments are required. For waste forms that do not show a significant trend and that fail tests for normality, either the database will have to be increased to approximately 600 experiments, or the use of a population coverage less than 99.5 percent will have to be applied to maintain the asserted confidence level.

4.2 DEGRADATION ANALYSIS MODELS

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) (CGC, described in Subsection 4.3.3, below). The CGC is, in general, the primary tool for determining the parameter ranges that characterize the potentially critical configurations. However, 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. Appendix C illustrates a case, which requires the CGC, and Appendix D illustrates a case, which does not. Acceptance is sought for the model validation process portion of the methodology described in Subsection 4.2.4.1, and for the industry standard geochemistry code, EQ3/6, for the environment of the proposed repository site at Yucca Mountain over the range of environmental conditions currently expected in the repository. The basis for this acceptance is presented in references to Subsection 4.2.4 and is summarized in that section. An example of the application of degradation analysis models to commercial SNF is given in Appendix C.

4.2.1 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 1996a, pp. 36-50) 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 1998o) was used in the examples shown in Appendix C. 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 subcritical limit. 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.

4.2.2 Internal Geochemistry Models

The internal geochemistry model consists of the industry standard non-equilibrium 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 current

version of the software (EQ3/6 v7.2b, Wolery 1992) is QA controlled as transferred software from LLNL with CSCI:UCRL-MA-110662. Future analyses, including those for License Application, will use the then current version after appropriate QA qualification. This portion of 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 1998e). 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 1998e), 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, waste form (WF) and other internal components (OIC), degrade.

To simulate the flow through, or flushing, of the waste package, water is also treated as a reagent that enters the reaction at a specified rate (taken to match the rate of water dripping into the waste package); this rate is simulated by a fixed increment of water at each time step. Since EQ3/6 does not have the capability to remove the added water, it will build up over a sequence of time steps. The removal of water is simulated by restarting the program with the total mass of water reduced to the original amount (e.g., 1 kilogram); the amounts of solids (precipitates) remain the same as at the end of the previous run, but the amounts of solutes (dissolved species) are adjusted downward so that their concentrations in the reduced water volume are the same as they were at the end of the previous run. The difference between the solute amounts before and after the restart (or rollover) determines the amount of each species removed from the waste package, and becomes the source term for the external geochemistry. As indicated previously, the results are re-scaled from 1 kilogram back to the total mass of water in the waste package (upwards of 1,000 kilograms).

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 4.4.1.1 and illustrated in Appendix C, where it is shown that for nominal drip rates of 5 to 10 mm/yr the evaporation rate will be much smaller than the drip rate, unless the temperature is elevated by some additional energy source (such as a criticality). For drip rates below the likely range (e.g., 0.1 mm/yr), evaporation could be a significant factor, and this possibility will be evaluated for License Application.

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 fissile materials and neutron absorbers.

The internal geochemistry model is nominally run with 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 this assumption will be considered in the more detailed analysis planned for License Application. 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.

4.2.3 External Geochemistry Model

The possibility of accumulating a critical mass of fissionable material outside of a waste package is evaluated by EQ3/6 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 1998p). 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. Any precipitation, or adsorption, of fissionable materials transported as colloids reported in TSPA will be added to the accumulations of dissolved material calculated by EQ3/6.

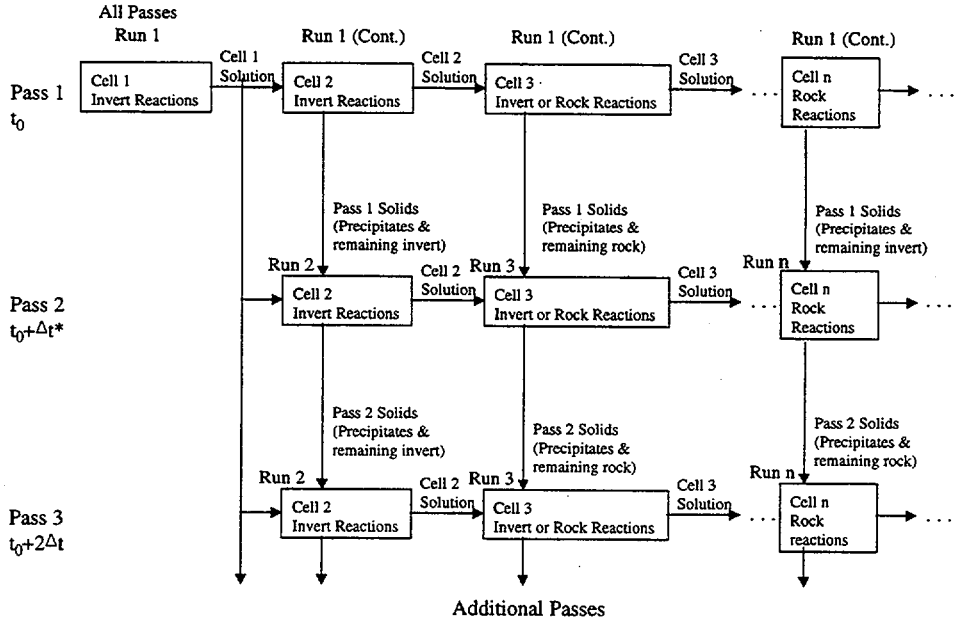
Cell, or layer, boundaries are then determined by distances (times) at which there is a change in the principal mineral being deposited. The process starts with the reacting material closest to the waste package, the invert (for example, crushed tuff) and any remaining drift liner; the passageway for 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 1998h)). 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 4-7. 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 4-7. 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.



Δt is the time difference between successive passes, which is also the time to traverse the principal cell (or layer)

Figure 4-7. Information Flow for External Geochemistry Model (open-system)

The application of this methodology to waste forms, which have both U and Pu, such as commercial SNF, leads to the following general results:

1. Precipitation of U, or Pu, or both, in the near-field and the far-field within a few meters of the drift will be primarily due to the decrease in pH caused by the chemical reaction of the carrier plume with the surrounding invert or host rock.

2. Pu precipitates closer to the source (at shorter times) than U because the pH decreases with distance from the source, and the Pu becomes insoluble at a higher values of the decreasing pH than does U.

3. A corollary to the previous item is that there can be some physical separation between U and Pu, as the Pu precipitates in cells closer to the source.

4.2.4 Validation of Degradation Methodology and Models

As explained in Subsections 4.2.2 and 4.2.3, the portion of the methodology for degradation analysis is based on the application of a geochemistry code, currently EQ3/6, to the materials present in the waste package and the repository environment. A key element of the portion of the methodology is the way in which the successive code runs are organized and interpreted. The validation of the portion of the methodology is concerned with this element and is summarized in Subsection 4.2.4.1. The validation of the specific EQ3/6 model is summarized in Subsection 4.2.4.2.

4.2.4.1 Validation of Degradation Methodology

Validation of the technique of using the waste package flow-through approximation is provided by a hand calculation to verify the correctness of the computer code on which that technique is based. That code adjusts the solute amounts downward from one EQ3/6 output to the next EQ3/6 input (rollover) (CRWMS M&O 1998q). It should be noted that this portion of the methodology could remain the same if the EQ3/6 were replaced by another geochemistry code; however, the geochemistry code (EQ3/6) is not expected to be replaced during this project, but may be modified to incorporate the flow-through mode internally and to include other options.

At the present time there has been no direct validation of the "open system" mode for external accumulations, but the calculations thus far are justified by their conservatism (CRWMS M&O 1997f). By the time of License Application, the EQ3/6 code will be upgraded to incorporate this capacity directly, and validation will be performed as part of the QA certification process for the upgraded version. There can be a large number of passes through any external groundwater pathway, limited only by the duration of the source term, and the accumulations at any one location can build up from each pass.

4.2.4.2 Validation of the EQ3/6 Geochemistry Code

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 4-2. They demonstrate the general validity of the code, particularly the computation of concentrations of solutes over a wide range of total dissolved solids.

Table 4-2. 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%	T.J. Wolery and S.A. 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	Within about 4% up to about 4m NaCl, and within 10% up to 6m NaCl	T.J. Wolery and S.A. Daveler (1992), pp. 144-156

Additional comparisons for chemistry conditions typical of a geologic repository at Yucca Mountain are summarized in Table 4-3. 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 rates are not well known, models used for waste package calculations utilize a range of rates to identify the most conservative cases.

Table 4-3. 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*	Precipitates formed, solution composition, including pH	Accurate prediction of mineral types: clays and calcite**	T.J. Wolery and S.A. Daveler (1992), pp. 166-179
Degradation of borosilicate (HLW) glass with J-13 Well Water*	Precipitates formed, solution composition, including pH	Accurate prediction of mineral types: clays and uranyl silicates**	W.L. Bourcier (1994)
Degradation of spent fuel with J-13 Well Water*	Precipitates formed, solution composition, including pH	Accurate prediction of mineral types: clays and uranyl silicates**	C.J. Bruton and H.F. Shaw (1988)
Natural geothermal alteration of welded tuff, (Burton 1996)†	Precipitates formed, solution composition, including pH	Accurate prediction of mineral types: clays and zeolites	C.J. Bruton (1996), Volume II, Chapter 3.4.2

*Experimental conditions intended to model the expected repository environmental parameters and degraded waste package component chemistry.

** For some reaction times quantitative agreement requires downward adjustment of reaction rates.

† Natural analog, also demonstrating conservative behavior with respect to high temperatures (up to 250°C).

4.3 PROBABILITY CALCULATION MODEL

An overview of the portion of the methodology for estimating the probability of a criticality event has been given in Section 3.5. 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. An illustrative example of this method for the calculation of the probabilities of criticality events is given in Appendix C. 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 have to be determined by the time of License Application.

4.3.1 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:

$$\Pr\{t \leq T \leq t+dt\} = f(t)dt \qquad \text{Eq. 4-6}$$

where $f(t)$ 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:

$$F(t) = \int_0^t f(\tau)d\tau \qquad \text{Eq. 4-7}$$

$$\text{or} \qquad F(t) = \Pr\{T \leq t\} \qquad \text{Eq. 4-8}$$

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 Subsection 4.3.2. 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.

4.3.2 Monte Carlo Technique

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.

As explained in Section 3.5, the Monte Carlo technique is used to develop statistics by randomly tracing through the steps of the scenarios leading to a potentially critical configuration. The sequence of steps in the application of the Monte Carlo technique is shown in Figures 4-8a and 4-8b 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 distribution of drip rates. The distribution of seepage fraction, seepage rate and their temporal variation will be obtained from a drift-scale seepage model, which will include the effects of thermal reflux. In practice, these distributions will be abstracted from the most recent version of the TSPA.

B. 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 RIP to combine the WAPDEG output with the value for drip rate sampled in the previous step.

C. 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.

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.

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 4.3.3), which 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.

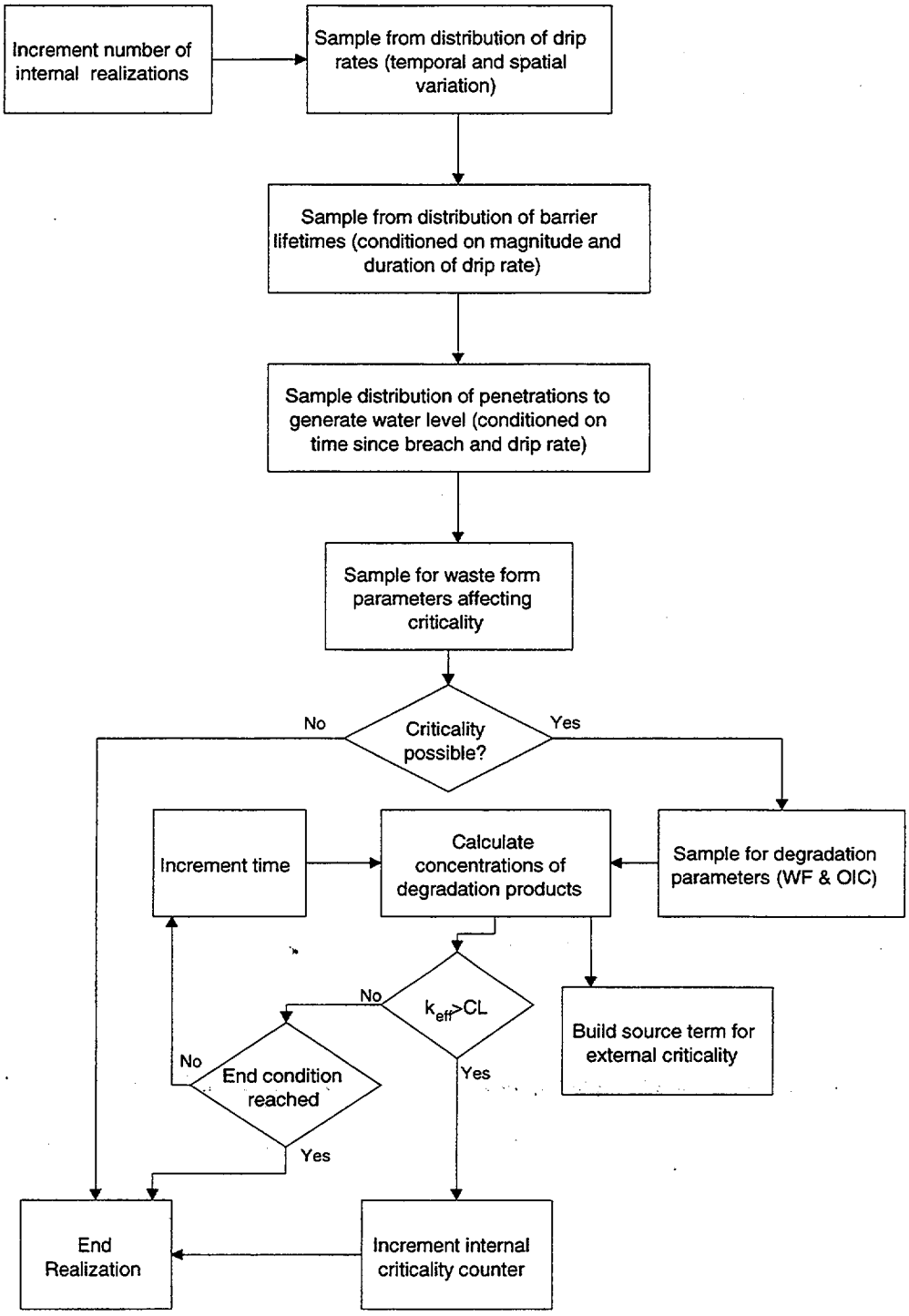


Figure 4-8a. Monte Carlo Technique Informational Flow, Internal

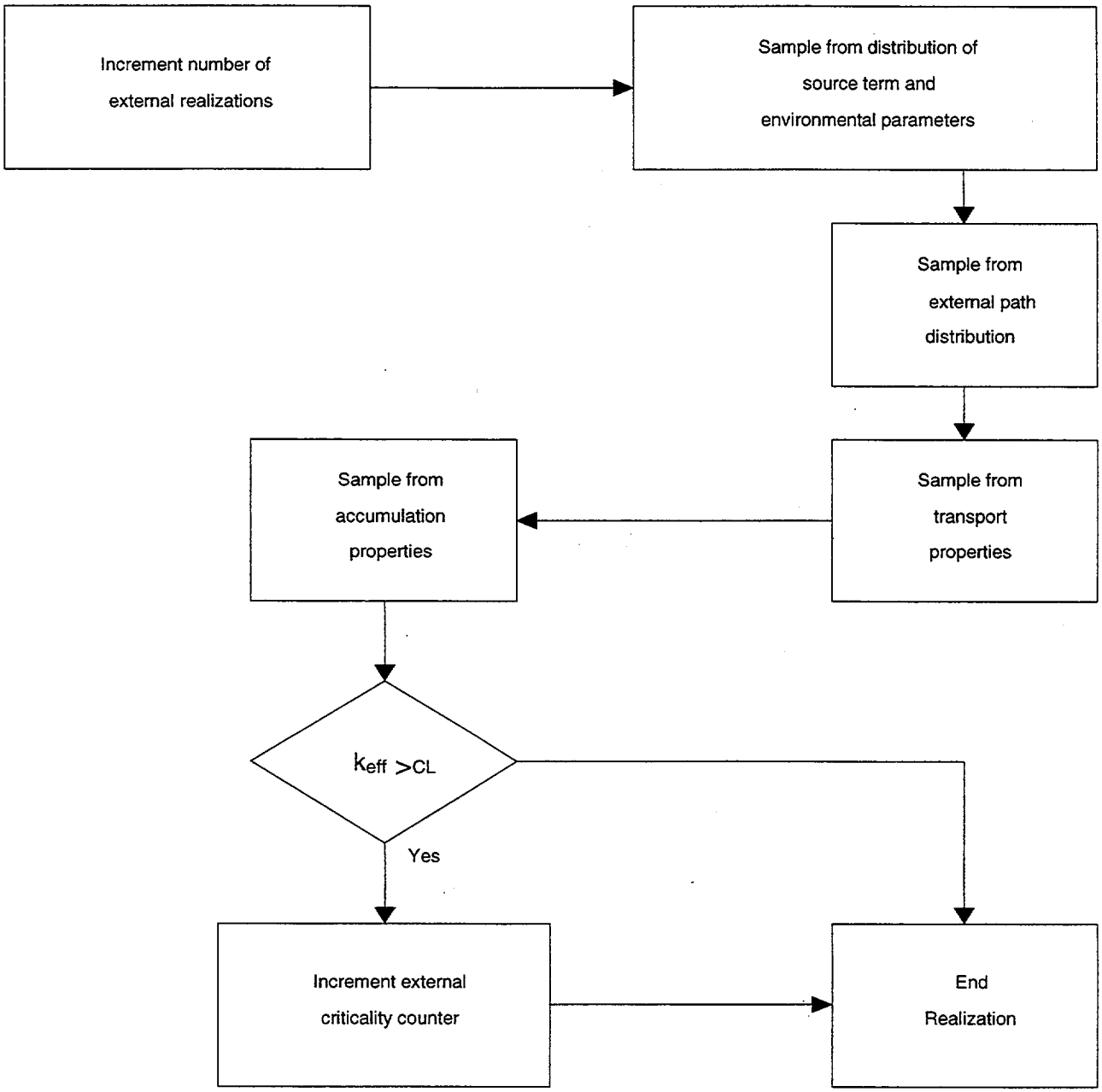


Figure 4-8b. Monte Carlo Technique Informational Flow, External

F. Evaluate criticality of the configurations defined by the previous step, using the k_{eff} regression developed as described in Section 3.5. If k_{eff}>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.

External Criticality

A. Sample from the distributions for the flow rate, concentration of fissile elements and pH for the source term (solution flowing out of the waste package). 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. The standard external locations will be established as part of the analysis for License Application. Preliminary analyses (CRWMS M&O 1998p) 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 4-8b. 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 principal difficulty with the Monte Carlo technique is the large number of trials (realizations) required to generate enough statistics when there are a large number of independent random parameters to be sampled. The identification of the worst case degraded configurations is intended to save time calculating the individual time steps of the degradation process, if the worst case will not be critical.

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.

4.3.3 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 fissile or neutron absorbing) and chemical species which can effect the solubility of the neutronically significant elements. As was mentioned in Subsection 3.3.4, 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 Subsections 4.2.2 and 4.2.3, above. 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; (2) to provide more rapid calculation of Monte Carlo statistics in situations where the EQ3/6 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 (only ^{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 (first external potential pond):

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.

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, 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.

4.3.4 Validation of the Criticality Probability Calculation Models

This report seeks NRC review and acceptance of the probabilistic criticality calculation portion of the methodology described in Subsections 4.3.2 and 4.3.3. To facilitate this review and acceptance process, the validation of a specific implementation of the portion of the methodology is described.

The validation of the criticality probability calculation models is conveniently divided into three parts: (1) the Monte Carlo framework for calculating probability, (2) several submodels, dealing primarily with environmental and material performance parameters, abstracted as part of the total system performance assessment (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 (discussed in Section 3.5) based on MCNP calculations. Validation of 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 also constitutes a validation of the CDFs used to generate the particular random variable values used in the Monte Carlo technique described in Subsection 4.3.2. Validation 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 (small computer code) *generate.c*, which is described in CRWMS M&O 1997c; 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 1997i. 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.

The most recent application of the probabilistic criticality evaluation portion of the methodology has been for the commercial PWR SNF, some of which is described in Appendix C. This application combined the configuration generator code (CGC) and the Monte Carlo probability calculation portion of the methodology, in the software routine PWRPROB described in CRWMS M&O 1998r and summarized in Appendix C of this document. The PWRPROB software routine has been verified for the specific case of the example 21 PWR waste package

with borated stainless steel plates for criticality control and containing the 15×15 assembly with Zircaloy clad fuel rods. Other characteristics of the problem are given in CRWMS M&O 1998r and summarized in Appendix C.

The verification of PWRPROB involved two calculations using MathCAD, Version 7 to check that the PWRPROB Monte Carlo simulation was producing correct output. These MathCAD calculations are described in Attachment IV of CRWMS M&O 1998r. First, the fully degraded basket k_{eff} regression expression was used, along with the waste stream data, to calculate the fraction of the waste stream that would exceed a k_{eff} of 0.98 in a fully degraded basket with oxide uniformly distributed at 33 volume percent. The results of this MathCAD calculation are shown in Attachment IV (page 2) of CRWMS M&O 1998r as a plot of the fraction of fuel assemblies exceeding the k_{eff} limit versus time (from 3,000 to 100,000 years). A similar case was executed for a single Monte Carlo trial of PWRPROB using specific input values that were used in the MathCad calculation (i.e., fixing the distributional inputs such that only a single value could be "sampled"). The results of the single trail of PWRPROB are provided in Figure 6-4 of CRWMS M&O 1998r. This figure shows nearly identical results to those in Attachment IV (of CRWMS M&O 1998r) following complete basket degradation, which occurs by approximately 20,000 years in this case. The peak occurs at 20,000 year for both plots. The similarity of shape and values of the two traces in Figure 6-4 of CRWMS M&O 1998r indicates that Monte Carlo framework of PWRPROB is properly processing the input and submodel outputs, and that the waste stream data and the regression expression are being properly used.

A more limited, but easier to understand, verification is provided by comparing the cumulative probability of k_{eff} exceeding 0.98 before 100,000 years for waste packages being loaded with the entire distribution of burnup-enirchment pairs for the inventory of PWR assemblies expected at the repository. This is called the noloadcurve strategy, since all of the fuel is loaded in the same type of waste package without using a loading curve to segregate the SNF with the highest criticality potential so that it can be handled in a waste package with more robust criticality control. The degradation process of the waste package is characterized as (1) the ion oxide becomes uniformly distributed, and (2) the boron is removed as the basket is corroded. The MathCAD calculation is given in CRWMS M&O 1998r, Attachment IV, and summarized in Table 4-4. 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 WP (last item in above table), which agrees very closely with that inferred from the Monte Carlo results presented in Figure 6-1 of CRWMS M&O 1998r (also reproduced as Figure C-31 of Appendix C of this document). In that figure, the no-loading curve gives a cumulative probability of 6×10^{-4} at 100,000 years.

The probabilistic criticality calculation models, as described in Subsections 4.3.2 and 4.3.3, can not be fully validated without the specific waste form, waste package design, and repository features that are to be licensed. Therefore the final validation process for the probabilistic models will be completed for License Application.

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

Parameter	Value	Variable Name	Source[1]
Mean Percolation Drip Rate	38.8 mm/yr		Section 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}	Section 5.1.5
Mean Stainless Steel Corrosion Rate	$1x10^{-4}$ 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	$1.4x10^{4}$ years		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	$8.2x10^{-4}$		P_{drip} x P_{breach} x P_{bath} x P_{dur} x P_{crit}

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

4.4 CRITICALITY CONSEQUENCE MODEL

Acceptance is sought for the validation of the portion of the methodology for the steady-state consequence models (equations representing physical material and heat balance processes) are acceptable for the range of environmental conditions expected in the repository, for both internal and external criticality. Acceptance is sought for the validation of the portion of the methodology for consequence evaluation of transient criticalities for both internal and external criticalities for the range of environmental parameters expected in the repository although it is expected that the specific models used by the methodology will be refined for License Application. This portion of the methodology incorporates equations of heat, mass, and momentum transfer plus equations of state for the materials involved. The validation of this portion of the methodology and models is given in Subsection 4.4.3.

There are two different time dependent behaviors of a criticality: transient and steady-state. 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 exponential increase in power, until the negative feedback mechanisms cause the k_{eff} to drop back below unity. The steady-state model applies when the approach to criticality is so slow as to permit

the negative feedback mechanisms to hold the k_{eff} very close to unity, so that there is no impulsive energy release (as is illustrated by the example in Subsection 4.4.1.1). For such a steady state criticality the only concern is with the increased radionuclide content remaining after the duration of the criticality event.

The transient model is concerned with the characterization of the energy release in the possibly very high power pulse over the short duration of the peak, as well as the cumulative buildup of radionuclide increments over a periodic pulsing. The insertion rate distinguishing between these two regimes will be determined by the analyses for License Application. Both transient and steady-state models will be developed in three versions, corresponding to the general locations where a criticality event may occur: internal to the waste package, external in the near-field, and external in the far-field. The status of the development of the current versions of these models is indicated in the following subsections. The models will all be refined by the time of the LA, so that the region of applicability can be demonstrated.

4.4.1 Consequences of Internal Criticality

4.4.1.1 Steady-State Criticality

As the criticality power level increases, the temperature will increase and the evaporative water loss will increase. Therefore, the steady-state temperature is that at which the evaporative water loss is just equal to the total (net) water infiltrating into the waste package. If the temperature were to increase beyond this point, the net decrease in moderator would shut down (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 the criticality process is conservatively bounded by the length of the high moisture part of a climatological cycle, which might be as long as 10,000 years (CRWMS M&O 1997h). It should be noted that this concept can be applied to a criticality event in which there is no standing water, but only water loosely bound to clay. Such water can be removed by evaporative heating, although the evaporation rate as a function of temperature and clay composition has not been sufficiently measured to support quantitative analysis at this time.

The principal direct consequence of a steady-state criticality is an increase in radionuclide inventory, which is computed from a point-depletion code, such as ORIGEN-S (part of the SCALE package (ORNL 1995) , for a given initial set of isotopes with a criticality event (or process) of a specified power level and duration. In using the point-depletion code, the isotope concentrations are taken as those, which lead to the criticality event. Since criticality was assumed at a threshold value of k_{eff} which was significantly less than 1.0 (either 1.0 or 0.95 less the correction for bias and uncertainty), the isotopic concentrations are not consistent with a steady-state criticality at $k_{eff}=1$. The inconsistency is acceptable because it errs on the side of conservatism.

4.4.1.2 Transient Criticality

Analysis has shown (CRWMS M&O 1997e) that the flow conditions in a waste package undergoing a transient criticality may be modeled by the reactor transient code, RELAP5/MOD3.2 (Idaho National Engineering Laboratory). This code is used to calculate the time dependent increase in k_{eff} with the following negative feedback mechanisms: Doppler broadening, void coefficient, thermal expansion, evaporation or boiling at the heated, free water surface. Although the RELAP5/MOD3.2 computer code has not yet been certified according to the OCRWM QARD (DOE 1998), the following facts of its acceptance by the nuclear industry indicate that there will be no obstacle to gaining that certification.

A. It was developed for the U.S. Nuclear Regulatory Commission as a basis for a nuclear plant analyzer.

B. Typical applications include simulations of operational transients in PWR systems such as loss of coolant and anticipated transients without scram for nuclear powerplant licensing. One such reference is Thompson and Kmetyk (1984).

C. The code has been developed and maintained under a QA code configuration system that incorporates a review and check process for code modifications and validation of both theory and numerical models thorough assessment cases comparing calculated results with test results.

D. The RELAP/MOD3.2 code has been installed on HP workstations in the M&O, and the 10 installation test cases have been run successfully.

Since the criticality events involving PWR SNF within a waste package are similar to the situations for which the RELAP5/MOD3.2 code was developed to analyze, there is reasonable confidence in the capability of RELAP5/MOD3.2 to provide conservative results for the applications within this analysis.

The OCRWM QA certification for RELAP5/MOD3.2 is presently in process. Future analyses with this code will use only the QA certified version. If any future revision (versions or mods) of the code are found to be more suitable (than RELAP5/MOD3.2) to the waste package transient criticality problem, such revision will be used after appropriate OCRWM QA certification.

The analysis with RELAP5 included slow and relatively rapid reactivity insertion mechanisms such as one or more assemblies shifting (or falling) from above the waste package water level to below the waste package level due to some mechanical disturbance. Such a reactivity insertion mechanism might typically have a duration of approximately 0.3 seconds (the time it might take to fall such a short distance) (CRWMS M&O 1997e).

The additional analysis for License Application will include an evaluation of possible positive feedback mechanisms, particularly the so-called *autocatalytic effect,* which can arise in an over-moderated system (Gratton et al. 1997). Additional analyses will also include configurations in which the waste form is degraded and the fissionable material and moderator are intermixed. If a transient criticality (rapid reactivity insertion) is credible under such circumstances, the consequences will be evaluated using a combined thermal-hydraulic-neutronic code such as that developed for external transient criticality (Gratton et al. 1997).

4.4.2 Consequences of External Criticality

4.4.2.1 Steady-State Criticality

The analysis to determine operating temperature and power level for an external steady-state criticality is similar to that described above for internal steady-state criticality, except that the radiation and buoyant heat convection-heat dissipation mechanisms are not available for external criticality, and the evaporation mechanism is much weaker.

4.4.2.2 Transient Criticality

There are expected to be no mechanisms for rapid reactivity insertion in the external environment (to be demonstrated in the analysis for License Application). The only exception could arise from a stack of assemblies (remaining after complete degradation of the waste package) in the drift that filled to some intermediate level of water. Rapid insertion could occur if an assembly at the top of the stack were initially out of the water, but fell in due to a sudden shaking. The use of RELAP5 for such a transient event would be very conservative with respect to the validation conditions used for the internal transient criticality, since the peak amplitude of the pressure and temperature pulses will be reduced for external criticality because of the lack of any confining structure analogous to the waste package barriers.

4.4.3 Validation of Criticality Consequence Methodology

4.4.3.1 Validation of the Steady-State Criticality Consequence Methodology

The steady-state consequence portion of the methodology is validated by conservatism inherent in the methodology, which serves to define a range of configuration parameters to provide an upper bound on the increase in the radionuclide inventory. 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. The initial isotopic concentrations are derived from the WP source term calculation, using SAS2H; the radionuclides remaining at the end of the criticality are calculated from ORIGEN-S (both part of the industry standard SCALE package (ORNL 1995), which has been validated over the parameter range of interest here). Upper limits on the criticality power level and duration are derived using the following conservative assumptions:

A. The criticality duration extends over the period of high infiltration rate

B. The maximum credible water infiltration rate is maintained over the wet part of a climatological cycle

A wet cycle duration of 10,000 years has been postulated (CRWMS M&O 1996b), but the calculation in Appendix C, Section 7 shows that even a conservatively high flow rate supports only a power level of a few kilowatts. Under these conditions Appendix C, Section 7 shows the increments in the nuclides most important for long term MGR performance (^{129}I, ^{99}Tc, and ^{237}Np) were each less than 5 percent of the pre-criticality amounts of these three nuclides, and the total increment, for all the nuclides considered in performance assessment measured in curies at the time of criticality ending, is less than 11 percent even for this extreme case. 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.

4.4.3.2 Validation of the Transient Criticality Consequence Methodology

The consequence portion of the methodology for transient criticality is implemented by a computer code incorporating time dependent differential equations describing 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, and there will also be different implementations for internal versus external criticality. For transient criticality internal to a PWR waste package, the RELAP5 is an appropriate implementation, which can be validated in a manner acceptable for NRC acceptance.

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 WP 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 PWR SNF WP system was modeled with SNF assemblies immersed in a water system which, except for orientation, is similar to typical RELAP5 PWR core analysis configurations. The models provide interaction between energy generation, energy redistribution, and negative feedback to the energy generating mechanism.

The WP criticality analysis differs from the typical RELAP5 reactor plant analyses by having:

A. Initial conditions in the WP at atmospheric pressure and low temperature and
B. Static fluid conditions (zero flow rate)

RELAP5 state properties extend to the low pressure and low (liquid) temperature state conditions, so the code was being used in the WP analysis within the range of thermal-hydraulic design conditions.

The principal limitation of the RELAP5 code affecting the WP analyses is that the flow system is primarily one-dimensional. To extend the flow system to cover limited two-dimensional capability, the cross flow junction model was invoked in the WP analysis. In such situations, momentum flux terms in the mathematical models are normally neglected which was done in the PWR WP analysis.

Frictional effects in the PWR WP analysis are mainly due to flow across the fuel rods in assemblies. Loss coefficients specified for the analysis were derived from cross flow loss coefficient correlations (I.E. Idelchik 1993). The value calculated from the correlation for a 15 x 15 PWR assembly was approximately eight. An additional multiplier of nine was used in the consequence analysis for conservatism resulting in the final value of 72. The higher loss coefficient value increases the frictional effects resulting in higher calculated pressures than would result from lower values.

The maximum reactivity in the intact but degraded WP potentially available for driving a transient criticality event was from a shift of iron oxide moderator displacement material from a homogeneous to a settled distribution. Upper limits on the time scale for this reactivity insertion (and thus the severity of the event) were derived from the minimum times required for redistribution of solid particles within the WP which were on the order of seconds (CRWMS M&O 1997e, p. 29). While this driving mechanism is different from normal nuclear plant transient events (i.e., control rods, valve closure, or temperature changes), it is not critical to the analysis since the reactivity driving events in RELAP5, from whatever source, must be reduced to a generic time dependent functional form.

4.5 TOTAL SYSTEM PERFORMANCE 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-VA document (CRWMS M&O 1998s). 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.

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-VA (CRWMS M&O 1998s) for the potential radioactive waste repository makes use of the computer program RIP in conjunction with detailed process-level models. The methodology for this report will use the same codes. The RIP code (CSCI#30055v5.19.01), and the detailed process models are described in documents for TSPA-VA (CRWMS M&O 1998s). The RIP code was specifically developed by Golder Associates Inc. in order to evaluate the performance of a potential radioactive waste disposal facility at Yucca Mountain (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 RIP (see Figure 4-9) that comprise the performance assessment model are (1) waste package behavior and radionuclide release component model, (2) radionuclide transport pathways component model, (3) disruptive events model, and (4) biosphere dose/risk model. These models are summarized briefly below. For evaluation of the consequences of a criticality 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.

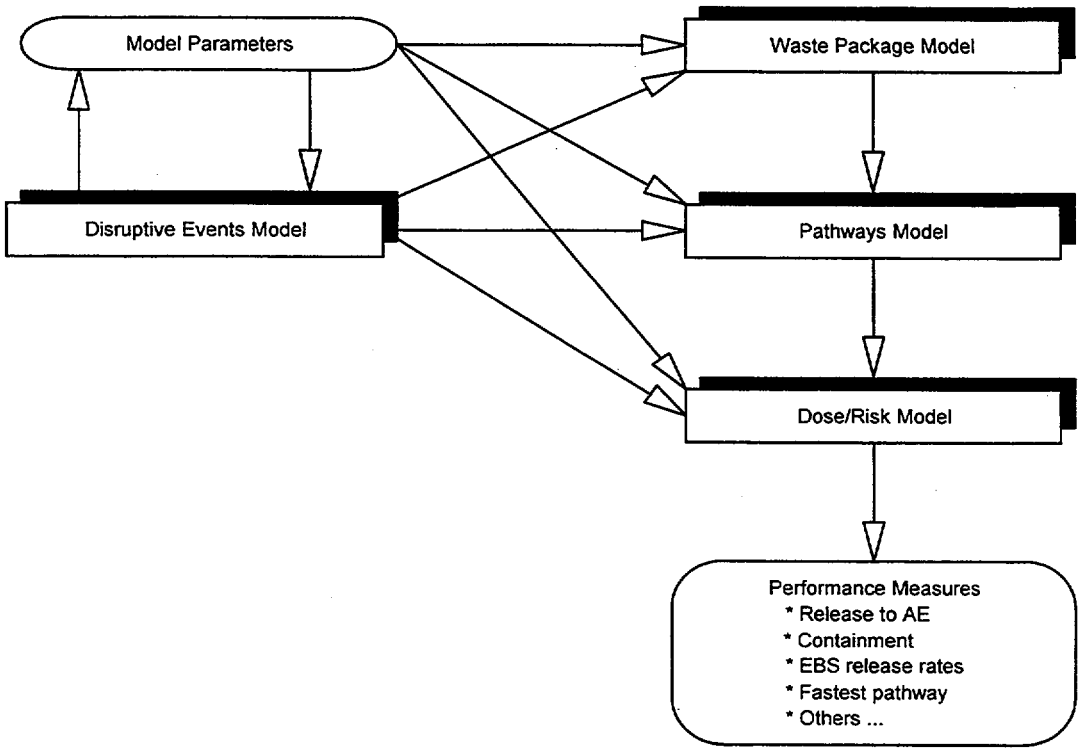


Figure 4-9. Components of the Repository Integration Program which are Used for Total System Performance Assessment

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, RIP computes the rate of mass transfer out of, and away from, the waste radionuclide 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.

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 RIP model uses a phenomenological approach that attempts to describe rather than explain the transport system. The resulting transport algorithm is based on a network of user defined pathways. The geosphere and biocell pathways reflect the major features of the hydrologic system and the biosphere, and are conduits through which transport occurs. The pathways may be used for

both flow balance and radionuclide transport purposes, and may account for either gas or liquid transport. The purpose of a pathway is to represent large-scale heterogeneity of the hydrologic system, such as geologic structures and formation-scale hydro stratigraphy (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-VA, the unsaturated zone (UZ) and saturated zone (SZ) transport is being simulated using the groundwater code FEHM1.0 (Zyvoloski et al. 1995, OCRWM QA Status TBV-564).

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 RIP 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).

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5.0 SUMMARY AND CONCLUSIONS

The proposed methodology for performing criticality analyses for waste forms for long-term disposal in the Yucca Mountain repository is presented in this report. The starting point for this 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 and degradation analyses are performed. The degradation analyses provide information on parameters that affect criticality potential. These parameters may include the amounts of fissionable material, neutron absorber material, corrosion products, and moderator. 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. Multivariate regressions are developed that cover the range of parameter values where the peak k_{eff} may exceed the critical limit criterion. 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 CL is the value of k_{eff} at which the configuration of fissionable materials is considered potentially critical. 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.

Additional performance-based criteria are also imposed so that proper consideration is given to events with a low probability of occurrence, but with a large associated consequence (increased radionuclide inventory). Thus, consequence analyses are performed when the probability criterion is satisfied, and the results of these analyses are measured against the performance-based criteria. The consequence analyses estimate changes in the radionuclide inventory that may impact the total system performance assessment (TSPA) and compares these changes with the criticality consequence criterion. Based on the results of these comparisons, either additional design options for reducing k_{eff} are implemented, or 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. The decisions concerning design features to reduce k_{eff} are based on risk, in conjunction with other information. Thus, the methodology is risk-informed.

The methodology presented is a blend of deterministic and probabilistic aspects. The evaluation of the various long-term processes, the combination of events, any potential criticality, and the consequences resulting from a potential criticality are all deterministic analyses. However, probabilistic analyses are performed to establish the likelihood of a criticality occurring.

The criticality calculations, degradation analyses, flow and transport analyses, probability evaluations, and consequence analyses supporting the methodology are based on specific models. Discussions of various models are provided in this report. The validation of models, including experimental data used for the validation, are also discussed. The applicability of the models for criticality analyses in the repository is defined by the range of the data used in the validation process. Limited validation of the following models: neutronic, degradation, configuration generator, and consequence is provided in this report and its references. Full validation awaits design information not yet available. The specific waste form, waste package design, and repository features that are to be licensed are needed for full validation.

This full validation will be provided in the License application and its references. The acceptance of specific models and their validation will be sought as part of the License Application.

The design criteria are based, in part, on the model validation process. For example, the CL criterion contains the criticality analysis method bias and uncertainty. The bias and uncertainty are established by analyzing experimental systems. The range of applicability of the CL is defined by the range of the parameters covered by the experimental database and trending analyses performed for this data. The criticality model validation process presented in this report analyzes 338 laboratory critical experiments and 45 commercial reactor critical experiments. This process will be followed to develop CL values for each waste package design. Acceptance of these CL values will be sought as part of the License Application.

Burnup calculations for the commercial reactor critical experiments that help validate the methodology were based on detailed core operations data, which included local burnup, fuel temperature, and moderator specific volume data. Thus, the isotopic concentrations representing burnup are an inherent property of the commercial SNF for the criticality model validation. This level of detail (i.e., the detailed core operation data) will not be available for the criticality evaluations performed for repository design. This will require assumptions to be made relative to the burnup characteristics of the commercial SNF for design applications of the isotopic model. Three requirements were proposed for design applications to ensure that the isotopic concentrations used for commercial SNF would be conservative with respect to k_{eff}. The first requirement addresses axial burnup distributions and their effect on k_{eff}. The second requirement addresses the quantities of isotopic concentrations present, as a function of burnup and enrichment. The third requirement addresses time effects relating to uncertainties in the half-life and branching fractions of the various isotopes and the resulting effects during the long disposal time period. The validation process for the isotopic model used for commercial SNF must satisfy these requirements.

Conclusions that can be reached based on this report are:

A. The following design criteria presented in Figure 1-1 (discussed in Section 1.5) 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 Section 3.4: the calculated k_{eff} for 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 *Probability* criterion discussed in Section 3.5: a criticality frequency of 10^{-4} per year for the entire repository will not be exceeded in any of 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 4.

   3. The *Criticality Consequence* criterion discussed in Section 3.6: the expected radionuclide increase from any criticality event will be less than 10 percent of the radiologically significant radionuclide inventory (curies present at time of criticality) that is available for release and transport to the accessible environment. This criterion is intended to ensure that the average radionuclide increment form any single criticality is much less than the uncertainty of the performance assessment dose

estimation, and is also 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 4.

4. The *Repository Performance Objectives* criterion discussed in Section 3.7: 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 presented in Section 3.1, and summarized in Figures 3-1a, 3-1b, 3-2a, and 3-2b comprehensively identifies degradation scenarios based on features, events, and processes associated with the proposed 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 Sections 3.2 and 3.3 is acceptable in general for developing a comprehensive set of potential postclosure configurations for disposal criticality analysis.

D. The portion of the methodology for performing criticality evaluations of postclosure configurations and using critical limits discussed in Section 3.4 is acceptable in general for disposal criticality analysis.

E. The portion of the methodology for estimating the probability of postclosure critical configurations and using multivariate regressions discussed in Section 3.5 is acceptable in general for disposal criticality analysis.

F. The portion of the methodology for estimating consequence of postclosure criticality events discussed in Section 3.6 is acceptable in general for disposal criticality analysis.

G. The neutronic model validation process described in Subsection 4.1.3 is acceptable in general for model validation. Specifically:

1. The process presented in Subsection 4.1.3.2 for calculating the CL values and the process presented in Subsection 4.1.3.3 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. Acceptance of the full range of CL values and their applicability for postclosure repository conditions will be sought as part of the License Application. Acceptance of a CL for a specific range is part of the model validation requested in item M.1 below.

2. The proposed requirements presented in Subsection 4.1.3.1.4 define the validation process for the isotopic model for waste packages containing commercial SNF.

H. The validation process for the degradation analysis portion of the methodology presented in Section 4.2 for calculating the chemical composition of fuel and waste-package component degradation products is acceptable in general for model validation. Specifically,

1. Validation of the flow-through mode (internal to the waste package) is provided by hand calculation to verify that the computer code that correctly adjusts the solute amounts downward from one output to the next input (rollover).

2. Validation of the open system mode (external to the waste package) is provided by the conservatism available in, and the application of, the methodology.

I. The validation process for the probability calculation and configuration generator models described in Subsection 4.3.4 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 4.4.3 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 4.1.3.1.4 for modeling burnup of commercial SNF for design applications are sufficient, if met, to ensure adequate conservatism in the isotopic model for burnup credit.

L. The principal isotopes selected to model burnup in intact commercial SNF, presented in Table 3-1 in Subsection 3.4.3, are acceptable for disposal criticality analysis. The process for selecting isotopes from the list of principal isotopes for degraded commercial SNF presented in Subsection 3.4.3 is also acceptable for disposal criticality analysis.

M. The following models are acceptable as described below. The validation of these models is for a range of the currently expected postclosure repository conditions for the proposed repository at Yucca Mountain, Nevada. The postclosure repository conditions are dependant upon the waste form, waste package design, engineered barrier design, data from material tests, data from natural systems tests, and Performance Assessment models of postclosure time dependent repository conditions. At the time this report is being released, all the waste forms are not fully defined, the final waste package and engineered barrier designs have not been finalized, data is still being collected from the material tests and natural systems, and the Performance Assessment models of postclosure repository conditions are still being refined. Thus, the conditions that will be presented for License Application are not fully defined, and the formal validation of these models for License Application will be provided or referenced in the License Application.

1. The neutronic models described in Subsection 4.1.1 and 4.1.2, including the SAS2H sequence of the SCALE 4.3 (CSCI:30011 V4.3, CRWMS M&O 1997g; Oak Ridge National Laboratory [ORNL] 1995) code system using the 44-energy group cross-section library and the MCNP 4B2 (CSCI:30033 V4B2LV, CRWMS M&O 1998t; ORNL 1997) computer code using the referenced cross section libraries, are acceptable for evaluating criticality potential for the range of neutronic parameters presented in Subsection 4.1.3.4.1. The applicability of these models to specific waste

package conditions in the repository will be demonstrated or referenced in the License Application using the validation process referred to in item G above.

2. The degradation model (the geochemistry code EQ3/6) described in Subsection 4.2.2 is acceptable for the range of environmental conditions currently expected in the repository. The bounding cases have been identified for the current range of environmental parameters and may be modified for the environmental parameters most suitable for License Application.

3. The configuration generator models described in Section 4.3 (equations representing physical and chemical release, transport, and accumulation processes), are acceptable for the range of environmental conditions currently expected in the repository. The bounding cases have been identified for the current range of environmental parameters and may be modified for the environmental parameters most suitable for the License Application.

4. The steady-state consequence models (equations representing physical material and heat balance processes) described in Section 4.4 are acceptable for the range of environmental conditions expected in the repository, for both internal and external criticality. The portion of the methodology for consequence evaluation of transient criticalities is acceptable for both internal and external criticality for the range of environmental parameters expected in the repository.

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M&O Procedures
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APPENDIX A

ACRONYMS AND ABBREVIATIONS

APPENDIX A
ACRONYMS AND ABBREVIATIONS

AENCF	Average Energy of a Neutron Causing Fission
Ag	Silver
Al	Aluminum
ALARA	As Low As Reasonably Achievable
ALF	Average Lethargy of a Neutron Causing Fission
AlOOH	Diaspore, a form of aluminum oxide
Am	Americium
ANS	American Nuclear Society
ANSI	American National Standards Institute, Inc.
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
AUCF	Advanced Uncanistered Fuel waste package design
B	Boron
B&W	Babcock and Wilcox or B&W Fuel Company
BOC	Beginning of Cycle
BOL	Beginning of Life
BONAMI	Name of a computer program, part of SCALE
B-SS	Borated Stainless Steel
BWR	Boiling Water Reactor
°C	Degrees Celsius
CASMO	Name of a computer program
CDF	Cumulative Distribution Function, for a probability distribution
CFR	Code of Federal Regulations
CGC	Configuration Generator Code
CH	Calico Hills
CHn1v	Calico Hills nonwelded unit 1 vitric
CHn1z	Calico Hills nonwelded unit 1 zeolitized
Ci	Curies
Cm	Curium
cm	Centimeter
COUPLE	Name of a computer program, part of SCALE
CRA	Control Rod Assembly
CRC	Commercial Reactor Critical
CRD	Contractor Requirement Document
CRWMS	Civilian Radioactive Waste Management System
DCRA	Disposal Control Rod Assembly
df	Variable in an equation, number of degrees of freedom
DFTL	Distribution Free Tolerance Limit
DHLW	Defense High-Level Waste
DI	Document Identifier
DOE	U. S. Department of Energy
DWPF	Defense Waste Processing Facility

EBS	Engineered Barrier System or Segment
EIA	Energy Information Administration
ENDF	Name of a nuclear cross section library set, Evaluated Nuclear Data File
EOC	End of Cycle
EPA	U. S. Environmental Protection Agency
EQ3/6	Name of a computer program
EQ6	Name of a computer code sequence, part of EQ3/6
eV	Electron Volt
Eu	Europium
Fe	Iron
Fe_nO_m	Iron oxide (n and m are integers less than 4)
FeOOH	Goethite, a form of iron oxide
FEP	Features, Events, and Processes
FEHM	Name of a computer program
FF	Far-field
Fig.	Figure
FM	Fissionable Materials
FR	Federal Register
FWF	Fissionable Waste Form
Gd	Gadolinium
$GdPO_4$	Gadolinium Phosphate
GWd/mtU	Gigawatt-Day per Metric Ton of Uranium
generate.c	Name of software routine
H	Hydrogen
HLW	High-level Waste
H/x	Water-to-fuel volume ratio
I	Iodine
ID	Inside Diameter
IOC	Interoffice Correspondence
IP	In-package
J-13	The designation of a well on Yucca Mountain
K	Degrees Kelvin
k_{eff}	Effective neutron multiplication factor
$k\infty$	Infinite neutron multiplication factor
kg	Kilogram
Kr	Krypton
kW	Kilowatt
LCE	Laboratory Critical Experiment
LEU	Low Enriched Uranium
LLNL	Lawrence Livermore National Laboratory
LTA	Long-Term Average Pluvial
LUTB	Lower Uniform Tolerance Band
LWR	Light Water Reactor

m	Meter
MCNP	Name of a computer program, Monte Carlo N-Particle
M&O	Management and Operating Contractor
MeV	Million Electron Volts
MGDS	Mined Geologic Disposal System
MGR	Monitored Geologic Repository
MIT	Massachusetts Institute of Technology
mm	Millimeter
MnO_2	Pyrolusite
Mo	Molybdenum
MOC	Middle of Cycle
MOX	Mixed Oxide
MTU	Metric Tons of Uranium
MWd	Megawatt Days
NAS	National Academy of Sciences
Nd	Neodymium
NDTL	Normal Distribution Tolerance Limits
NEMO	Name of a computer program
NF	Near-field
NLP	Nevada Site Administrative Line Procedure
NITAWL-II	Name of a computer program, part of SCALE
Np	Neptunium
NRC	U.S. Nuclear Regulatory Commission
NUREG	Designator for an NRC Document
O	Oxygen
OCRWM	Office of Civilian Radioactive Waste Management
OD	Outside Diameter
OIC	Other Internal Components of the waste package (not SNF)
ORIGEN-S	Name of a computer program, part of SCALE
ORNL	Oak Ridge National Laboratory
P	Variable in an equation, proportion of the population covered
PA	Performance Assessment
Pa	Protactinium
Pa	Pascals
PD	Present Day
pdf	Probability Density Function
ppmB	Parts per million of boron
PRA	Probabilistic Risk Assessment
PTn	Paintbrush Tuff Non-welded
Pu	Plutonium
PWR	Pressurized Water Reactor
PWRPROB	Name of software routine
pugdcr.c	Name of software routine
QA	Quality Assurance
QAP	Quality Administrative Procedure
QARD	Quality Assurance Requirements and Description

RELAP	Name of a computer program
REV	Revision of a document
Rh	Rhodium
RIP	Name of a computer program, Repository Integration Program
ROA	Range of Applicability
RSIC	Radiation Shielding Information Center
Ru	Ruthenium
RW	Radioactive Waste (referring to DOE/RW)
SAS2H	Name of a computer code sequence, part of SCALE
SCALE	Name of a computer program, Standardized Computer Analysis for Licensing Evaluations
SER	Safety Evaluation Report
SL	Subcritical Limit
Sm	Samarium
SNF	Spent Nuclear Fuel
SP	Super-Pluvial
SRS	Savannah River Site
SS-B	Stainless Steel Boron
SZ	Saturated-Zone
t	Time
TBD	To Be Determined
TBR	To Be Resolved
TBV	To Be Verified
Tc	Technetium
TCw	Tiva Canyon welded
TDSS	Assumption identifier, Technical Data Subsurface
Th	Thorium
TSbv	Topopah Springs basal vitrophyre
TSPA	Total System Performance Assessment
TSw	Topopah Spring welded
TSw2	Topopah Spring welded unit 2
TSw3	Topopah Spring welded unit 3 (Vitrophyre tuff)
U	Uranium
UnOm	Uranium Oxide (n and m are numbers)
UCF	Uncanistered Fuel
UCRL	University of California Research Laboratory
UNS	Unified Numbering System for Metals and Alloys
USL	Upper Subcritical Limit
UZ	Unsaturated-Zone
VA	Viability Assessment
Vol%	Volume Percent
WAPDEG	Name of a computer program, Waste Package Degradation model
WIPP	Waste Isolation Pilot Plant
WP	Waste Package
WF	Waste Form

WTAC	WIPP Technical Assistance Contractor
Wt.%	Weight Percent
XSDRNPM	Name of a computer program, part of SCALE
YMP	Yucca Mountain Site Characterization Project
yr	Year

Symbols

β	Bias or the reciprocal of the time duration over which there is a significant probability of criticality occurrence
D´	Normality test for data sets of 50 or more observations
df	Number of degrees of freedom
Δ	Change in
γ	The confidence level
P	The proportion of the population covered
$S(\alpha,\beta)$	Method for handling the thermal motion of scattering nuclei that also accounts for the binding effects of the nuclei
S_P	The square root of the pooled variance
S_P^2	The sum of the inherent 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

APPENDIX B

GLOSSARY

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

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.

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

Average energy of a neutron causing fission is the average of the energies at which neutrons cause fission.

Average lethargy of a neutron causing fission is the natural log of 10 MeV divided by AENCF expressed in units of MeVs.

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 poison designs are part of a core design that determines the location and amounts of the burnable poisons in a reactor core.

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 which accounts for the reduction in criticality potential associated with spent nuclear fuel relative to that of fresh fuel. Burnup credit reflects the net depletion of fissionable isotopes and the creation of neutron absorbing isotopes during reactor operations. Burnup credit also accounts for variations in the criticality potential of spent nuclear fuel produced by radioactive decay since the fuel was discharged from a reactor. Burnup credit is one of the licensing issues which will be addressed in the Topical Reports submitted to the U.S. Nuclear Regulatory Commission. For geologic disposal, burnup credit (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 a metal receptacle with the following purpose: (1) for solidified high-level radioactive waste, its purpose is a pour mold, and (2) for spent fuel, it may provide structural support for loose rods, nonfuel components, or confinement of radionuclides during preclosure operations.

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

Cell-spectrum-weight is a method used to homogenize cross-sections from two or more discrete regions into a single set of cross sections.

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

Cladding is the metal cylinder that surrounds the uranium pellets in commercial and some types of DOE fuels.

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

Convolution is a multiple integral in which the range of integration and integrand function arguments for one integral contain the variable of integration of another integral.

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.

Degraded fuel. See Spent nuclear fuel.

Discrete ordinates is a numerical approximation to the transport equation in which angular fluxes are solved on a finite-differenced spacial grid, for a discrete number of angles.

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.

Dose significant radionuclides are those radionuclides which provide the major contribution to dose at the accessible environment, due to their concentration in the waste form and long half life. The names and initial inventories of these radionuclides are specified in the TSPA.

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.

Effuent is the liquid or gas that flows out of some volume. It is used in this report for aqueous solutions exiting a waste package.

End effects are the differences between k_{eff} calculations for models based on axial variations and models based upon axial uniformity in fuel content distributions.

Engineered barrier system (EBS) is the waste packages and the underground facility (10 CFR 60.2).

Engineered barrier system 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.

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.

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

Fissile materials are those materials which will fission with slow neutrons (e.g., ^{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.

Free gas method is a method for handling the thermal motion of scattering nuclei that assumes the nuclei are in the form of a monatomic gas.

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 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) *Mined Geologic Disposal System Requirements Document* (YMP 1998).

Hydration is the adding of OH ions or H_2O molecules.

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

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

Intact fuel. See Spent nuclear fuel.

Invert is the level bottom placed in the drifts.

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

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).

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

Localized corrosion is a type of corrosion induced by local variations in electrochemical potential on a microscale over small regions. Variations in electrochemical potential may be caused by localized irregularities in the structure and composition of usually protective passive films on metal surfaces and in the electrolyte composition of the solution that contacts the metal.

Long-term-average-climate is one of three sets of conditions used to represent climate changes through time. Representative of the expected typical climate conditions at Yucca Mountain, with precipitation twice that of the present day climate.

Methodology as used in this document methodology refers to the systematic procedures proposed to evaluate the risk of criticality in the respository. 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. See engineered barrier system near-field.

Negative feedback is an element of a dynamic system that tends to reverse the current direction of evolution.

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.

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

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

Positive feedback is an element of a dynamic system that tends to reinforce the current direction of evolution.

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.

Prompt critical is a critical configuration in which $k_{eff} > 1$ from reliance on the prompt fission neutrons only.

Radial zone loaded fuel is a fuel design in which the enrichment of the fuel varies in the radial direction (e.g., assembly to assembly or fuel pin to fuel pin).

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).

Resonance is a peak in the cross section data at certain incident neutron energies.

Retrieval is the act of intentionally removing radioactive waste from the underground location at which the waste had been previously emplaced for disposal (10 CFR 60.2).

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

S(α,β) is a method for handling the thermal motion of scattering nuclei that also accounts for the binding effects of the nuclei.

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.

Sorption coefficient (K_d). Coefficient for a term for the various processes by which one substance binds to another.

Spectral parameter is a neutronic parameter that provides an index that may be used to characterize a neutron in system.

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.

Superpluvial is one of three sets of conditions used to represent climate changes through time. Representative of wetter-than-normal climate conditions at Yucca Mountain, with precipitation three times that of the present day climate.

Surface discharge is a release to the surface from an acquifer.

Topographic is the physical features of a district or region.

Transient criticality is a criticality event that is time-dependent.

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.

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

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.

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

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.

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APPENDIX C

EXAMPLE APPLICATION OF THE METHODOLOGY FOR COMMERCIAL SPENT NUCLEAR FUEL

APPENDIX C

EXAMPLE APPLICATION OF THE METHODOLOGY FOR COMMERCIAL SPENT NUCLEAR FUEL

This appendix provides an example application of the disposal criticality analysis methodology for commercial pressurized water reactor (PWR) spent nuclear fuel (SNF). Some comparison between PWR fuel and preliminary boiling water reactor (BWR) fuel results is also provided. Further refinements and details will be provided for License Application. Refer to Appendix A for the list of acronyms and abbreviations, and Appendix B glossary of terms.

1.0 INITIAL INPUTS

The first section of this appendix discusses the initial inputs used in the disposal criticality analysis methodology. The inputs include the Waste Form Characteristics, Waste Package/Engineered Barrier Design, Repository Site Characteristics Material Degradation Characteristics, and the Master Scenario List.

1.1 WASTE FORM CHARACTERISTICS

The category of commercial spent nuclear fuels encompasses the commercial light water reactor (LWR) SNF generated in BWRs and PWRs. Although some non-LWR fuel has been used for commercial applications (e.g., Fort St. Vrain), the non-LWR fuel has been reclassified as DOE SNF. There is a great deal of variability in the characteristics of commercial SNF. For purposes of this example, a single commercial waste form will be used for each LWR type.

The commercial PWR waste form used in the example is B&W 15 × 15 Mark B4 PWR SNF assemblies. The mechanical characteristics of the B&W 15 × 15 fuel assembly used for the example are listed in Table C-1a. Figure C-1a shows a B&W 15 × 15 fuel assembly, with a cut-away of a fuel rod.

The commercial BWR waste form used in the example is GE 8 × 8 BWR SNF assemblies with a central water rod. The mechanical characteristics of a representative GE 8 × 8 fuel assembly used for the example are listed in Table C-1b. A graphical representation of a BWR fuel assembly is provided in Figure C-1b.

1.2 WASTE PACKAGE/ENGINEERED BARRIER DESIGN

The current concept of operations of the proposed Yucca Mountain Repository calls for multiple combinations of waste package and engineered barrier designs to accommodate the different waste forms. The designs are designated by the type of waste package (WP). The engineered barrier system (EBS) outside the waste package does not vary for different waste packages in the current concept of operations.

Table C-1a. Mechanical Parameters of B&W 15 x 15 Fuel Assembly (CRWMS M&O 1996g, p. 6)

Parameter	Value	Units	Metric	Units	Radius (cm)
Fuel rods	208	/assembly	208	/assembly	-
Fuel Rods on a Lattice Side	15	/side	15	/side	-
Guide Tubes	16	/assembly	16	/assembly	-
Instrumentation Tubes	1	/assembly	1	/assembly	-
Total Guide + Instrument Tubes	17	/assembly	17	/assembly	-
Instrument Tube Thickness	0.16764	inches	0.066	cm	-
Clad/Tube Material	Zirc-4		Zirc-4		-
Fuel Pellet OD	0.3686	inches	0.936244	cm	0.468122
Fuel Stack Height	141.8	inches	360.172	cm	-
Fuel Assembly Height	165.625	inches	420.7	cm	-
Mass of U	1023	lb	464	kg	-
Mass of UO_2	1160.64	lb	526.38	kg	-
Percent of Theoretical Density	95	%	95	%	-
Fuel Clad OD	0.430	inches	1.0922	cm	0.5461
Clad Thickness	0.0265	inches	0.06731	cm	-
Fuel Clad ID	0.377	inches	0.95758	cm	0.47879
Fuel Rod Pitch	0.568	inches	1.44272	cm	0
Guide Tube OD	0.530	inches	1.3462	cm	0,6731
Guide Tube Thickness	0.016	inches	0.04064	cm	-
Guide Tube ID	0.498	inches	1.26492	cm	0.63246
Instrumentation Tube OD	0.493	inches	1.25222	cm	0.62611
Instrument Tube Thickness	0.16764	Inches	0.066	cm	-
Fuel Assembly Envelope	8.536	inches	21.68144	cm	-
Displaced Volume per Fuel Assembly	4927	$inches^3$	0.081	m^3	-

The inner diameters (IDs) above are calculated by subtracting 2 · thickness from the outer diameter (OD).

Table C-1b. Mechanical Parameters of Example GE 8 x 8 Fuel Assembly (CRWMS M&O 1998o, p. 7)

Parameters	Value
Fuel pellet radius	0.5207 cm
Active fuel length	368.9096 cm
Clad thickness	0.0813 cm
Clad outside radius	0.6134 cm
Rod pitch	1.6256 cm
Water rod outside radius	1.3094 cm
Water rod inside radius	1.2281 cm
Initial uranium loading	171177 g/assembly

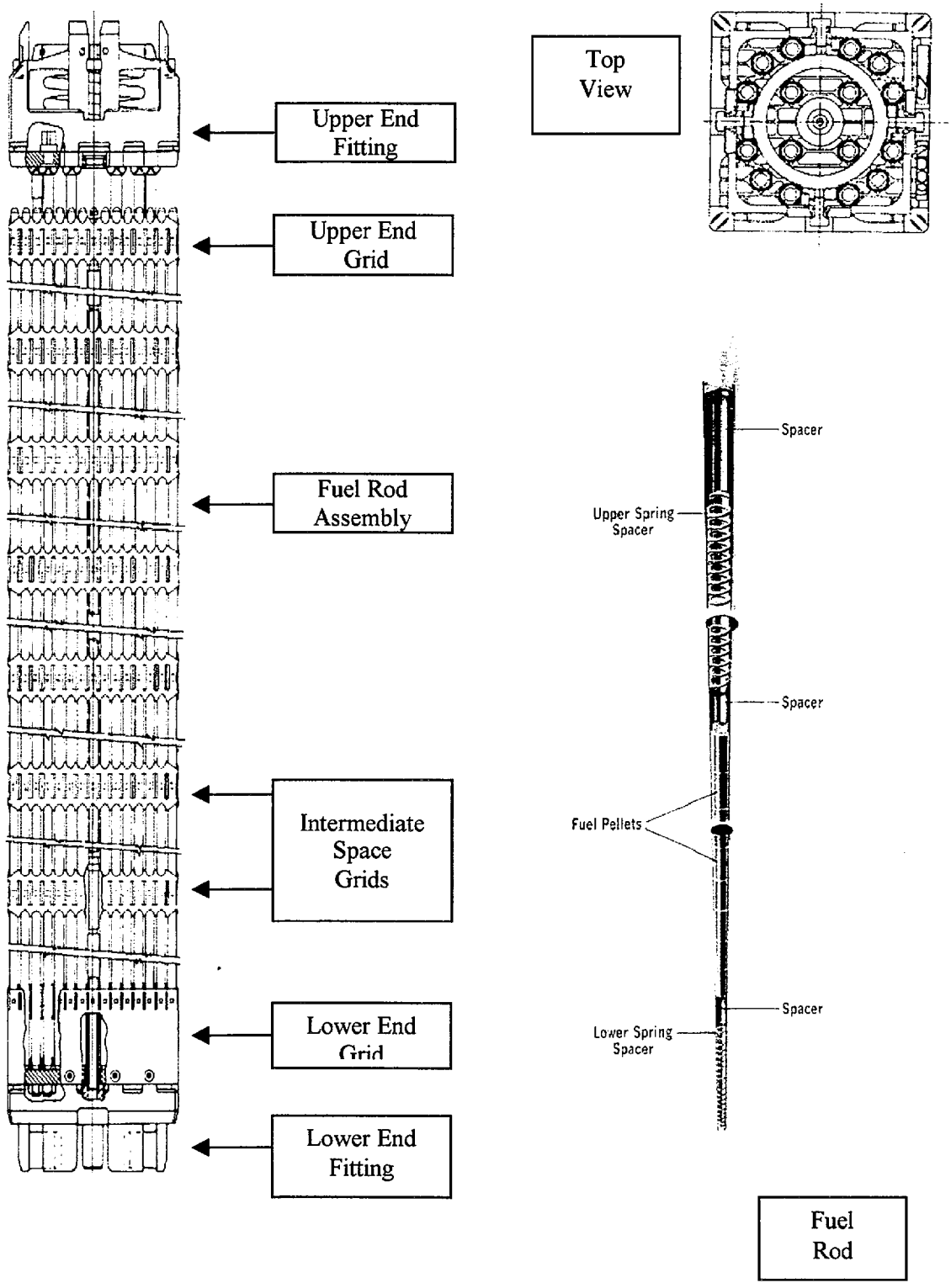

Figure C-1a. B&W 15 x 15 Fuel Assembly

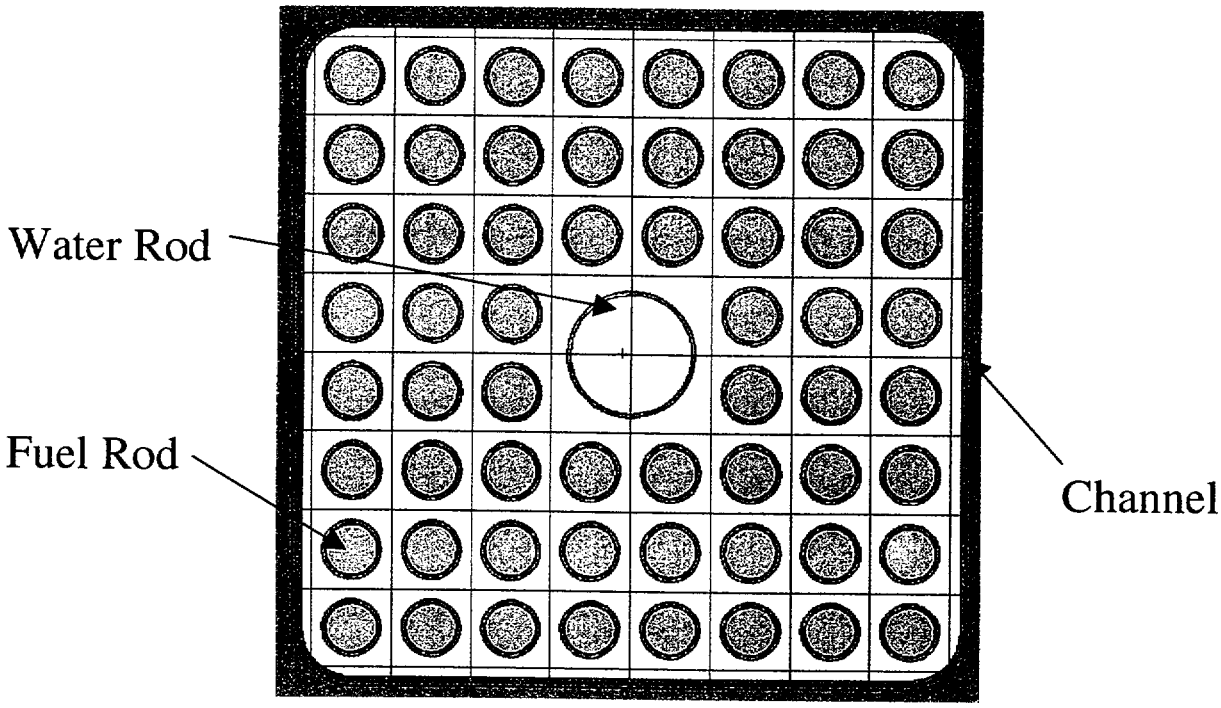

Figure C-1b. Example GE 8 x 8 Fuel Assembly

The waste package design selected for evaluation in the example is the 21 PWR Uncanistered Fuel (UCF) design. Figure C-2a provides a graphical description of the 21 PWR UCF Absorber Plate design. The design relies on burnup credit and neutron absorbers to provide disposal criticality control. Figure C-2a identifies the major components of the UCF waste package design. The material call outs for the components in the waste package (CRWMS 1997j, p. 125) are listed under the components (A 516, Stainless Steel Boron, and Alloy C-22). Not shown in this picture are the thermal shunts, which are fabricated from aluminum alloy 6061. A 516 refers to the type of the carbon steel, the Stainless Steel Boron is a Type 316 stainless steel alloy with 1.6 weight-percent boron, and Alloy C-22 refers to a specific type of nickel-based alloy (ASTM B 575 is commonly known by the trademark name C-22) that was used for this example. Figure C-2b shows a cross-section of the 44 BWR UCF Absorber Plate waste package design used for the preliminary comparison between BWR and PWR fuel. The materials used for this waste package are the same as for the PWR package discussed above.

Figure C-3 provides an example criticality loading curve for the intact 21 PWR UCF Absorber Plate waste package design loaded with B&W 15 x 15 fuel assemblies. The intact loading curve was generated as part of the preclosure criticality safety evaluation (intact WP flooded with unborated water) performed in CRWMS M&O 1998j. Assemblies with average burnup and enrichments below the line would not be acceptable for loading in the Absorber Plate WP without supplemental Disposal Control Rods. No loading curve for the intact 44 BWR UCF Absorber Plate waste package has been defined at this time.

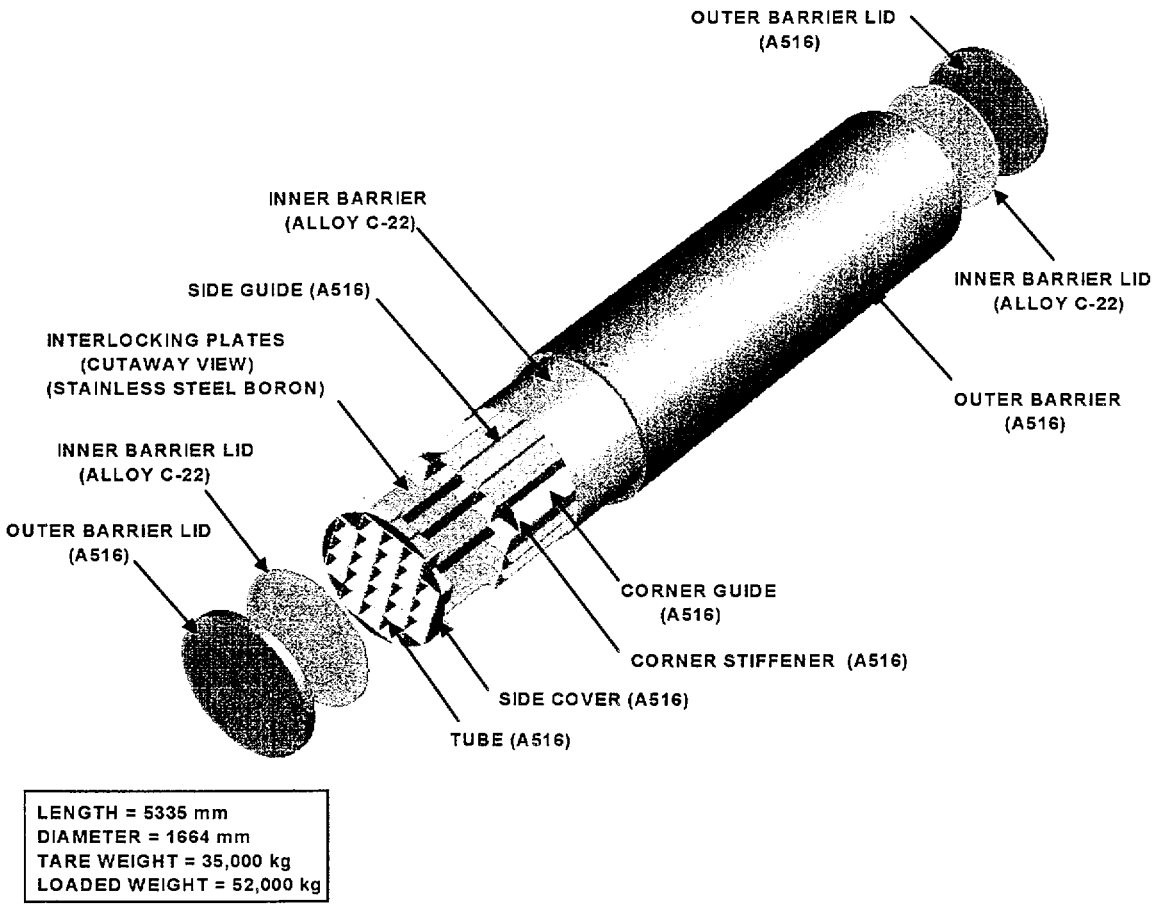

Figure C-2a. 21 PWR UCF Disposal Container

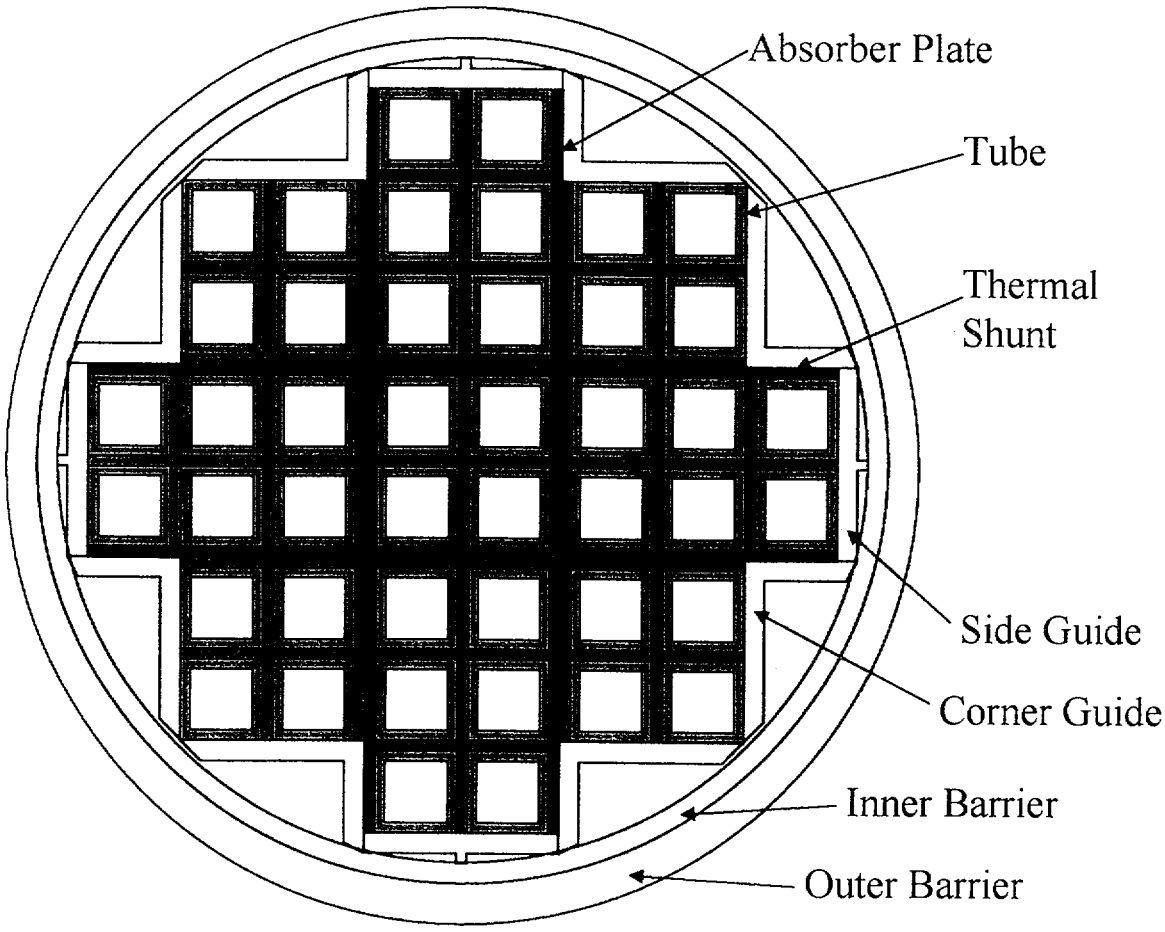

Figure C-2b. 44 BWR UCF Disposal Container

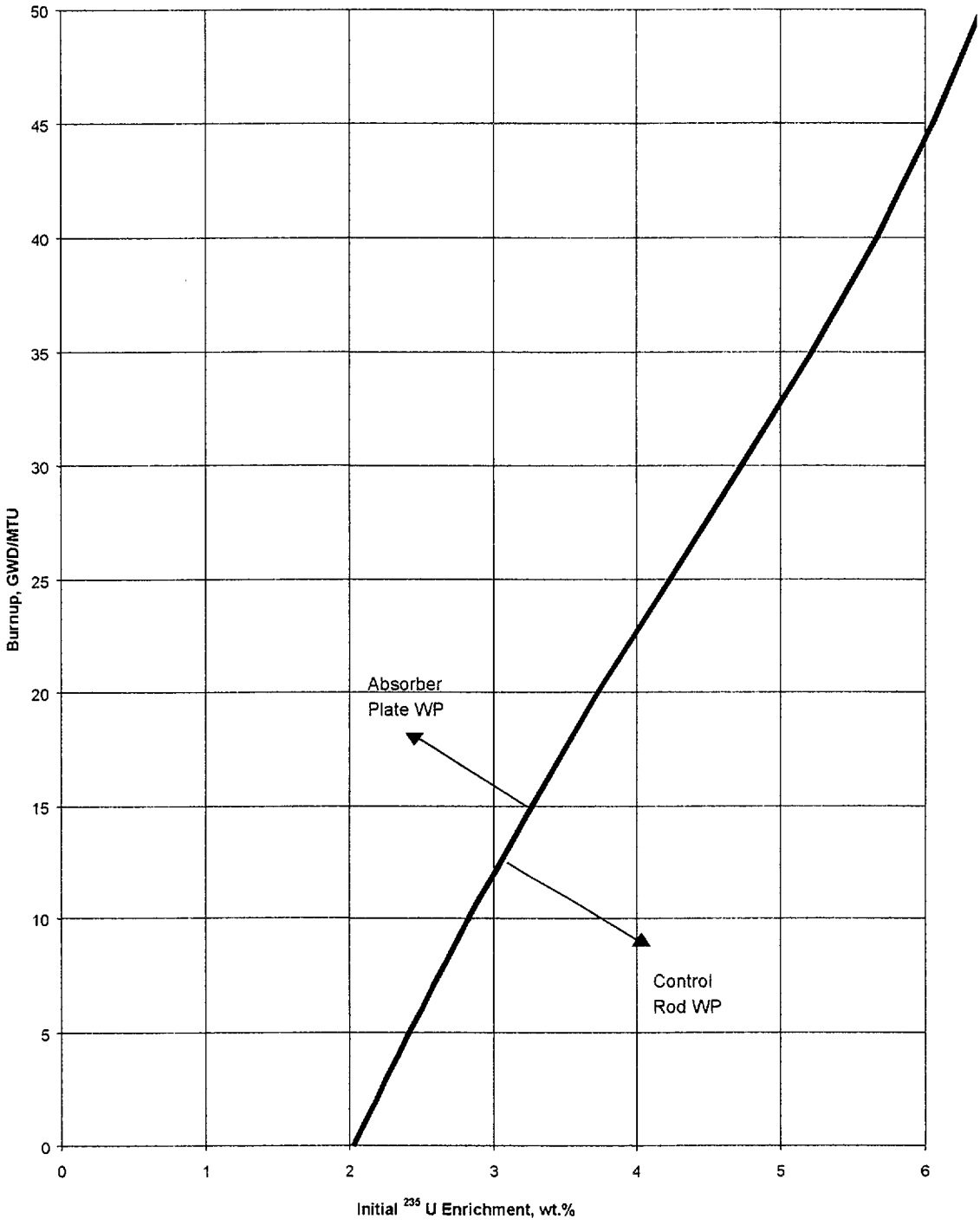

Figure C-3. Example Loading Curve For the 21 PWR UCF Waste Package

1.2.1 Engineered Barrier System Design

The EBS design (the underground structures) used in the example is the EBS Viability Assessment design (CRWMS M&O 1997a). Figure C-4 shows a view of the EBS design used in the example evaluation. The EBS design for the example has the following properties:

- 5.5 meter diameter emplacement drifts (CRWMS M&O 1997a, Fig. 7-20)
- ~1200 meter long drifts (CRWMS M&O 1997a, Fig. 7-1)
- Pier emplaced waste packages (CRWMS M&O 1997a, Fig. 7-20)
- Piers consist of a carbon steel box filled with concrete resting on a pre-cast concrete invert segment (CRWMS M&O 1997a, Fig. 7-20)
- Waste package pedestal supports are made of carbon steel and are attached to the piers (CRWMS M&O 1997a, Fig. 7-20)
- Invert material is pre-cast concrete (CRWMS M&O 1997a, Fig. 7-20)
- 15.4 meter nominal center-to-center spacing between emplaced 21 PWR waste packages (CRWMS M&O 1997k, Table 7.5-2)
- 28 meters nominal spacing between emplacement drifts (CRWMS M&O 1997a, Fig. 7-20)
- No backfill in the emplacement drifts (CRWMS M&O 1998m, Key 0046).

Figure C-4 shows three types of waste packages in the drift; however the PWR waste package was the only type specifically addressed in the example evaluation.

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

1.3 REPOSITORY SITE CHARACTERISTICS

The repository site used in the example is the proposed Yucca Mountain Site in Nevada. The Yucca Mountain site is an unsaturated site in volcanic tuff.

1.3.1 General Physical Description

The repository emplacement horizon is situated in Topopah Spring welded Unit 2 tuff (TSw2). The emplacement horizon is more than 200 meters below the ground surface and 200 meters above the water table (CRWMS M&O 1996f p. 5-4). Figure C-5 provides a sketch of the Waste Package (WP) Emplacement Concept used for the sample evaluation, including a cutaway pillar showing the different types of rock layers found between the surface and water table at the Yucca Mountain site. A detailed description of the rock layers can be found in Determination of Available Volume for Repository Siting analysis (CRWMS M&O 1997b, p. 30). The pillar in Figure C-5 shows only a portion of a single emplacement drift.

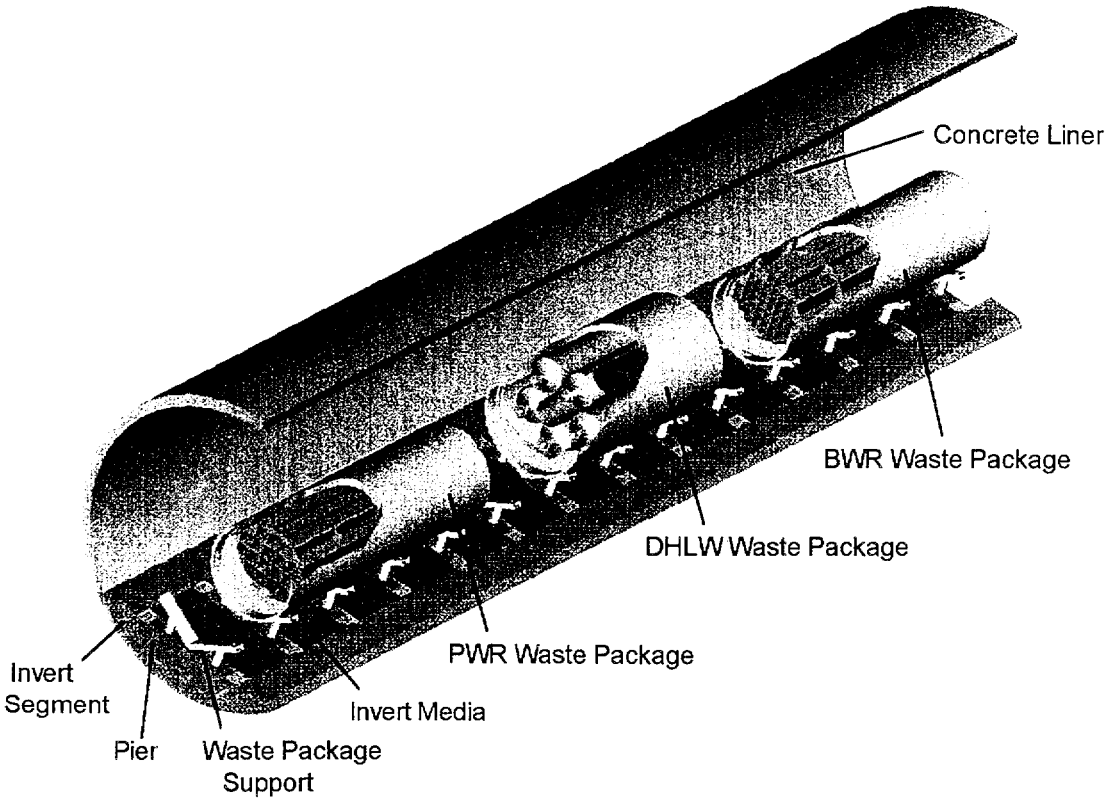

Figure C-4. Engineered Barrier Segment

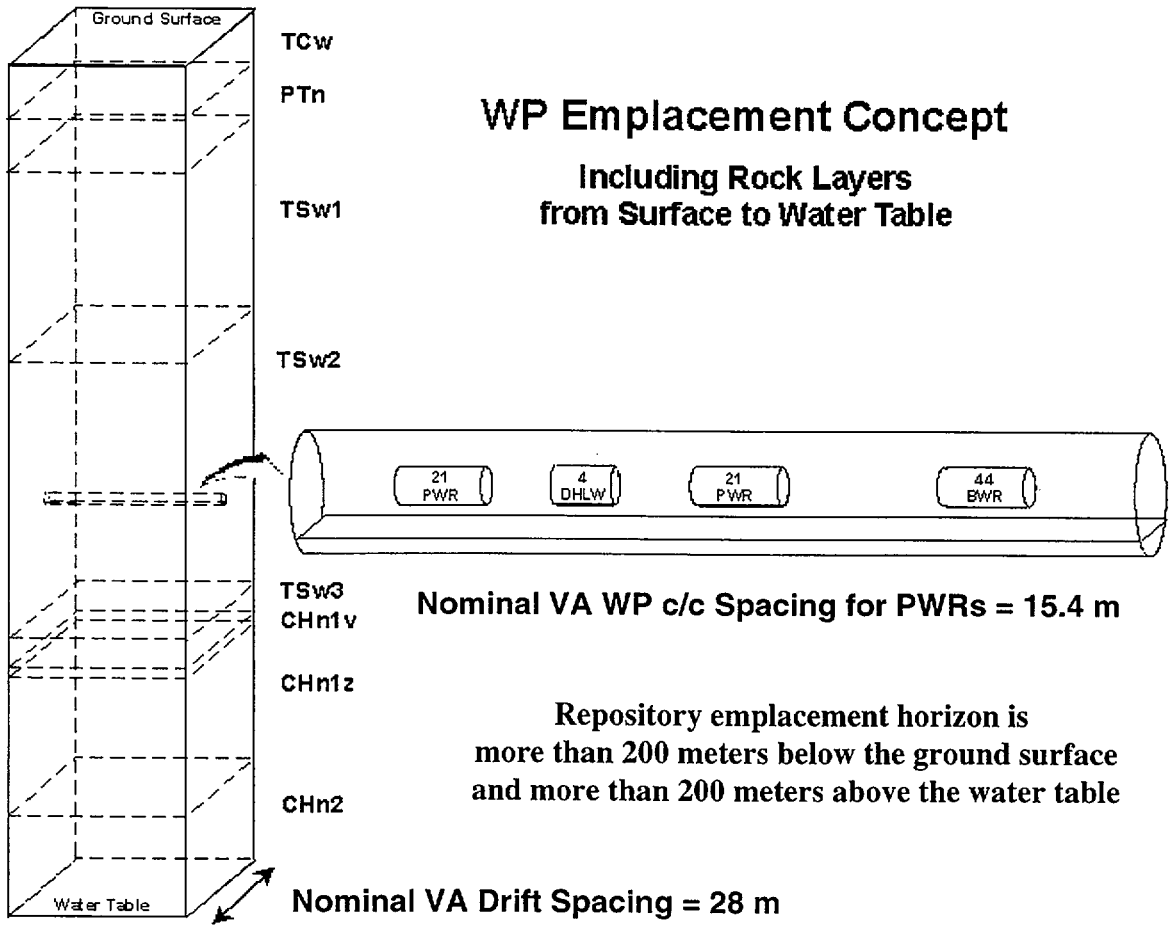

Figure C-5. WP Emplacement Concept

Figure C-6 provides a graphical representation of a sample repository layout for the potential Yucca Mountain repository. The ramps, emplacement blocks, Yucca Mountain ridge, and water table are all identified in the figure. The parallel lines shown in the areas identified as emplacement blocks are the drifts where waste packages would be emplaced. A detailed description of the conceptual repository layouts can be found in CRWMS M&O 1997a (Section 7).

1.3.2 Range of Site Characteristics

A large number of repository site characteristics are considered in the example. The range of the repository site characteristics or parameters used are consistent with the models used for the total system performance assessment (TSPA).

1.3.2.1 Climate Changes and Associated Percolation Rates

The climate model utilized was obtained from the draft TSPA-VA abstraction of the unsaturated zone (UZ) flow model.[1] In this model, future climate is modeled as a sequence of discrete states lasting for long periods of time. Only three discrete climate states were considered: present, long-term average, and super pluvial. Present climate represented relatively dry, interglacial conditions. The long-term average represented the typical conditions at Yucca Mountain, between the wet and dry extremes. Because glacial climates have dominated globally over the last million years, the long-term average represented an average pluvial period at Yucca Mountain. The super pluvial represented periods of extreme wetness. A detailed summary of the duration, frequency, and percolation rate probability distributions for each climate state is provided below.

Present Day (PD)

Duration: Uniformly distributed from 0 to 20,000 years, except for the current cycle which has already lasted for 10,000 years and has a remaining duration that is uniformly distributed from 0 to 10,000 years ([1] pp. 2.3-14).

Frequency: Three out of every four 100,000 year cycles ([1] p. 2.3-14).

Percolation Rate:	Minimum:	≈0.50 mm/yr ([1] Table 2.3-101)
	Mean:	7.01 mm/yr ([1] Table 2.3-38)
	95%:	14.6 mm/yr ([1] Table 2.3-38)
	Maximum:	19.5 mm/yr ([1] Table 2.3-38)

Long Term Average Pluvial (LTA)

Duration: 80,000 to 100,000 years (100,000 years – duration of PD or super-pluvial [SP]) ([1] pp. 2.3-14).

[1] The climate model utilized was obtained from *Preliminary Draft Chapter of the Unsaturated Zone Flow Abstraction for the TSPA-VA*. 1998. MOL.19980428.0202.

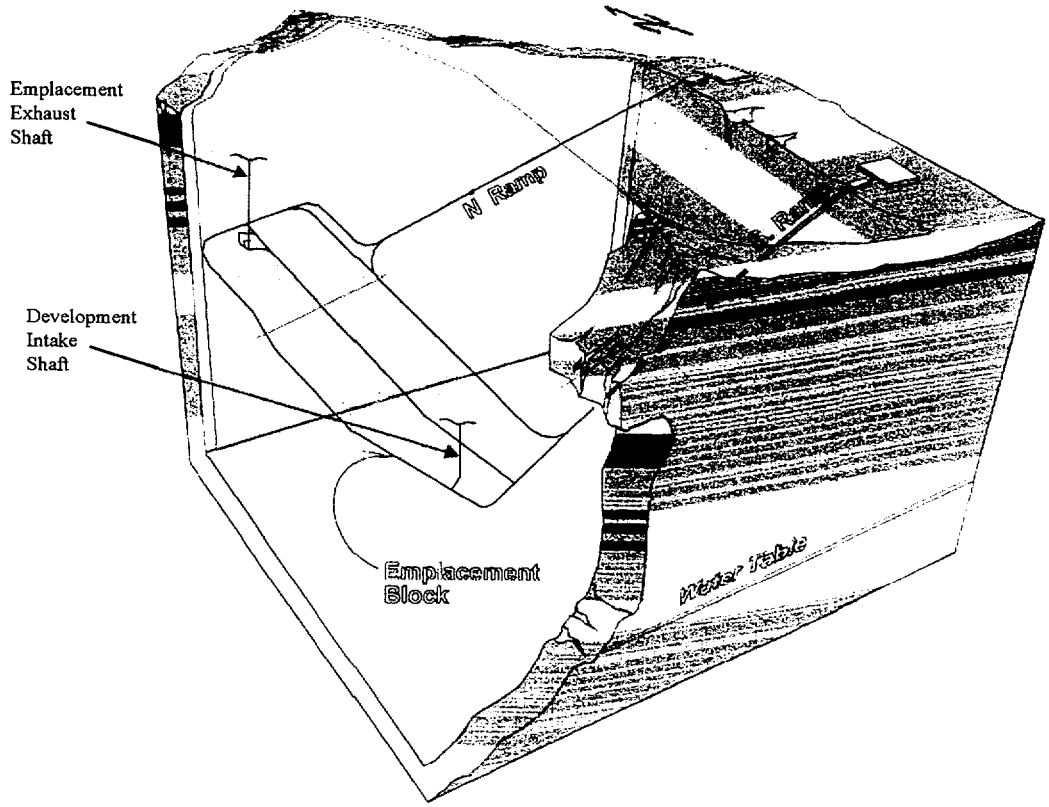

Figure C-6. Sample Repository Layout

Frequency: Occurs every 100k year cycle between two PD climates or between a PD and an SP climate ([1] pp. 2.3-14).

Percolation Rate:	Minimum:	≈7.5 mm/yr ([1] Table 2.3-102)
	Mean:	38.8 mm/yr ([1] Table 2.3-38)
	95%:	67.9 mm/yr ([1] Table 2.3-38)
	Maximum:	83.8 mm/yr ([1] Table 2.3-38)

Super-Pluvial

Duration: Uniformly distributed from 0 to 20,000 years ([1] pp. 2.3-14).

Frequency: One out of every four 100k year cycles ([1] pp. 2.3-14).

Percolation Rate:	Minimum:	≈10 mm/yr ([1] Table 2.3-103)
	Mean:	105.8 mm/yr ([1] Table 2.3-38)
	95%:	213.4 mm/yr ([1] Table 2.3-38)
	Maximum:	287.9 mm/yr ([1] Table 2.3-38)

To facilitate the use of the percolation rate uncertainty data in the probability calculation performed later in this appendix, a least-squares fit of the data to a three-parameter Weibull distribution was performed (CRWMS M&O 1997g, Section 5.1.1). The Weibull distribution was chosen for this application because of its ability to fit a wide variety of distribution shapes, and the ability to set a minimum value for the distribution. Figure C-7 shows the Weibull Cumulative Distribution Function (CDF) for the present day climate percolation rate, and the data points used in the fit. Figures C-8 and C-9 provide the same information for the LTA and SP climates, respectively.

1.3.2.2 Seepage Fraction

The draft TSPA-Viability Assessment (VA) base case seepage model is based on abstraction of the results of a large number of three dimensional unsaturated zone flow process-model calculations. The process-model results were abstracted in Tables 2.3-49 and 2.3-50[1] by fitting the calculated seepage fraction (the fraction of WPs under dripping fractures) with beta probability distributions for which the mean and standard deviation are functions of the percolation rate in the fractures. Figure C-10 shows the mean seepage fraction and the associated uncertainty (one standard deviation).

1.3.2.3 Seepage Flow Rate

As with the seepage fraction, the seepage flow rate abstraction was developed in Tables 2.3-49 and 2.3-50[1] by fitting the seepage flow rate results from the UZ flow process model with beta probability distributions for which the mean, standard deviation, and maximum are functions of the percolation rate in the fractures. Figure C-11 shows the maximum and mean flow rates and the associated uncertainty (one standard deviation).

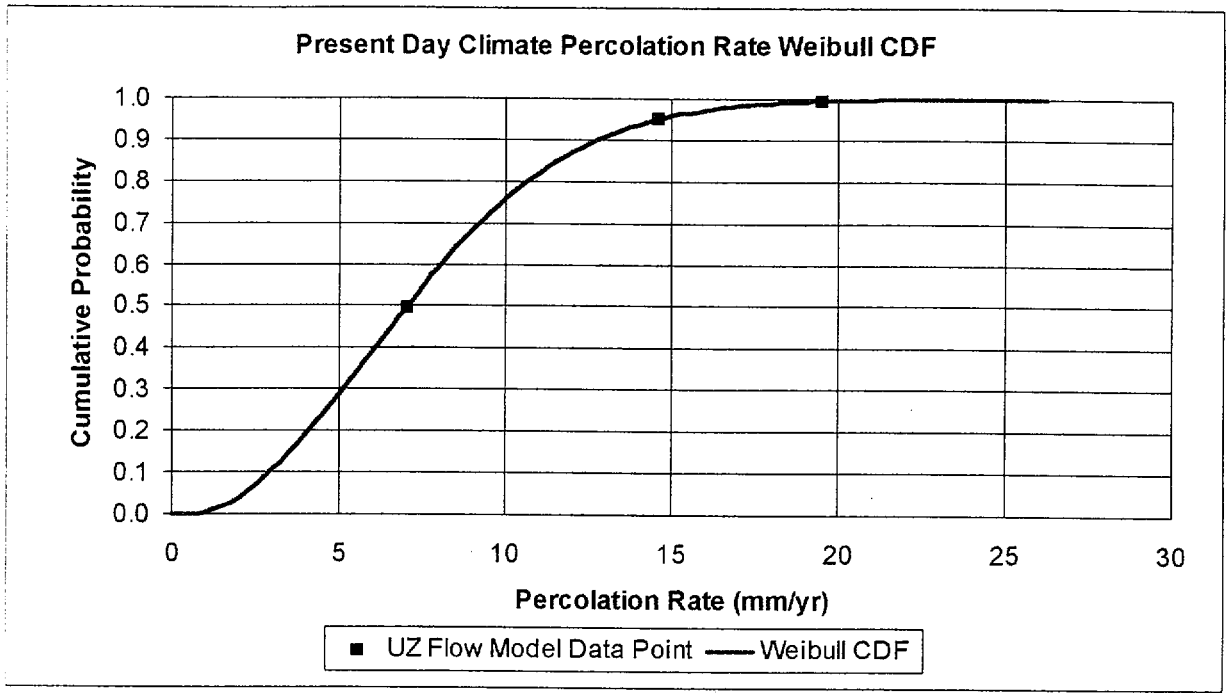

Figure C-7. Present Day Climate Percolation Rate

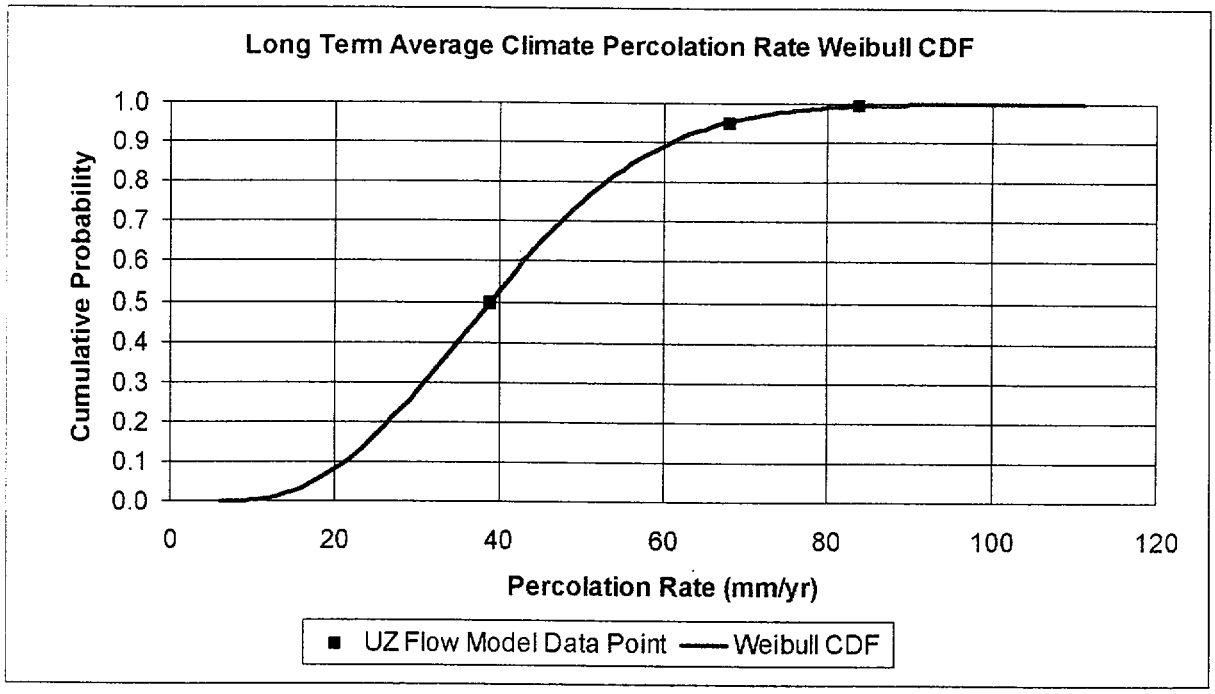

Figure C-8. Long-Term Average Climate Percolation Rate

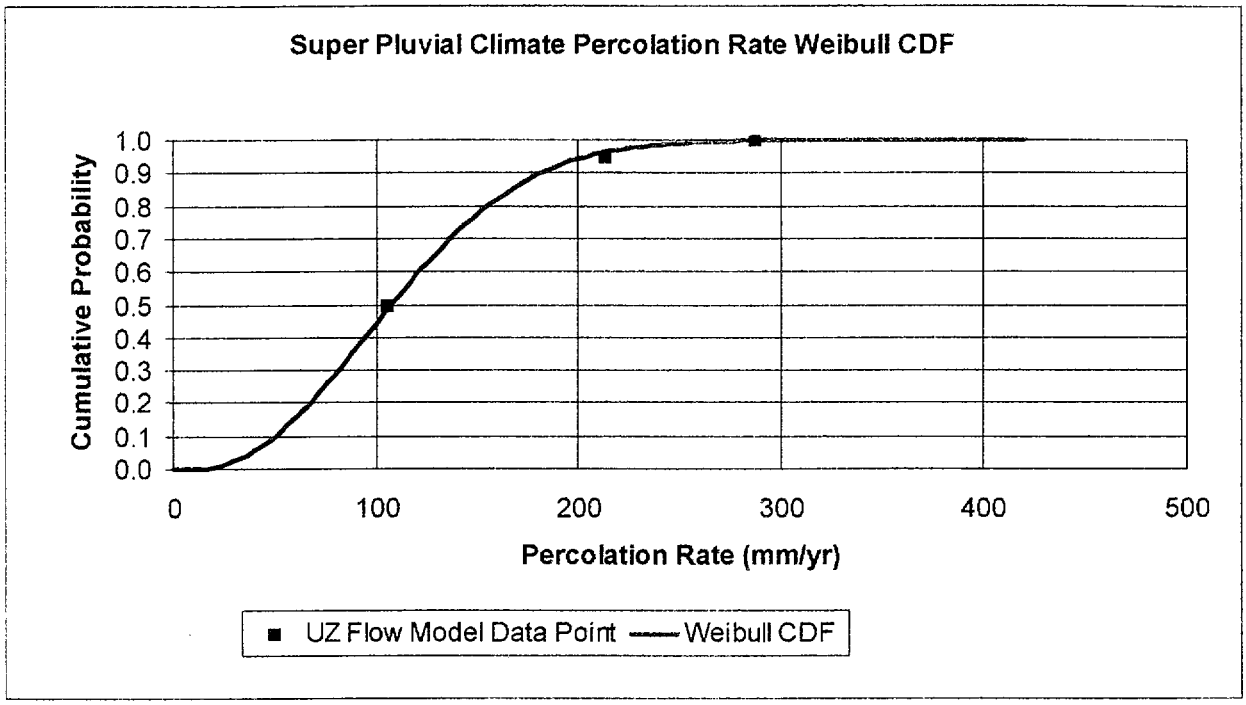

Figure C-9. Super Pluvial Climate Percolation Rate

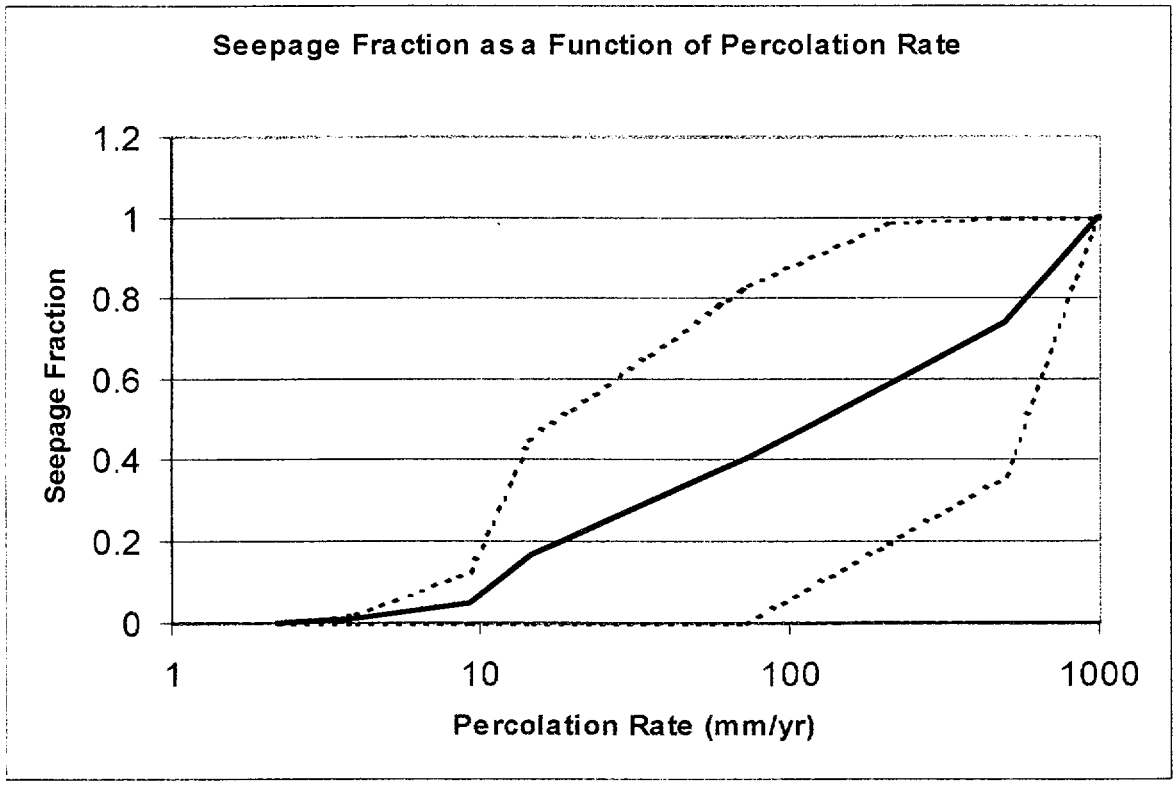

Figure C-10. Seepage Fraction as a Function of Percolation Rate

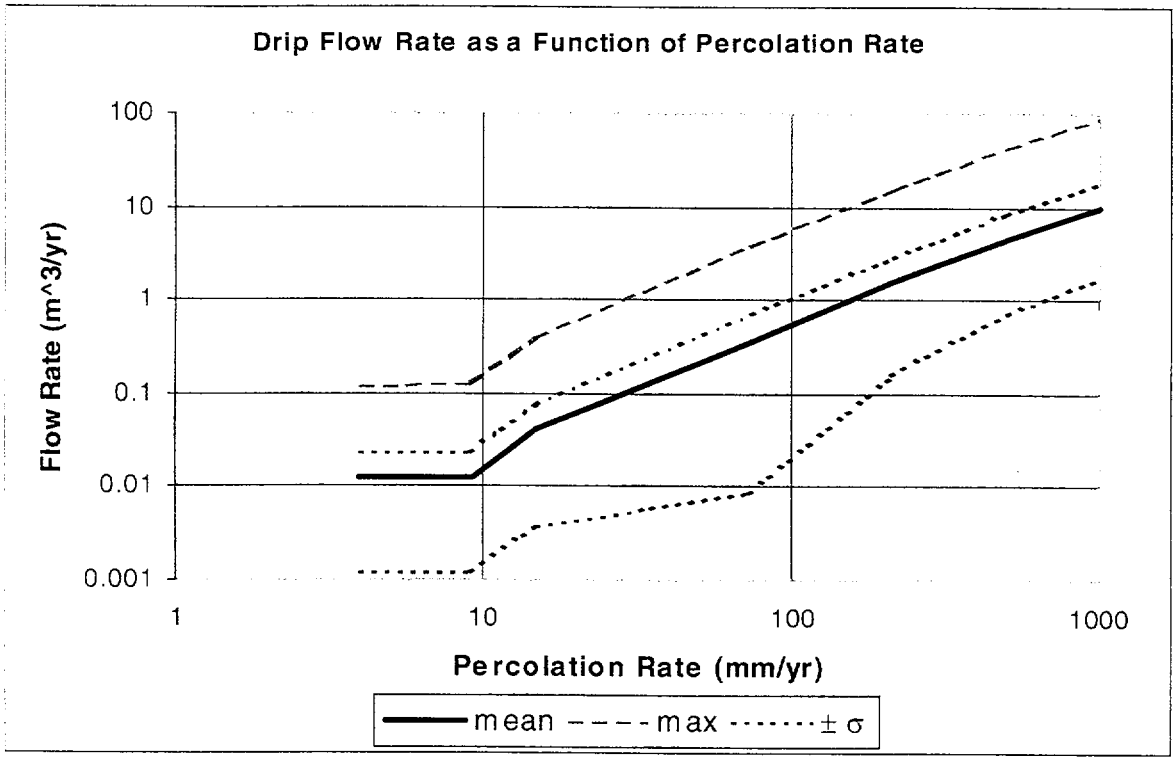

Figure C-11. Drip Flow Rate as a Function of Percolation Rate

1.3.2.4 Water Chemistry

Geochemistry calculations of basket corrosion products assumed that the water composition entering the waste package would be the same as for water from well J-13. This water has been analyzed repeatedly over a span of at least two decades, as explained in CRWMS M&O 1997d (and the references cited therein). The average composition is reproduced in Table C-2 (CRWMS M&O 1997d, Table 4.1.4-1).

Table C-2. Analyzed Composition of J-13 Well Water

J-13 Water	Molality	Mole Fr.
Na	1.99e-03	1.20e-05
Si	1.02e-03	6.11e-06
Ca	3.24e-04	1.95e-06
K	1.29e-04	7.74e-07
C	1.45e-04	8.69e-07
F	1.15e-04	6.89e-07
Cl	2.15e-04	1.29e-06
N	1.42e-04	8.53e-07
Mg	8.27e-05	4.97e-07
S	1.92e-04	1.15e-06
B	1.24e-05	7.44e-08
P	1.27e-06	7.63e-09
H	1.11e+02	6.67e-01
O	5.55e+01	3.33e-01
Total	1.67e+02	1.00e+00

1.4 MATERIAL DEGRADATION CHARACTERISTICS

The means of material degradation considered include corrosion, physical deformation, and combinations. The forms of corrosion considered include general corrosion, pitting corrosion, stress corrosion cracking, metal embrittlement, etc. Causes of physical deformation considered include rock falls, static loads, and seismic events. The combinations look at the physical deformations applied to a material weakened by corrosion.

1.4.1 Barrier Material Degradation Characteristics

As described in Section 1.2, the containment barriers in the example waste package design consist of two metallic materials: ASTM A 516, a low-carbon steel for the outer barrier and ASTM B 575 N06022, a nickel-based alloy for the inner barrier (CRWMS M&O 1997j, p. 125). ASTM B 575 is commonly known by the trademark name C-22. The A 516 low-carbon steel is considered a corrosion allowance material. A 516 has a well known general corrosion rate. Alloy C-22 is a corrosion resistant material, which resists general corrosion, but is susceptible to pitting corrosion in harsh environments.

The time to breach both the outer and inner barriers is determined for TSPA-VA using the waste package degradation simulation code WAPDEG. Figure C-12 provides a sample distribution of waste package breach times for packages under dripping fractures developed using WAPDEG v3.06, CSCI:30048 (CRWMS M&O 1998k), and the associated Weibull fit used in the probabilistic analysis discussed later in this appendix (CRWMS M&O 1998g, Section 5.1.4). WAPDEG also tracks the spatial location of penetrations on the surface of the waste package, which can be utilized to determine the fraction of packages, which may experience internal flooding. In this sample, 52.3 percent of the packages had the first penetration occur on the bottom of the package, and thus would not be capable of flooding. This expectation is based on information in CRWMS M&O 1996f which indicates that corrosion product plugging of pits would not significantly extend the time required for draining of the package, as corrosion products were only found to completely plug small aperture cracks if they were compacted by high water pressure. For the remaining 47.8 percent which breached on the top first, the distribution of time between the top penetration and the first bottom penetration is shown in Figure C-13 (CRWMS M&O 1998g, Section 5.1.5).

1.4.2 Basket Material Degradation Characteristics

The basket for the example waste package design consists of three metallic materials: ASTM A 516 low-carbon steel for the fuel cell tubes and structural side and corner guides, aluminum alloy for the thermal shunts, and a borated austenitic stainless steel for the criticality control plates (CRWMS M&O 1997j, p. 125).

CRWMS M&O 1996d, (p. 59) indicates that the 10 mm thick carbon steel side guides in the PWR waste package will fail by bending at a thickness of 2.9 mm if there is no other material loading the basket (which would only be the case after the upper portion of the WP barriers have collapsed, allowing backfill and/or rockfall rubble to enter). CRWMS M&O 1996d, (p. 59) estimated that this failure would occur within 60 to 340 years following WP breach using the TSPA carbon steel corrosion model (CRWMS M&O 1995a, Subsection 5.7.3). Failure of the side guides will cause the bottom row of fuel assemblies to shift downward to touch the inside of the inner barrier. As the criticality control plate assemblies also rest on the top of the side guides, the entire basket structure should also shift downward. Since the corner guides are under less loading, their failure should occur shortly after failure of the side guides.

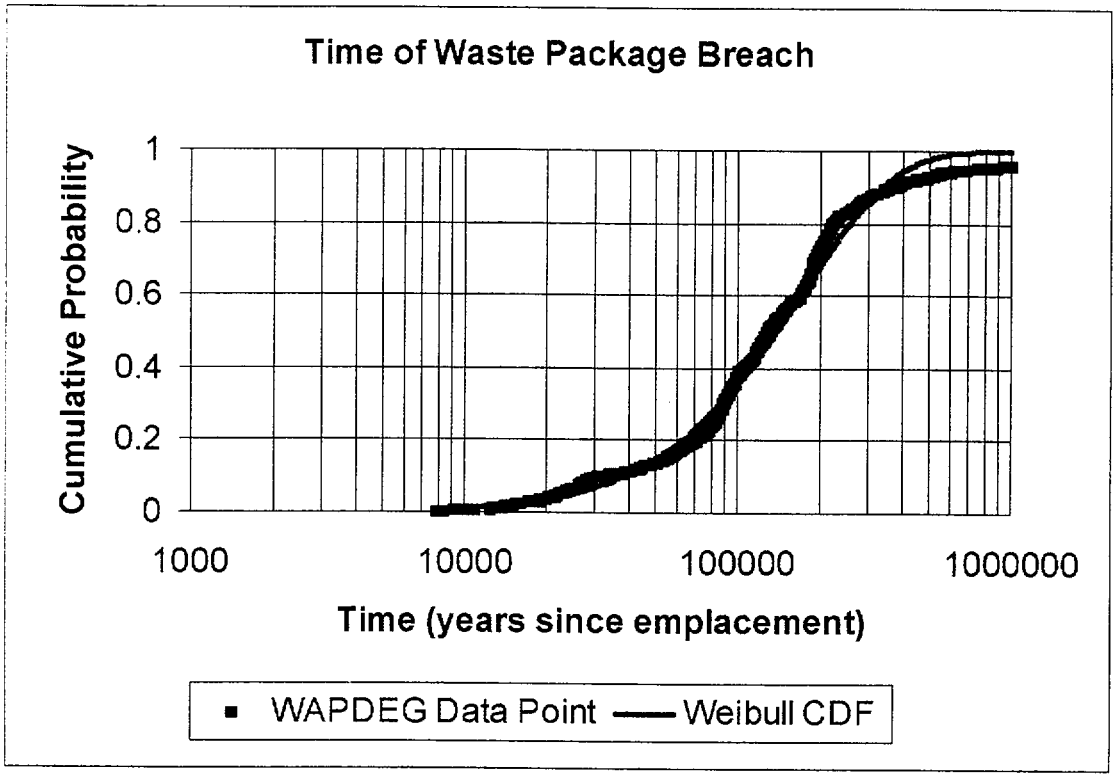

Figure C-12. Time of Waste Package Breach

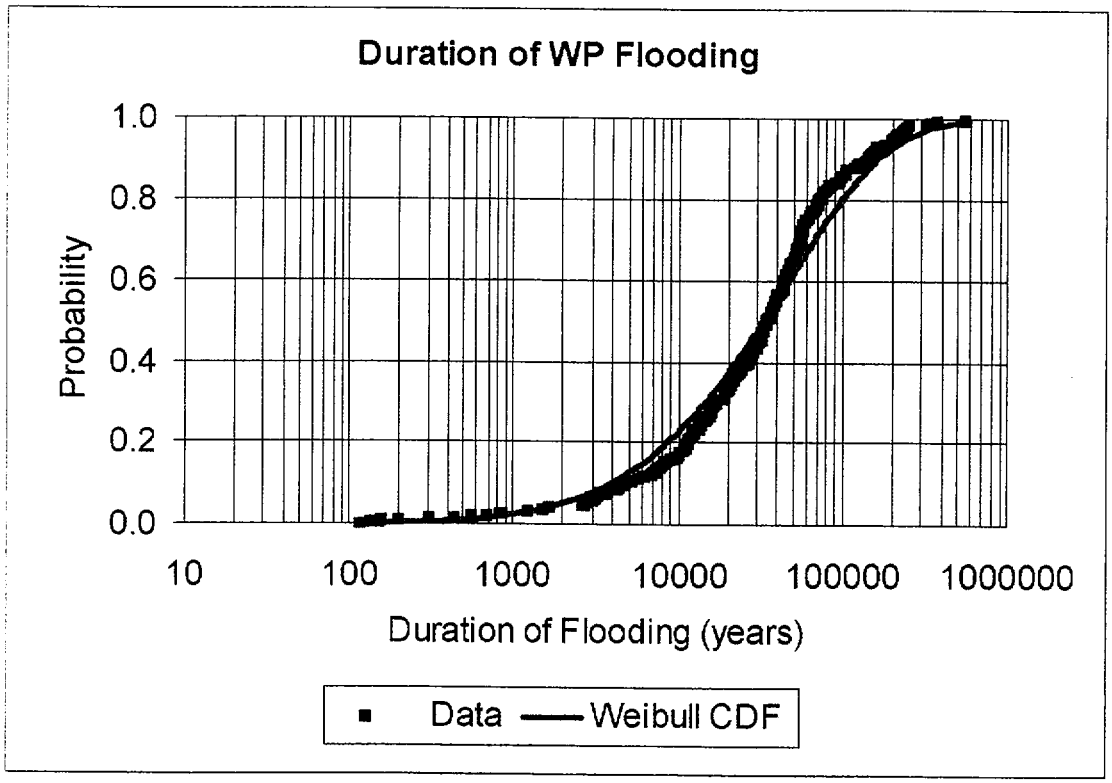

Figure C-13. Duration of Waste Package Flooding

Failure of the corner guides will result in the assemblies on the end of the second row from the bottom to shift downward to touch the inside of the inner barrier. The assemblies above them should remain in place until sufficient degradation of the criticality control plates, which support them has occurred. A similar sequence and timing of degradation and collapse would be expected for the BWR waste package as well.

The 5 mm thick carbon steel fuel cell tubes are expected to fully degrade before the failure of the side guides (because they are thinner) or the criticality control plates. In structural analysis of the criticality control plates for the PWR waste package, it was determined that the plates could maintain the basket and SNF assembly configuration without structural support from the tubes (CRWMS M&O 1998j, p. 60). Failure of the tubes will, therefore, not cause collapse of the basket, so no specific structural analyses were performed for the tubes. Any insoluble corrosion products from the carbon steel tubes would be expected to remain in their respective fuel cells until complete degradation of the criticality control plates occurs. While not specifically evaluated, this would also be expected to remain true for the BWR waste package due to the overall lower mass of the BWR assemblies to be supported.

The borated stainless steel criticality control plates are fabricated from a corrosion resistant material, and localized forms of corrosion are the primary cause of corrosion induced failure in most applications. For example, while CRWMS M&O 1998d, (p. 60) indicates that several thousand years (after breach) would be required for general corrosion to remove sufficient material to cause final collapse of the basket structure, localized corrosion in the crevice regions at the corner of each cell would likely cause this collapse to occur earlier. However, exposure and degradation of the metal boride particles in the borated stainless steel can only occur as a result of bulk degradation of the stainless steel matrix, which is best represented by the general corrosion rate. Preliminary corrosion tests have shown that the borides corrode at a rate similar to that of the stainless steel matrix. However, due to their extremely small size, the boride particles are not expected to last for more than a few hundred years after exposure (CRWMS M&O 1996g, p. 32).

The corrosion model used for the borated stainless steel is based upon the general corrosion rates measured for unborated 304 and 316 stainless steels (see Figure C-14) in repository-relevant environments (CRWMS M&O 1996g, Subsection 4.1.4 and CRWMS M&O 1998g, Subsection 5.1.6). Corrosion tests comparing the performance of borated and unborated stainless steels have generally shown little difference in corrosion rates (CRWMS M&O 1996g, Subsection 4.1.4). However, in one test with low pH conditions, borated stainless steel was found to have a corrosion rate four times that of unborated stainless of the same type (CRWMS M&O 1996g, Subsection 4.1.4). Therefore, to more conservatively model the corrosion of borated stainless steel with the available data, the corrosion rates sampled from the 304/316 stainless steel distribution will be multiplied by a unitless "boron factor." This boron factor will be sampled from a uniform distribution ranging from 1 to 4.

The aluminum thermal shunts are expected to corrode at a rate similar to that of the carbon steel (CRWMS M&O 1998e, Subsection 5.2.3). However, as they do not perform a structural or neutronic function no significant changes in basket geometry would be expected as a consequence of their degradation.

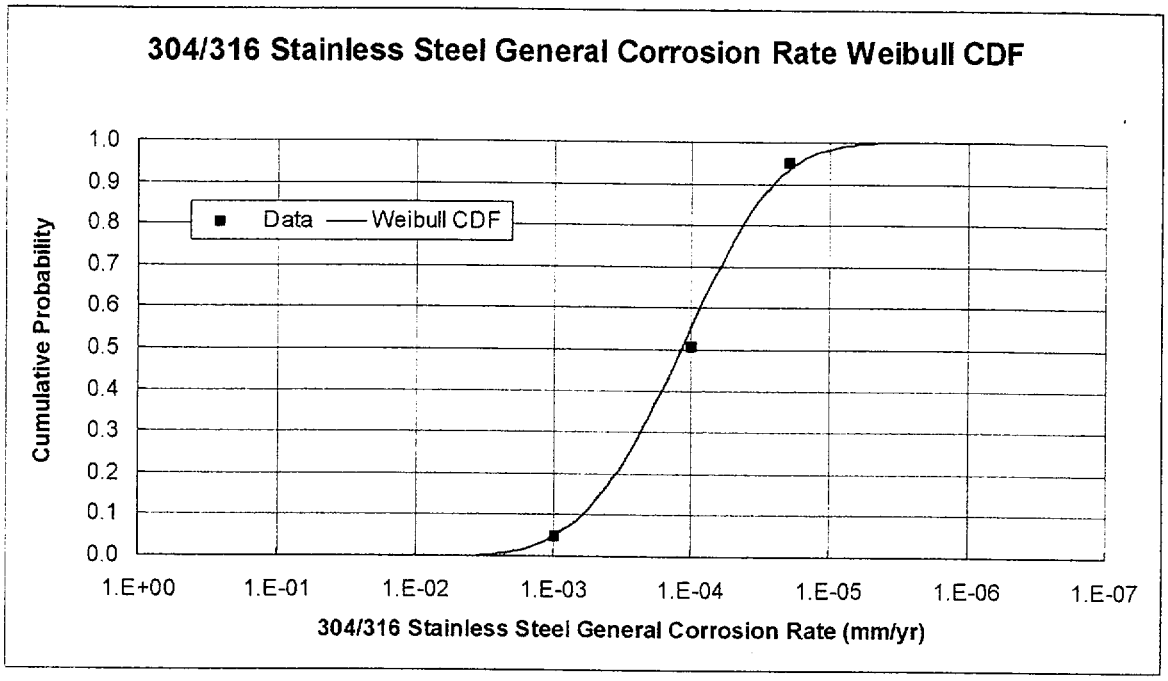

Figure C-14. Stainless Steel Corrosion Rate

1.4.3 Waste Form Degradation Characteristics

The components of the commercial SNF waste form in the example include the cladding, the spacer grids and end plates, and the oxide (fuel pellets). The end plates are made of austenitic stainless steel (SS302). The spacer grids and fuel cladding are made of a zirconium-based alloy (Zircaloy-4). The fuel pellets are uranium dioxide (UO_2) with a mixture of activation and fission products.

Structural calculations for PWR assemblies have shown that a Zircaloy clad Westinghouse 17 × 17 assembly on the bottom of the PWR WP would be capable of supporting the entire static load of the basket corrosion products and all assemblies above it (CRWMS M&O 1997b, Section 3.5). CRWMS M&O 1998d, (Section 7.8) has performed further structural analysis to demonstrate that other vendors' assemblies are at least as robust as the Westinghouse 17 x 17 assembly, and that the top assembly can support the load of 3.1 m of tuff rubble. Significant losses of PWR assembly structural integrity due to corrosion would not be expected because of the high corrosion resistance of Zircaloy. Zircaloy clad BWR fuel would be expected to have even greater structural integrity due to the presence of a Zircaloy channel around each assembly. CRWMS M&O 1998d, (p. 44) indicates that at the below-boiling temperatures that would be expected in the time frames considered for WP breach, studies have found no localized corrosion in aqueous environments across a pH range of 1 to 12, and in the presence of a variety of ions including lithium, sodium, potassium, ammonium, nitrate, sulfate, chloride, and fluoride. Since Zircaloy has an extremely low general corrosion rate, the Zircaloy components of the fuel assembly would be expected to last much longer than any other internal components of the WP (Hillner et al. 1998, p. 17).

Assembly degradation is still credible, however, as not all assemblies have cladding and spacer grids that are fabricated from highly corrosion resistant Zircaloy, and because of the potential

for rockfall, some assemblies may be exposed to dynamic loads. Based on information in CRWMS M&O 1998d, (p. 30) there are 1,846 PWR and 333 BWR assemblies with stainless steel cladding. This represents approximately 1.85 percent and 0.20 percent of the total PWR and BWR historical and projected populations, respectively. The structure of these assemblies would be expected to degrade at the same rate as the absorber plate components. Finally, while the Zircaloy fuel rods are relatively robust under static loads, they are not capable of withstanding significant dynamic loads. The energy to break one rod varies from a few joules to tens of joules (CRWMS M&O 1998d, p. 47). Thus, some collapse of the assembly structure would be expected once the upper portion of the waste package is no longer capable of providing protection from rock falls.

The fuel pellet fragments are also subject to degradation once the cladding has been breached. At sufficiently high temperatures in an oxidizing environment, the fragments will oxidize, from UO_2 to U_4O_9 and from U_4O_9 to U_3O_8 (Einziger 1994, p. 554). The first step results in a slight reduction in volume and opening of grain boundaries. The second step results in a large increase in volume and reduction of the fragments to powder. The increase in volume could result in splitting of the cladding. The oxides are also subject to dissolution. Oxidation (particularly oxidation to U_3O_8) and dissolution are coupled effects. By splitting the cladding, the formation of U_3O_8 will increase exposure of the fuel to water, and by breaking the fuel fragments into powder, it will greatly increase the surface area and dissolution rate. Fuel oxidation cannot occur until the disposal container is breached because the container provides an inert environment for the fuel while the temperature is in the range where oxidation could be significant.

All the waste form degradation characteristics used in the degradation analyses (CRWMS M&O 1998e, Subsection 5.1.1.1) are consistent with the TSPA evaluations (CRWMS M&O 1998d, p. 6-2).

1.5 MASTER SCENARIO LIST

The master list of scenarios and associated configuration classes are discussed in Section 3.1 of the topical report. No additional information will be provided here.

2.0 DEVELOP CONFIGURATION CLASS DEFINITIONS

2.1 INTERNAL CONFIGURATIONS

This section summarizes those scenarios/configurations, which are applicable to the 21 PWR and 44 BWR Absorber Plate waste packages and must be considered in the degraded mode criticality evaluation.

2.1.1 Identify Applicable Scenarios

Moderation is a required condition for criticality in commercial SNF with an enrichment of less than 5 weight-percent (Knief 1993, p. 68). Hence, of the internal criticality scenarios in Figure 3-1 of the main report, only the scenarios under the branch "Liquid accumulates in waste package" can lead to criticality for commercial PWR or BWR fuel (scenarios IP-1, 2, 3). The choice of scenarios is further narrowed by the review of basket material and fuel assembly degradation mechanisms performed in Section 1.4. Figure C-15 illustrates the expected sequence of degradation of the PWR fuel and basket components based on the discussions in

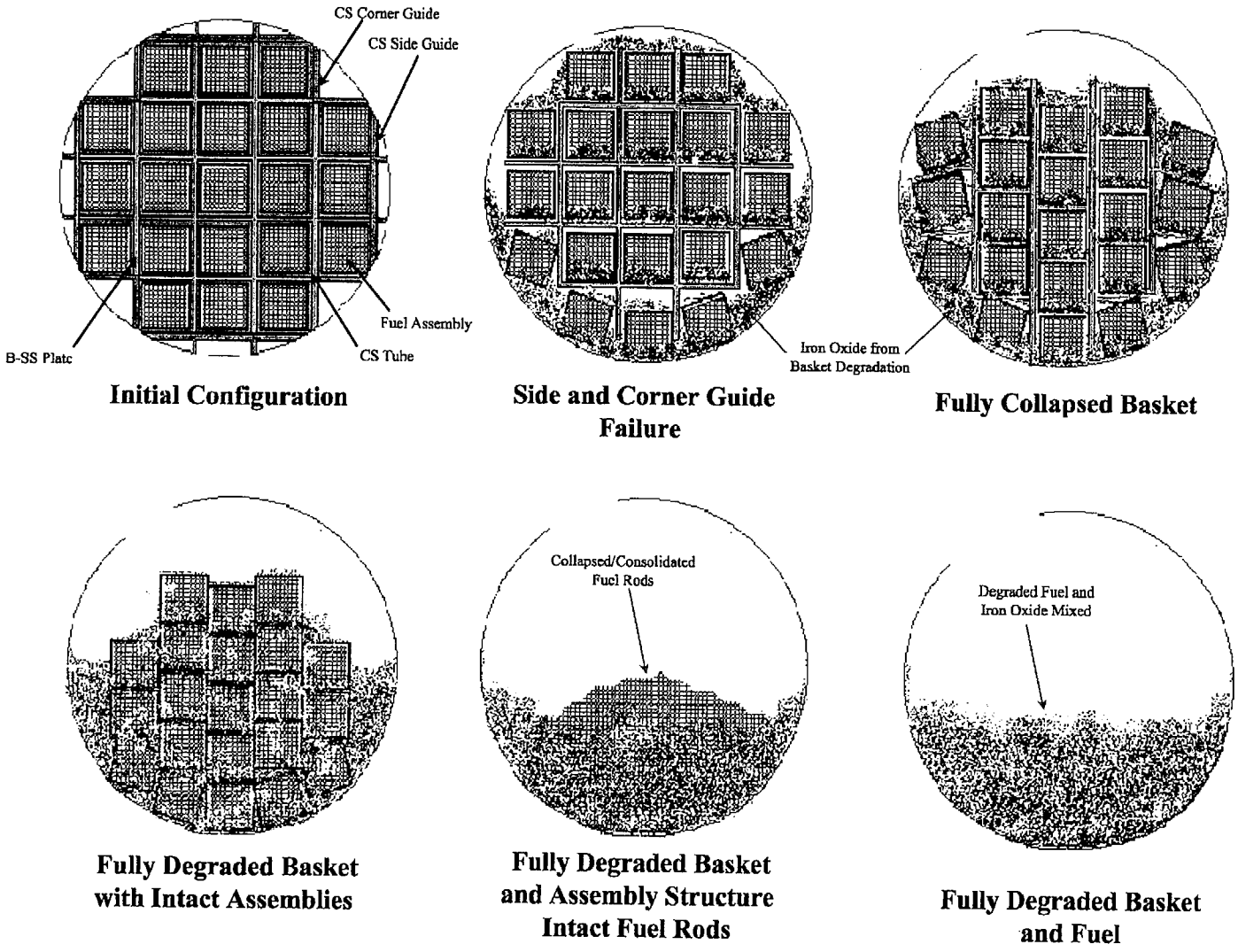

Figure C-15. Illustration of Expected 21 PWR WP Internal Degradation Sequence

Subsections 1.4.2 and 1.4.3. Physically possible variations on the expected sequence (e.g., rockfall crushing basket or fuel, different oxide distributions) are discussed in Subsection 2.1.3. The aluminum and carbon steel components are much less corrosion resistant than the borated stainless steel, and thus will completely degrade prior to significant degradation of the absorber plates. Similarly, the absorber plates are less robust with respect to aqueous corrosion than the Zircaloy clad fuel (except for stainless steel clad fuel). The above information is also true for the BWR fuel and basket components. Based on the expected sequence of internal degradation, only the IP-3 scenarios will be applicable to PWR and BWR fuel.

2.1.2 Identification of Configuration Classes

The following are the configuration classes associated with scenario IP-3 that must be evaluated for the 21 PWR Absorber Plate waste package:

1. Degraded basket but intact SNF. The amount of neutron absorber remaining is either all (configuration IP-3a), part (IP-3b), or none (IP-3c). All three of these configurations belong to the first configuration class, according to the listing in Section 3.1.1 of the main report. IP-3d does not apply because the basket structural supports degrade prior to the neutron absorber material.

2. Degraded basket and degraded SNF. There is only one configuration, and that has the degraded SNF at the bottom of the waste package and the soluble neutron absorbers flushed from the waste package (IP-2a). This configuration is also the only configuration in the second configuration class listed in Section 3.1.1 of the main report. It should be noted that, although this configuration has the IP-2 label, it actually starts in the IP-3 scenario group and gets to the IP-2 configuration via the D2-D link.

For the present example, only configuration IP-3c has been evaluated for the 44 BWR waste package.

2.1.3 Configuration Specification: Parameter Ranges

This section summarizes the parameter ranges which must be considered in the criticality evaluation of the configurations in the above mentioned classes. Geochemistry analyses (CRWMS M&O 1998e, Section 5.3.1) of the basket degradation process performed with EQ3/6 have demonstrated that the iron from corrosion of the carbon steel and borated stainless steels will remain in the waste package as the insoluble iron oxide hematite (Fe_2O_3). While goethite (FeOOH) is also possible, it will essentially be equivalent to the water/hematite mixtures already considered. The aluminum from the thermal shunts will also remain as insoluble diaspore (AlOOH), but was not initially considered in most of the PWR criticality evaluations because it is present in much lower concentrations than iron and has a significantly lower absorption cross section. Figure C-16 indicates the percentage of voidspace in a loaded 21 PWR waste package occupied by corrosion products from the degraded basket materials as a function of time since breach (CRWMS M&O 1998e, Section 5.3.1).

Based on examination of archaeometallurgy literature (Knight 1982, Watkins 1972), lamination and flaking of the corrosion products from the carbon steel would be expected to redistribute this material within the waste package voidspace (primarily within the assembly voidspace as most of the corroding metal will be between assemblies). There are several possible variations for the distribution of the basket corrosion products within the PWR waste package voidspace.

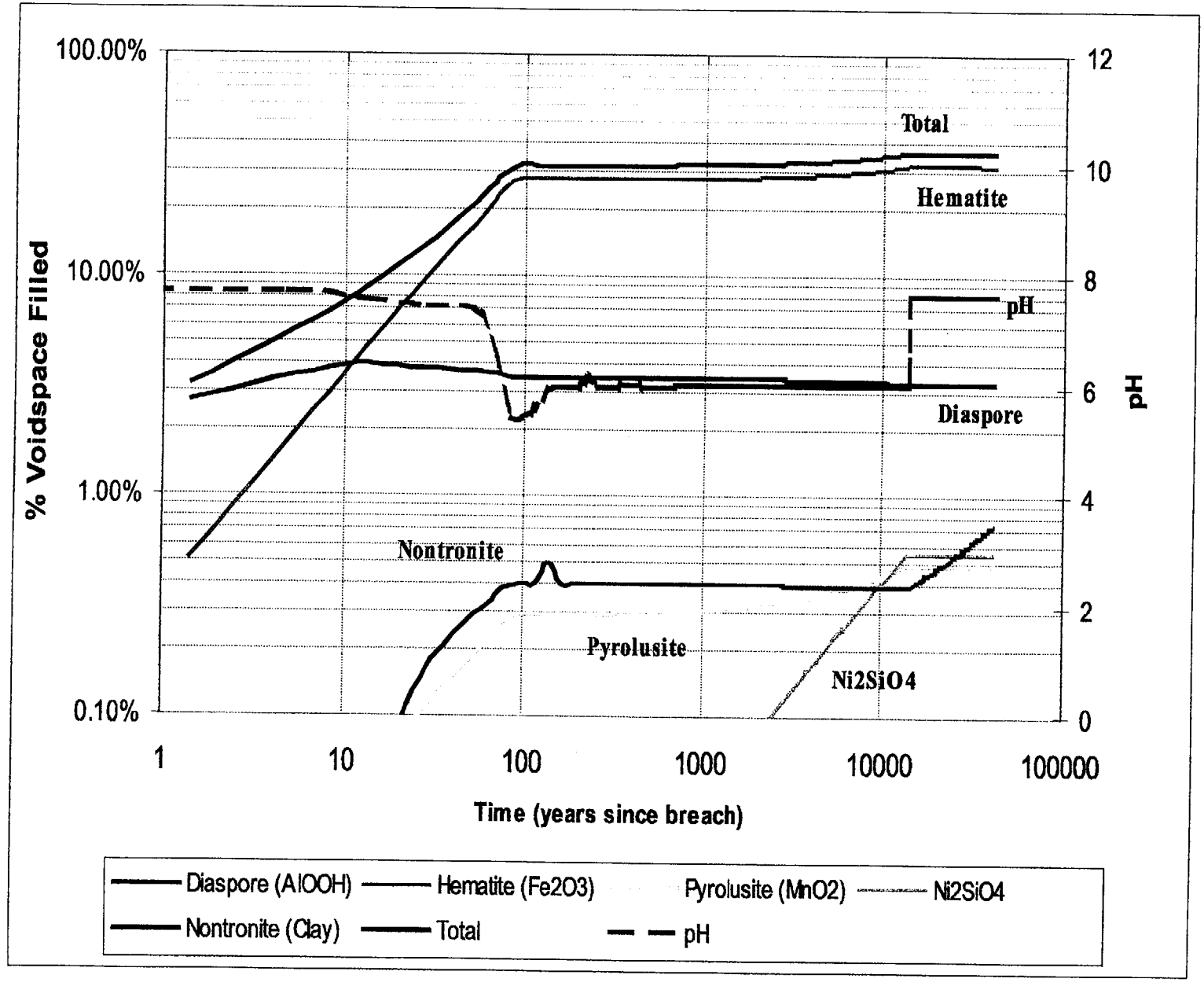

Figure C-16. Percent Internal Voidspace Occupied by Basket Corrosion Products

At the extremes are uniform distribution of the corrosion products within the waste package voidspace, and settling of the oxide to the bottom of the waste package, or to the bottom of a fuel assembly before all of the criticality control plate has corroded. For the settled case, a maximum packing factor of 58 percent is specified based on the solids fraction of tightly packed sand (CRWMS M&O 1996g, p. 29).

Based on the geochemistry analysis of the degradation products discussed above, and the sequence of structural changes discussed in Section 1.4.2, the specific parameter ranges to be considered for the PWR waste package in addition to the characteristics of the fuel are as follows (CRWMS M&O 1996g, p. 30):

1. Collapsed PWR Basket with Partial Thickness Borated Stainless Steel (B-SS) Remaining (configuration classes IP-3a and 3b)

    a) Uniformly distributed oxide (Fe_2O_3) occupying 30-40 volume-percent of the assembly void space (30 percent = carbon steel tube degradation only, 40 percent = carbon steel tube and all B-SS degradation), depending on the amount of B-SS plate remaining, with the remainder as water, and

    b) Settled oxide covering the bottom 8 to 10 rows of an assembly (8 rows = carbon steel tube degradation only, 10 rows = carbon steel tube and all B-SS degradation), depending on the amount of B-SS plate remaining. The oxide occupies 58 percent of the covered void, with the remainder being water.

For both partial basket configurations, various thicknesses of borated stainless steel should be considered.

2. Fully Degraded/Oxidized PWR Basket (configuration class IP-3c):

    a) Uniformly distributed oxide occupying 30, 33, or 40 volume-percent of the waste package void space (33 percent base volume-percent for the current amount of basket material excluding AlOOH), and

    b) Settled oxide covering the bottom 3, 3.5, 4, and 4.5 rows of assemblies (3.5 is the base case for the current amount of basket material excluding AlOOH). The oxide occupies 58 percent of the covered void, with the remainder being water.

Based on the borated stainless steel corrosion information discussed in Subsection 1.4.2, the fully degraded basket configurations were evaluated without consideration for any remaining boron. However, the boron from the degraded boride particles may still remain in solution for some time, or become adsorbed onto the iron oxide (0.67 percent retained in the oxide at the peak adsorption rate for Fe_2O_3 from Goldberg and Glaubig 1985), so the effects of these mechanisms on degraded waste package k_{eff} will also be evaluated. The amount of adsorption may increase by over an order of magnitude if AlOOH and FeOOH are considered (Goldberg and Glaubig 1985). In addition, the effects of water level will also be considered.

The following geometries involving full degradation of the PWR basket structure and various degrees of rod consolidation were also evaluated for the limiting fuels to address the effects of degraded or crushed fuel assemblies by mechanisms discussed in Section 1.4.3 (configuration class IP-2a):

1. Various amounts of assembly crushing (i.e., reduced fuel rod pitch) in the vertical direction, and both the vertical and horizontal directions for the fully degraded basket.

2. Fuel rods piled at the bottom of the fully degraded basket waste package (simulates complete spacer grid degradation).

Discussion of the criticality evaluations performed for the above configurations are provided in Section 3.

Since the BWR WP contains the same materials as the PWR waste package, and the BWR fuel assemblies being evaluated are also Zircaloy clad, the above geochemistry results are considered applicable to the BWR WP being evaluated. However, due to the presence of the Zircaloy channels around each BWR assembly, these corrosion products will not be able to expand into the void space between the fuel rods. Removing the volume within the 44 BWR assembly channels from the available void space inside the package inner diameter indicates that a Fe_2O_3/AlOOH corrosion product mixture will occupy 53.86 percent of the remaining void space. An FeOOH/AlOOH mixture would occupy 72.39 percent of the void space outside of the assembly channels. As the corrosion product forms, there are two possibilities for its physical location within the waste package. In one case, the weight of the assemblies may force the corrosion product out from between the horizontal portions of the channel, leaving no vertical gap between assemblies once the basket has collapsed. However, forcing the corrosion product out from the vertical space between the assemblies will require that the spacing between vertical columns of collapsed assemblies be maintained to accommodate this material. In the other extreme, all of the corrosion product from degradation of the carbon steel tubes, borated stainless steel plates, and aluminum thermal shunts will remain between vertically adjacent assemblies. Considering only the expansion of the carbon steel and borated stainless steel between each assembly indicates that the vertical separation will be 2.7 cm if Fe_2O_3 is formed, and 3.7 cm if FeOOH is formed. The vertical separation between some assemblies may actually be greater than these values because of the presence of corrosion products from the aluminum thermal shunts and the fact that oxides generally do not pack to theoretical densities. Finally, based on the boron adsorption rates in Goldberg and Glaubig (1985), 0.87 percent of the original boron may be adsorbed if an Fe_2O_3/AlOOH mixture is present, and 15.79 percent of the original boron in the basket may be adsorbed if an FeOOH/AlOOH mixture is present. Degradation of the BWR assembly structure has not been considered at the present time.

In all of the above configurations, the package is considered to be resting on a level surface. Since the waste package supports are fabricated from carbon steel tubes (see Subsection 1.2.3) which have wall thicknesses much less than that of the outer barrier, they would be expected to have completely degraded prior to waste package breach. After failure of the supports, the waste packages would still be expected to remain on the relatively level surface provided by the piers and invert media (see Figure C-4). Consideration of the effects of any long-term deformation of the invert surface, or the emplacement drifts themselves, on the orientation of the package will be performed for License Application. Such orientation changes would only be expected to effect the k_{eff} in configurations involving settled corrosion products, where

differences in the oxide level along the length of the package may make the effects of axial differences in assembly burnup significant.

2.2 EXTERNAL CONFIGURATIONS

The limited scoping analyses of external criticality have not yet provided a screening that could serve to narrow the range of possible scenarios and configuration classes.

2.2.1 Identify Applicable Scenarios

All of the external criticality scenarios shown in Figure 3-2 of the main report are possible for commercial SNF, but none have been found critical in the external criticality scoping analyses thus far.

2.2.2 Identification of Configuration Classes

The only configuration classes examined thus far are:

- NF-1b; the precipitation of uranium or plutonium in the near-field was found to be many orders of magnitude below what would be required for a critical mass (CRWMS M&O 1998f, Section 7.2).

- FF-3c; if there is any possibility of precipitating a critical mass from the water flowing out of the waste package in the far-field, it would be at an organic reducing zone, but the probability of encountering a sufficient amount of reducing material in one place would be less than one in 10 million (CRWMS M&O 1996a, p. 41).

2.2.3 Configuration Specification: Parameter Ranges

The Pu and U concentrations that would be required for criticality in configuration NF-1b have been examined in some detail (CRWMS M&O 1998f, Section 7.2). For example, it was found that for a typical worst case geometry for accumulation of U or Pu beneath the waste package (a 1 meter cube containing a three dimensional fracture network of 1 mm aperture and 30 mm spacing in all three dimensions) a critical mass would require at least 1 percent of the fracture volume to be occupied by the Pu and/or U, which implies a total Pu or U mass of approximately 10 kg. Geochemical analysis shows the maximum concentration/mass attainable in the rock immediately beneath a commercial PWR waste package to be several orders of magnitude below this amount (CRWMS M&O 1998f, Section 6.1).

3.0 CRITICALITY ANALYSIS

3.1 CONFIGURATION CRITICALITY EVALUATIONS

Representative cases based upon the configurations developed in Section 2.0 were evaluated. Cases were evaluated that spanned the range of parameter values for the configuration class parameters identified in Section 2.0.

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

1. The configurations internal to the waste package determined in Section 2.1 were modeled with the criticality model (MCNP4A CSCI:30006 V4A, CRWMS M&O 1997i was used for these analyses, since MNCP4B CSCI:30033 V4B2LA was not qualified at the time).

2. Conservative SNF isotope concentrations from the SNF isotopics model (ORIGEN-S/SCALE 4.3) at the appropriate cooling times (modified according to the applicable degradation and transport models) were entered into the criticality models. The accuracy of isotopic model results for long decay times is discussed in the main report.

3. Criticality analyses of the configurations were performed and the appropriate subcritical limits were applied to the results. Regressions for predicting k_{eff} as a function of various configuration parameters were developed for configurations which exceeded the subcritical limit over some portion of the parameter ranges discussed in Subsection 2.1.3.

3.1.1 Commercial SNF Isotopics

This section identifies the different fuel isotopic sets which were used in the example criticality analysis. Burnup and enrichment pairs were selected for analysis such that the population of fuel to be placed in the absorber plate waste package was spanned. Burnup and enrichment pairs, which bound 100 percent of the PWR fuel population (high enrichment, low burnup) were also identified. The PWR burnup and enrichment pairs evaluated are summarized in Table C-3 (CRWMS M&O 1996g, Section 7.2). For the example BWR calculation, only enrichments in the range of 3.5 to 4.5 weight-percent were considered, with burnups in the range of 20 to 45 GWd/mtU.

Table C-3. Burnup and Enrichment Pairs Evaluated in PWR Criticality Analysis

Type	Burnup and Enrichment Pairs Evaluated
Absorber Plate Bounding	9 GWd/mtU, 1.7 wt.%; 27 GWd/mtU, 3.9 wt.%; 34 GWd/mtU, 4.9 wt.%; 3 GWd/mtU, 0.8 wt.%; 23.5 GWd/mtU, 3 wt.%; 35 GWd/mtU, 4.5 wt.%; 12 GWd/mtU, 1.5 wt.%; 28 GWd/mtU, 3.25 wt.%; 39 GWd/mtU, 4.6 wt.%; 32.5 GWd/mtU, 3.5 wt.%; 44 GWd/mtU, 4.9 wt.%; 38.5 GWd/mtU, 3.85 wt.%; 48 GWd/mtU, 4.9 wt.%
100% PWR Bounding	3 GWd/mtU, 4.3 wt.%; 13 GWd/mtU, 4.7 wt.%

The calculation of the PWR and BWR spent fuel isotopics was performed with the SAS2H code sequence, which is a part of the SCALE 4.3 code system. The basic SAS2H model used to perform the depletion and decay of the PWR assemblies are identical to those defined in CRWMS M&O 1996b (Section 7.3) with only those portions relating to the burnup and enrichment of the assembly changed as indicated in CRWMS M&O 1996g (p. 38). The BWR SAS2H model used was for a representative 8 × 8 assembly with a central water rod, several gadolinium bearing rods, and utilized 10 axial nodes for each burnup/enrichment combination (CRWMS M&O 1998o, Section 5.3). For License Application, the depletions will be performed consistent with the methods discussed in Section 4.1 of the main report. The decay out to 1 million years was run as a separate case from the SAS2H burnup calculation with ORIGEN-S, which is also part of the SCALE 4.3 code system. The decay case is a stand-alone ORIGEN-S problem, which utilizes the output from SAS2H and decays to a number of specified times. The grams/assembly per time step from the combined SAS2H/ORIGEN-S output was used to calculate the number density of each principal isotope at the times of

interest for each burnup and enrichment pair. These number densities were used as input to the fuel region for MCNP criticality calculations.

3.1.2 Partially Degraded Basket with Intact Fuel

The purpose of this section is to describe the MCNP cases performed in CRWMS M&O 1996g (Section 7.3) to evaluate the range of parameters indicated in Subsection 2.1.3 for the partially degraded PWR basket configurations. Note that at this point in the process, no estimation of the likelihood of obtaining a specific combination of parameters is developed. The degraded 21 PWR absorber plate waste package was modeled in MCNP by explicitly modeling one-quarter of the package and then using two reflective planes to represent the entire package (Figure C-17 shows the location of one of the reflective planes and the other plane divides the package in half along the axial length). The composition and dimensions of the containment barriers are modeled explicitly. The details of the outer barrier's skirt were not modeled in detail, since the skirt would not affect the criticality results appreciably (less than the standard deviation in the Monte Carlo method). The fuel assemblies are modeled as part of a lattice array, with the lattice positioned such that it represents a basket structure, which has uniformly collapsed towards the bottom of the waste package. The assemblies were not modeled as resting on the bottom of the waste package because some oxide from corrosion of the side guides may be there to support them, and the approximate cylindrical geometry is more reactive than that which would occur if all assemblies were touching the bottom. Each fuel assembly is treated as a heterogeneous system with the fuel rods, control rod guide tubes, and instrument guide tubes modeled explicitly. Fuel rods are modeled with water in the gap region, and guide and instrument tubes are also filled with water only (no oxide). The remaining borated stainless steel plate is modeled at the edge of the assembly lattice cell. Figure C-17 shows the MCNP model for the partially degraded basket configuration with settled oxide. Both the uniformly distributed oxide and the settled oxide configurations were evaluated for 7 plate thicknesses. For the uniformly distributed configurations, iron oxide concentrations of 30 volume-percent, 35 volume-percent, and 40 volume-percent were evaluated for several burnup and enrichment pairs. Figure C-18 shows the results for the 4.9 weight-percent/34 GWd/mtU burnup and enrichment pair at 30 volume-percent and 40 volume-percent uniform oxide. For the settled scenarios, 58 volume-percent iron oxide fully covering the bottom 8, 9, and 10 rows of fuel rods in an assembly were evaluated for several burnup and enrichment pairs. Figure C-19 shows the results for the 4.9 weight-percent/34 GWd/mtU burnup and enrichment pair with the bottom 8 and 10 rows of fuel rods covered by 58 volume-percent oxide. For most cases, each burnup and enrichment pair was only evaluated for the 14,000 year decay time, as this has been the time of peak postclosure k_{eff}.

3.1.3 Fully Degraded Basket with Intact Fuel

The purpose of this section is to describe the MCNP cases performed in CRWMS M&O 1996g (Section 7.4) to evaluate the range of parameters indicated in Subsection 2.1.3 for the fully degraded 21 PWR basket configurations. In addition, some discussion of the evaluations performed to date on the 44 BWR fully degraded basket configurations is also provided. Note that at this point in the process, no estimation of the likelihood of obtaining a specific combination of parameters is developed.

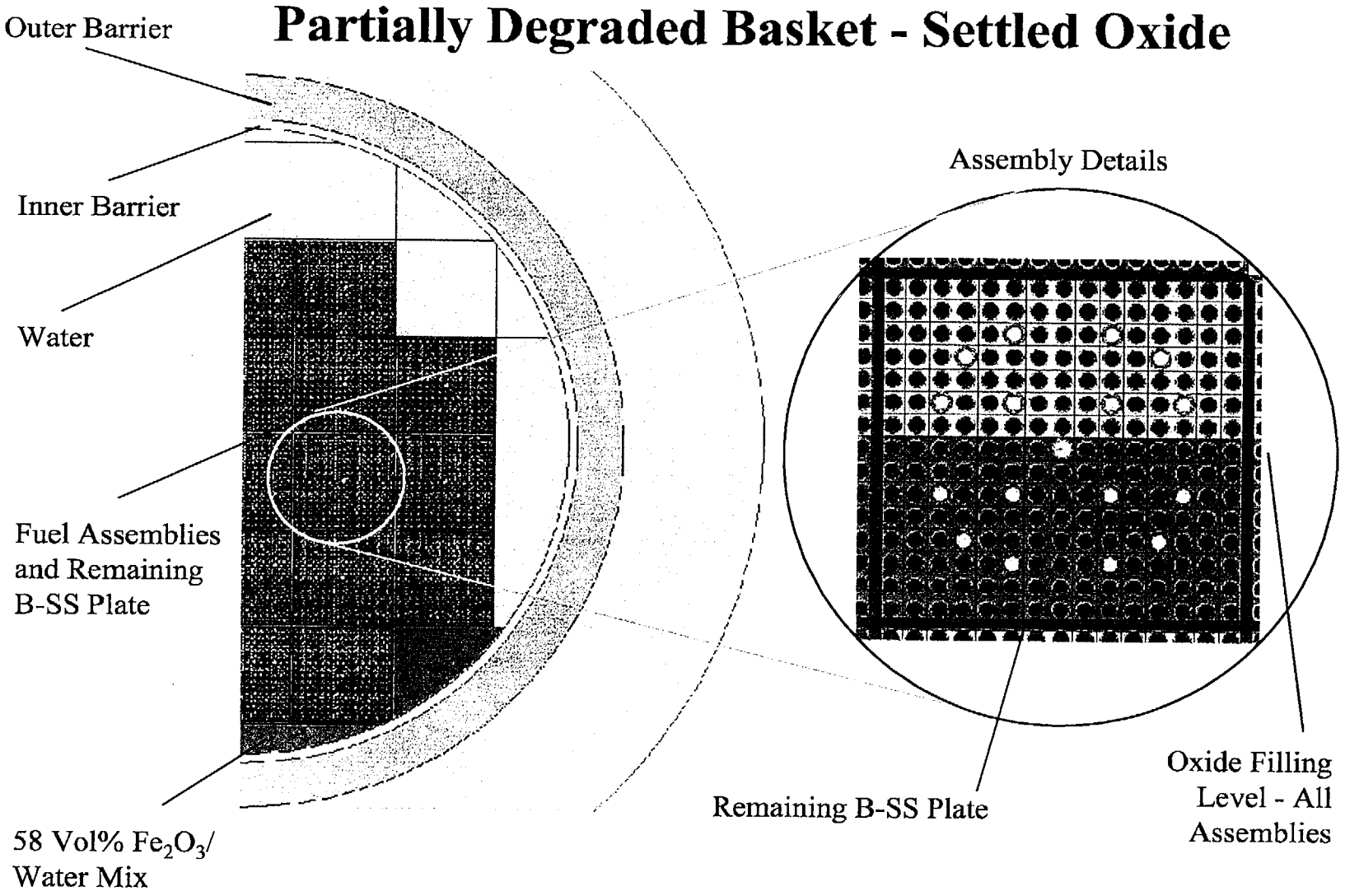

Figure C-17. MCNP Model for Partially Degraded Basket with Settled Oxide

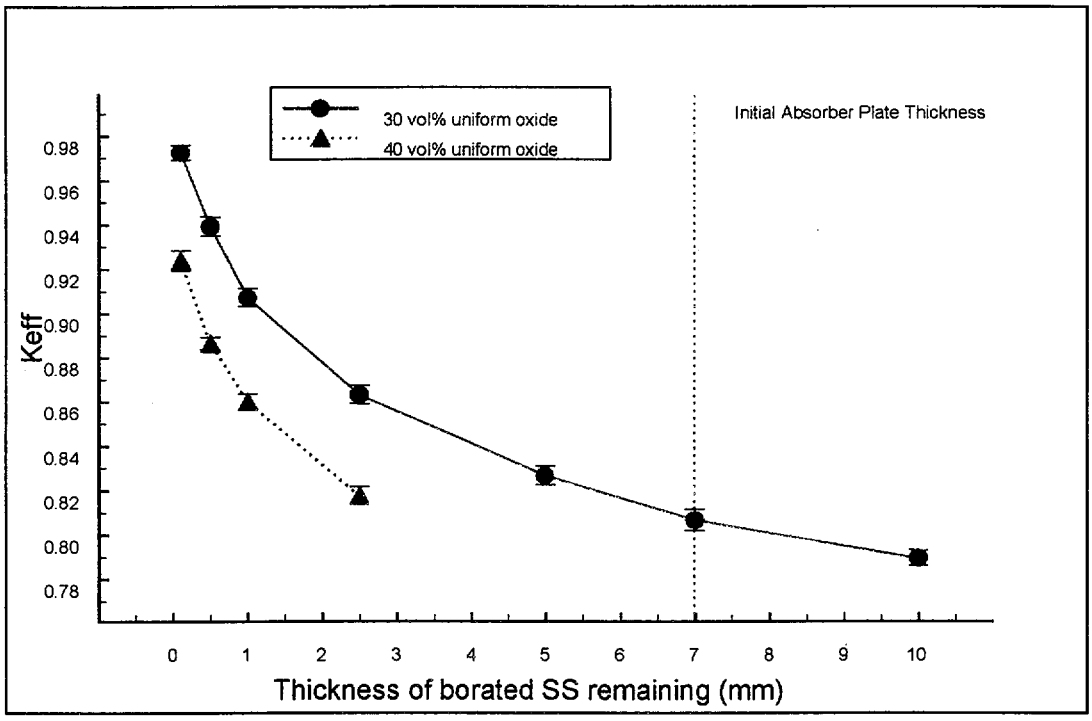

Figure C-18. k_{eff} as a Function of Remaining Absorber Plate Thickness for the 4.9 wt.%/34 GWd/mtU Fuel at 14,000 years with 33 vol.% Uniform Oxide

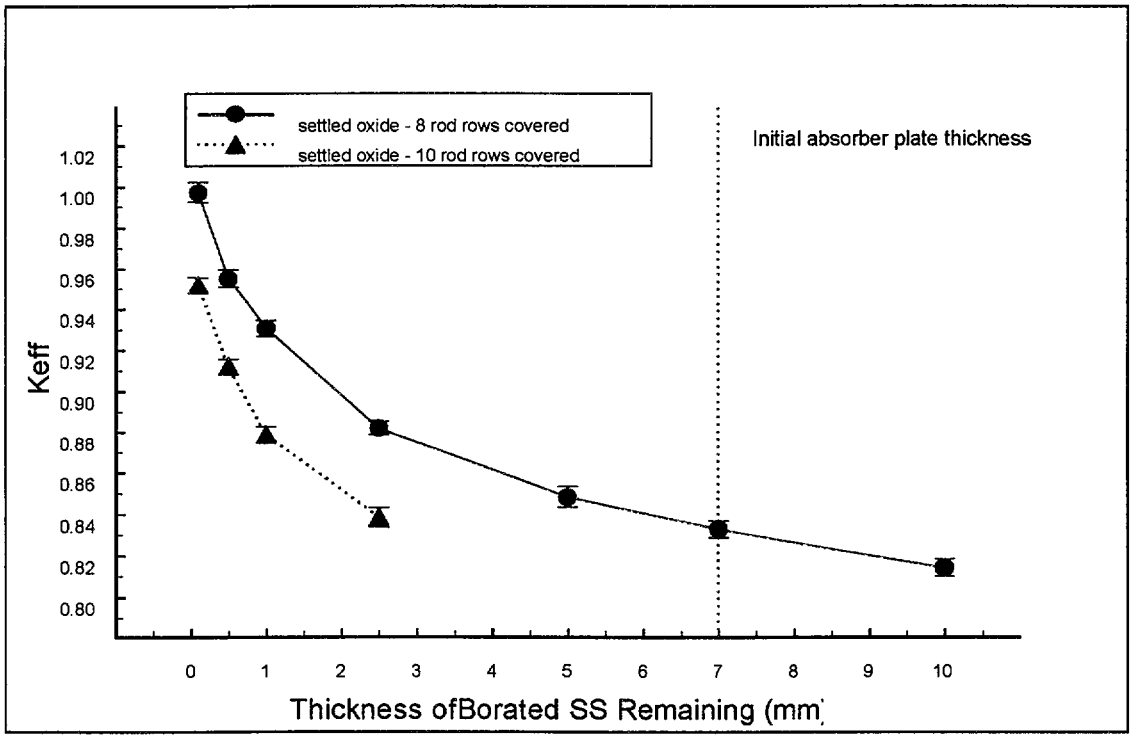

Figure C-19. k_{eff} as a Function of Remaining Absorber Plate Thickness for the 4.9 wt.%/34 GWd/mtU Fuel at 14,000 years with 58 vol.% Settled Oxide

As with the partial basket model, the fully degraded 21 PWR absorber plate waste package was modeled in MCNP by explicitly modeling one-quarter of the package and then using two reflective planes to represent the entire package. The composition and dimensions of the containment barriers are modeled explicitly. The details of the outer barrier's skirt were not modeled in detail, since the skirt would not effect the criticality results appreciably (less than the standard deviation in the Monte Carlo method). The fuel assemblies are modeled as part of a lattice array, with the lattice positioned such that it represents a basket structure, which has uniformly collapsed towards the bottom of the waste package. The assemblies were not modeled as resting on the bottom of the waste package because some oxide from corrosion of the side guides may be there to support them, and the approximate cylindrical geometry is more reactive than that which would occur if all assemblies were touching the bottom. Each fuel assembly is treated as a heterogeneous system with the fuel rods, control rod guide tubes, and instrument guide tubes modeled explicitly. Fuel rods are conservatively modeled with water in the gap region, and guide and instrument tubes are also filled with water only (no oxide). Figure C-20a shows an example of the MCNP model for the fully degraded PWR basket with 58 volume-percent settled oxide configuration. Figure C-20b shows a model of similar detail for the fully degraded 44 BWR WP with uniform oxide distribution. A settled oxide configuration was not modeled because the channels prevent settling of the basket corrosion products within the BWR assembly. Other differences include modeling of one-half of the package, with a reflective plane to represent the other hemicylinder, to allow the full 10 axial node fuel region to be modeled explicitly.

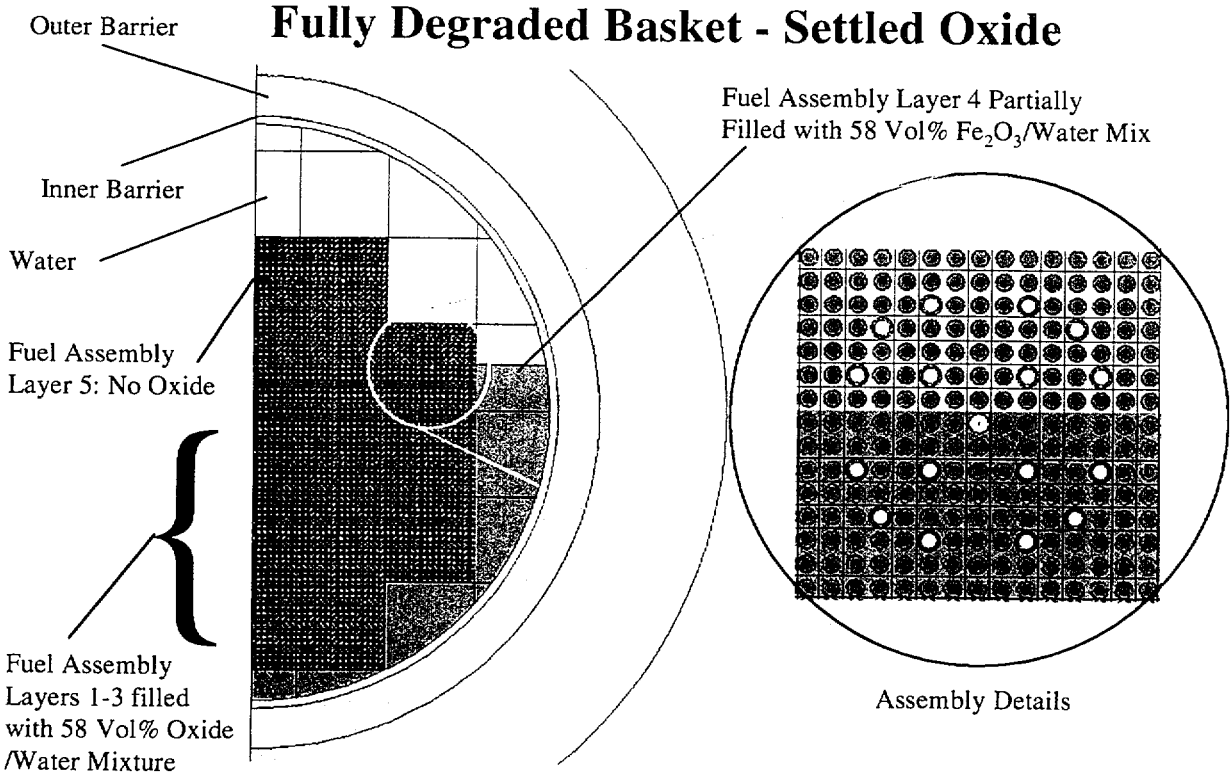

Figure C-20a. MCNP Model for Fully Degraded 21 PWR Basket with Settled Oxide

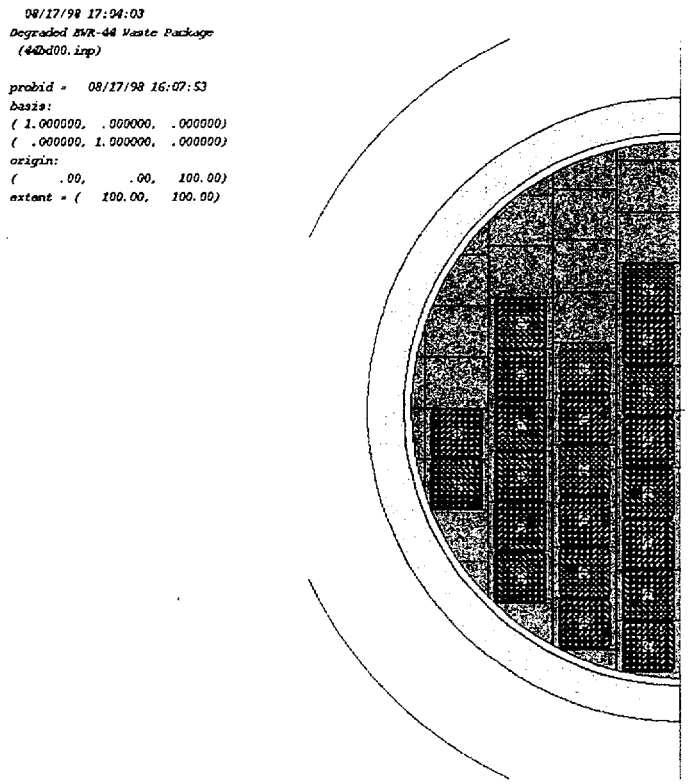

Figure C-20b. MCNP Model for Fully Degraded 44 BWR Basket with Uniform Oxide and No Vertical Separation Between Assemblies

Results of some of the cases evaluated in CRWMS M&O 1996g (Section 7.4) are provided in Figures C-21 through C-24 to demonstrate the behavior of k_{eff} as a result of varying certain parameters. Figure C-21 shows the time effects on k_{eff} for several burnup and enrichment pairs for the 33 volume-percent base uniform oxide configuration. Figure C-22 provides the same information for the 58 volume-percent settled oxide configuration. In all of the configurations, the peak k_{eff} generally occurs between 10,000 and 35,000 years. One noticeable feature is the increasing prominence of the postclosure peak-and-valley in k_{eff} as burnup increases. This effect primarily results from the decay of ^{241}Pu, ^{240}Pu, and ^{239}Pu isotopes which are present at higher concentrations in higher burnup fuels. Figures C-23 and C-24 show the effects of varying the amount of iron oxide in the waste package for the 58 volume-percent settled and uniform oxide configurations, respectively, for two burnup enrichment pairs at the time of peak k_{eff}. As expected, the results show that increased amounts of oxide in both configurations result in reduced k_{eff} due to moderator exclusion and the modest absorption cross section of iron. As discussed in Section 2, the amount of oxide resulting from basket degradation covers 3.5 layers of assemblies in the settled configuration, and takes up 33 volume-percent in the uniform configuration. CRWMS M&O 1996g determined that an addition of 2,659 kg of carbon steel basket material would produce sufficient oxide upon degradation to reduce the peak k_{eff} below 0.91 for both fully degraded configurations. Other general observations from this part of the evaluation were (1) the settled configuration is more limiting than the uniform, (2) for burnup and enrichment pairs with the same k_∞ per the relationship in ORNL 1987 (p. 7), the one with the highest burnup will have the highest k_{eff} in the degraded configurations, and (3) the 4.9 weight-percent enrished 34 GWd/mtU PWR fuel was bounding for the absorber plate waste package under the loading scheme defined in CRWMS M&O 1997e (Section 8).

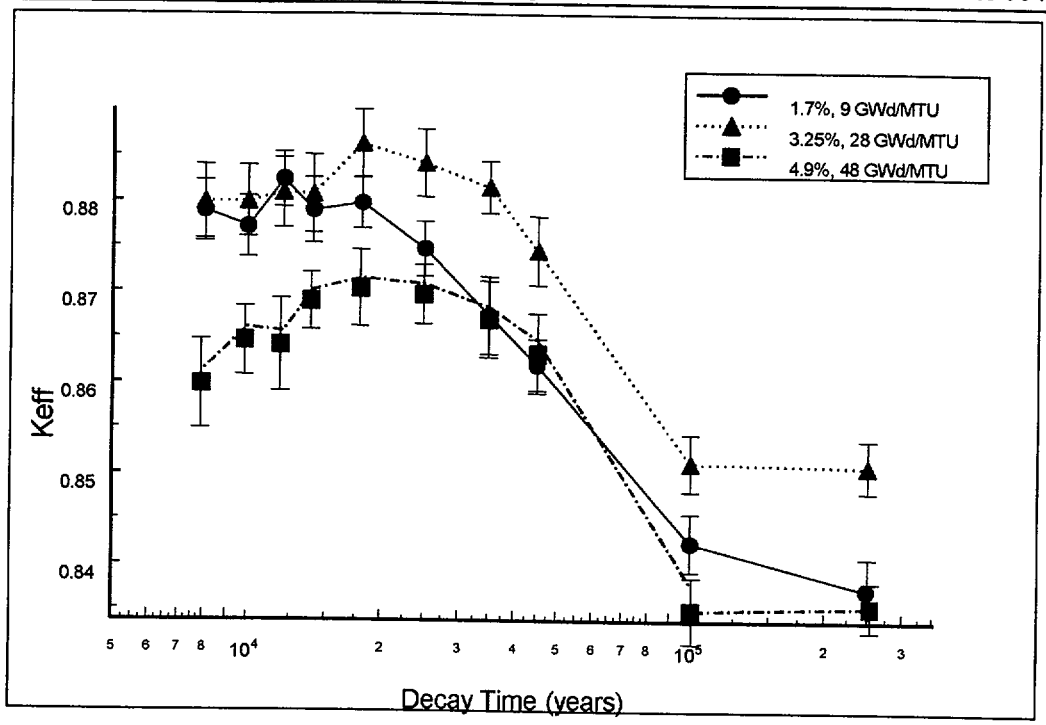

Figure C-21. Time Dependence on k_{eff} as a Function of Assembly Burnup for the Fully Degraded PWR Basket with 33 vol.% Uniform Oxide Distribution

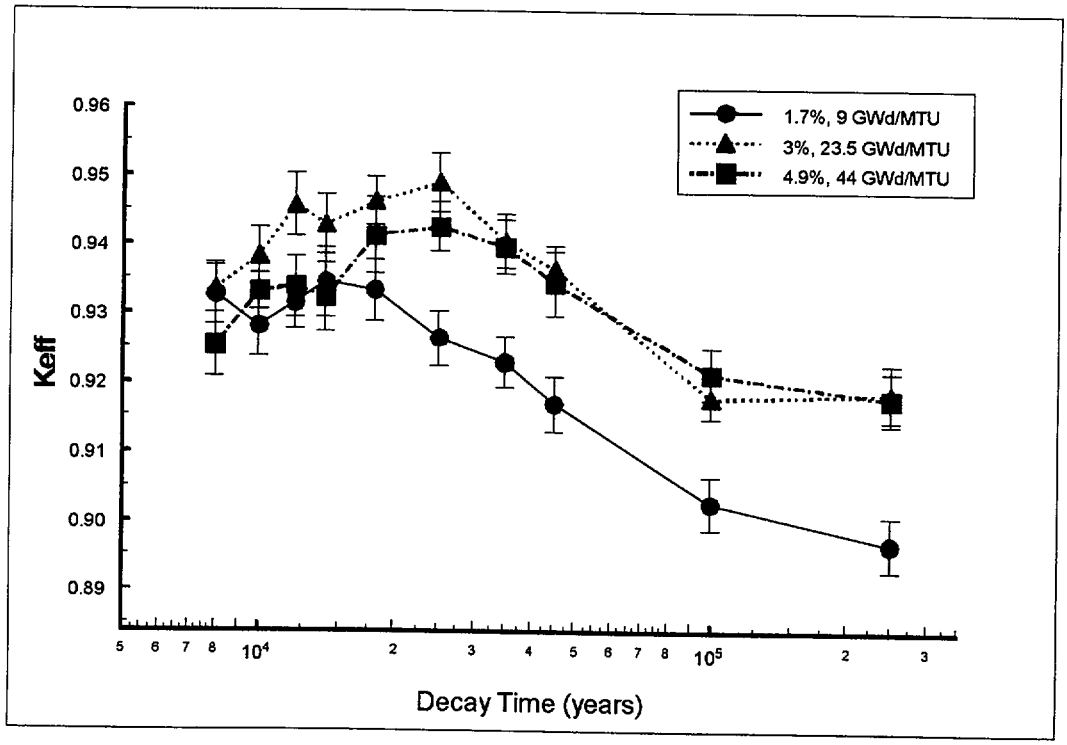

Figure C-22. Time Dependence on k_{eff} as a Function of Assembly Burnup for the Fully Degraded PWR Basket with 58 vol.% Settled Oxide Distribution

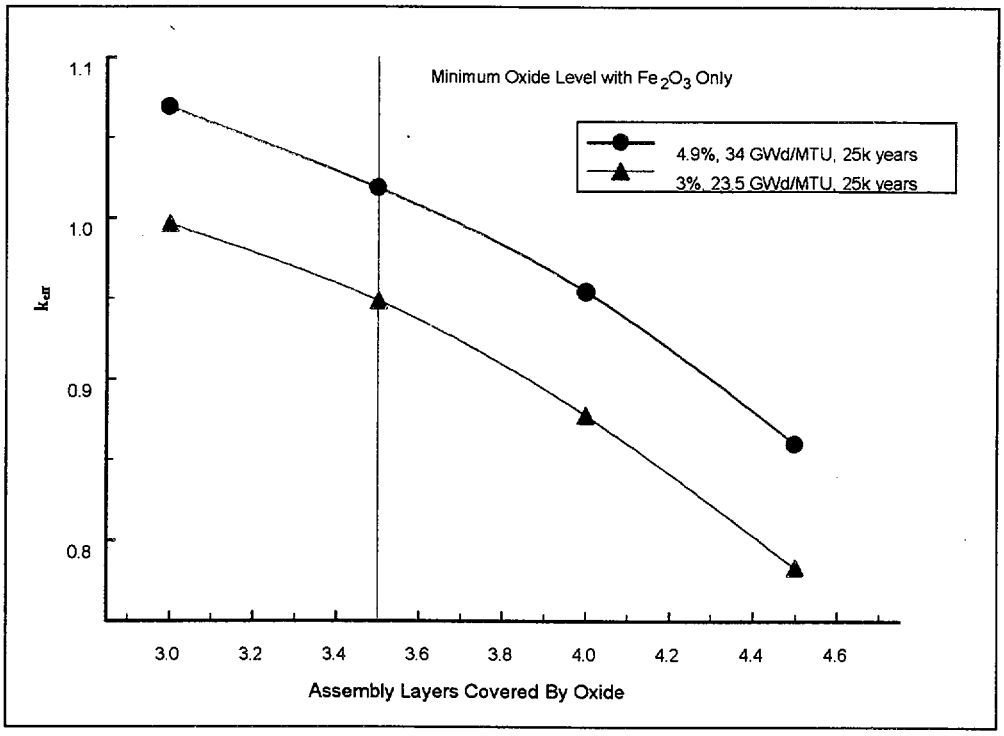

Figure C-23. Effects of Oxide Level on Fully Degraded PWR Basket k_{eff} for 58 vol.% Settled Configuration

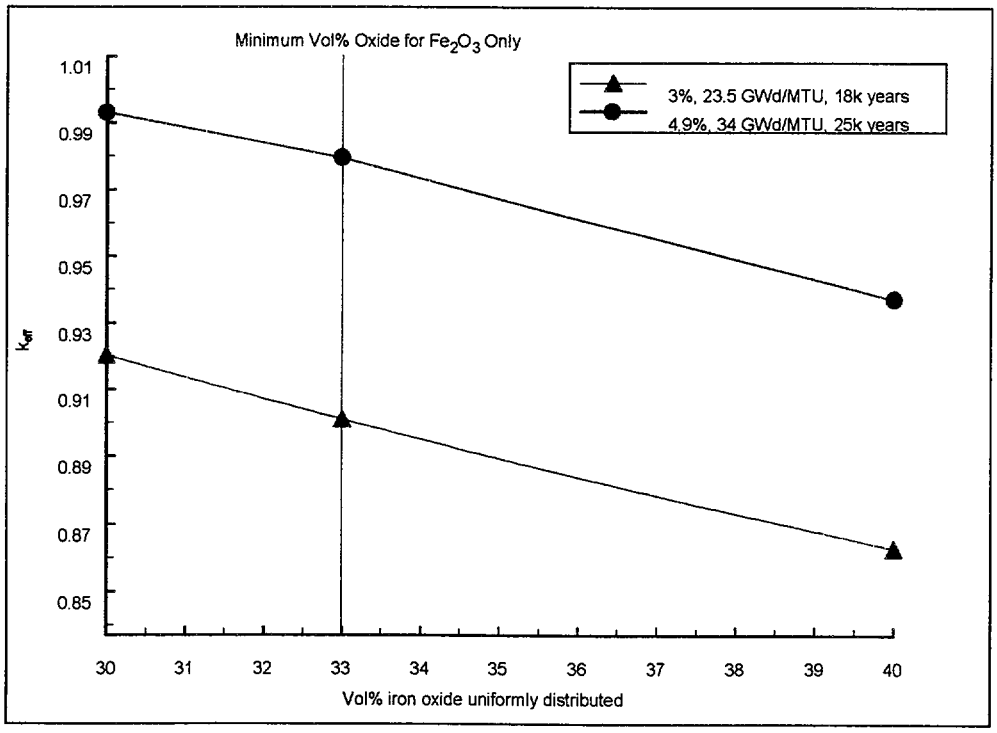

Figure C-24. Effects of Uniformly Distributed Oxide vol.% on Fully Degraded Basket k_{eff}

However, it should be noted that in the case of the first item, consideration of the additional volume occupied by the corrosion products of the aluminum thermal shunts (≈4 volume-percent) would increase the settled oxide level to the point of almost covering the 4th layer of assemblies. Based on the results shown in Figures C-23 and C-24, this would be expected to reduce the k_{eff} of the settled oxide case to approximately the same value as the uniform oxide case for the same fuel type.

To evaluate the effects of 0.67 percent boron absorption onto the iron oxide, both 33 volume-percent uniform and 58 volume-percent settled PWR configurations were evaluated for time of peak k_{eff} for several burnup and enrichment pairs. Table C-4 presents the k_{eff} and $\Delta k_{eff}/k_{eff}$ results for 0.67 percent ^{10}B adsorption onto the iron oxide. The results indicate that this amount of boron adsorption provides less than a 1.4 percent reduction in k_{eff} for the uniform cases, and a 0.2 percent reduction for the settled cases. Boron adsorption is less effective for the settled configuration because the assemblies contributing to the high k_{eff} are those which are above the level of the oxide, and thus not affected by the boron adsorbed therein. Based on these results, this boron retention mechanism cannot be counted on for significant criticality control for either oxide distribution scenario.

Table C-4. Effects on k_{eff} of Peak Boron Adsorption on Iron Oxide

Burnup/ Enrichment Pair	Decay Time (years)	33 vol.% Uniform			58 vol.% Settled		
		k_{eff}	σ	$\Delta k_{eff}/k_{eff}$	k_{eff}	σ	$\Delta k_{eff}/k_{eff}$
4.9 wt.%/34 GWd/mtU	25000	0.96586	0.00175	-0.0139	1.01598	0.00218	-0.0026
3.9 wt.%/27 GWd/mtU	35000	0.94447	0.00134	-0.0120	0.99602	0.00188	-0.0016
1.7 wt.%/9 GWd/mtU	14000	0.8695	0.00167	-0.0107	0.93223	0.00122	-0.0022

Depending on the amount and distribution of holes on the upper surface, the waste package may not be entirely flooded. Figure C-25 presents the k_{eff} results for the 4.9 weight-percent/34 GWd/mtU fuel in the 58 volume-percent settled oxide configurations at the time of peak k_{eff} for various water levels. The results indicate that, for the settled configuration, uncovering the top layer of PWR assemblies drops k_{eff} below 0.90. Analysis of the 33 volume-percent uniform configuration for the same burnup and enrichment pair indicates that the water level must drop below the middle of the third layer to achieve the same result. However, this is partially an artifact of maintaining 33 volume-percent oxide as the water level is reduced. These cases also verify that a fully degraded unflooded absorber plate waste package which contains only a hydrated oxide will not be a criticality concern (scenario IP-6).

Figure C-26 presents the $\Delta k_{eff}/k_{eff}$ results for various concentrations of dissolved ^{10}B in the entire water volume for the 58 volume-percent settled oxide cases for several burnup and enrichment pairs at the time of peak k_{eff}. Based on the few cases run, it appears that there is a slight trend towards decreasing boron worth with increasing burnup. This is likely the result of the fact that higher burned fuels have higher ^{239}Pu concentrations, and thus a harder spectrum (more epithermal fission) which makes the boron less effective.

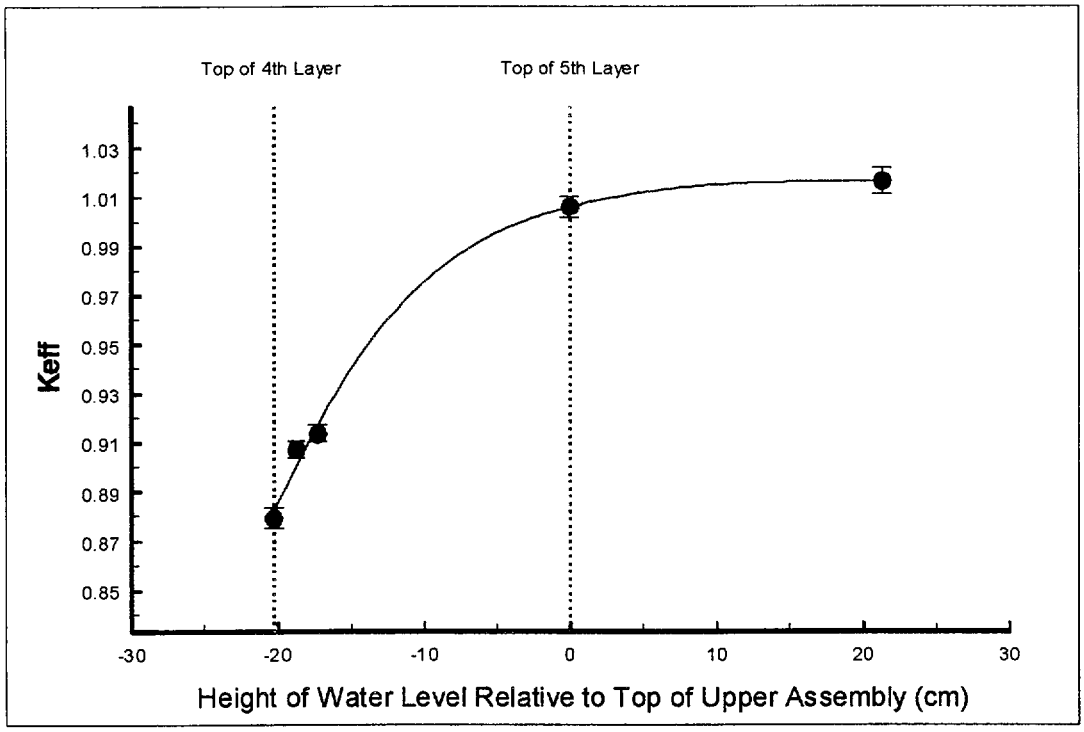

Figure C-25. Effects of Internal Water Level on Fully Degraded PWR Basket k_{eff} (4.9 wt.% Enrichment, 34 GWd/mtU, 35,000 Years Decay)

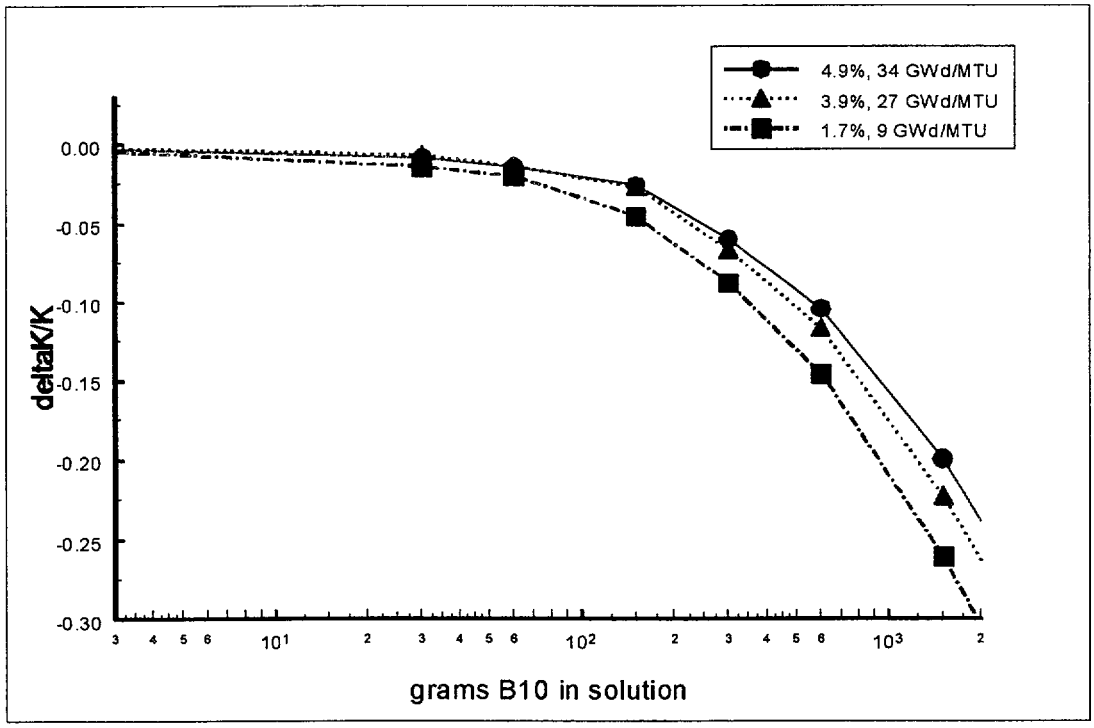

Figure C-26. Effects of Dissolved ^{10}B on Fully Degraded Basket k_{eff} for the 58 vol.% Settled Oxide Configuration

Finally, Table C-5a presents k_{eff} results for the two 100 percent PWR bounding burnup and enrichment pairs (4.3 weight-percent/3 GWd/mtU and 4.7 weight-percent/13 GWd/mtU) in the 58 volume-percent settled oxide and 33 volume-percent uniform oxide configurations. Results are presented with and without the 16 rod disposal control rod assemblies (DCRAs) in the assembly guide tubes, indicating that the DCRAs provide ≈24-25 percent reduction in k_{eff} for these fuel compositions in the settled configuration, and ≈26-27 percent reduction for the uniform configuration. k_{eff} results for the bounding burnup and enrichment pair for the absorber plate waste package, 4.9 weight-percent/34 GWd/mtU, are also shown in Table C-5a. These results indicate that use of DCRAs eliminates any criticality concern for this fuel in any degraded configuration with intact fuel.

Table C-5a. k_{eff} Results for with and without 16 Rod DCRAs

Burnup/ Enrichment Pair	58 vol.% Settled				33 vol.% Uniform			
	Without DCRAs		With 16 rod DCRAs		without DCRAs		With 16 rod DCRAs	
	k_{eff}	2σ	k_{eff}	2σ	k_{eff}	2σ	k_{eff}	2σ
4.3 wt.%/3 GWd/mtU	1.21464	0.00410	0.91253	0.00418	1.18004	0.00446	0.86228	0.00494
4.7 wt.%/13 GWd/mtU	1.16360	0.00430	0.87859	0.00470	1.12942	0.00484	0.83002	0.00432
4.9 wt.%/34 GWd/mtU	1.01860	0.00486	0.7599	0.00448	0.97950	0.00370	0.71312	0.00458

The preliminary results for 44 BWR waste package with a fully degraded basket indicate that the k_{eff} values for the base case configuration (no vertical separation between assemblies and 54 volume-percent uniform Fe_2O_3/AlOOH corrosion product mixture) are comparable to those of the 21 PWR waste package with a fully degraded basket. Comparison of 25,000 year-old BWR fuel with 4.5 weight-percent enrichment and 35 GWd/mtU burnup, to PWR fuel of the same age, enrichment, and burnup indicates that the k_{eff} values for the base BWR configuration were 1 percent lower than the 58 volume-percent settled PWR configuration and 3 percent higher than the 33 percent uniform PWR configuration. Like the PWR fuel, the time of peak postclosure k_{eff} values occurred in the 10,000 to 35,000 year time frame. Table C-5b shows the effects on k_{eff} of the other variations in the fully degraded basket configurations for the 44 BWR waste package that were discussed in Section 2.1.3. Both the possibility of BWR assembly separation by corrosion products, and the potential for boron adsorption on FeOOH/AlOOH, may produce significant reductions in degraded BWR waste package k_{eff}.

Table C-5b. k_{eff} Results for Various Configurations of a 44 BWR WP with a Fully Degraded Basket Containing 4.5 wt.% initial ^{235}U Enrichment, 35 GWd/mtU SNF at 25,000 Years (CRWMS M&O 1998o, Section 6.1)

Case	k_{eff}	2σ	$\Delta k_{eff}/k_{eff}$
Base case – no vertical separation and 54 vol.% uniform Fe_2O_3/AlOOH	0.9709	0.0031	0.0000
2.7 cm vertical separation and 54 vol.% uniform Fe_2O_3/AlOOH	0.8858	0.0029	-0.0876
2.7 cm vertical separation and 72 vol.%FeOOH/AlOOH	0.8691	0.0027	-0.1049
3.7 cm vertical separation and 72 vol.% FeOOH/AlOOH	0.8327	0.0026	-0.1424
3.7 cm vertical separation and 72 vol.% uniform FeOOH/AlOOH with 15% of ^{10}B Absorbed	0.7660	0.0022	-0.2111

3.1.4 Fully Degraded Basket with Degraded Fuel

The purpose of this section is to describe the MCNP cases performed in CRWMS M&O 1996g. (Section 7.5) to evaluate the range of parameters indicated in Section 2.1.3 for the fully degraded basket configurations with degraded fuel assemblies. Note that at this point in the process, no estimation of the likelihood of obtaining a specific combination of parameters has been developed. Only the 33 volume-percent uniform configuration was evaluated, as consolidation of the fuel rods in the 58 volume-percent settled case would cause the rods in the top 1.5 assembly rows that are currently in clear water to settle below the oxide layer. Thus, evaluation at 33 volume-percent uniform is bounding for the settled oxide scenario as well. As this evaluation of sensitivity to consolidation is performed primarily to demonstrate that collapsed assemblies are less reactive than intact assemblies, only the bounding for the absorber plate waste package fuel was evaluated at a decay time of 25,000 years. A rod clearance of 73 percent corresponds to a 0 cm clearance between guide tubes and adjacent fuel rods. Fuel rod consolidation in only the vertical direction and in both vertical and horizontal directions was evaluated. Variations in spacing of the consolidated assemblies was also performed. The results are provided in Table C-6, and as expected, show a decreasing k_{eff} as the rods move closer together.

Table C-6. Effects of Reduced Rod Spacing for the 4.9 wt.%, 34 GWd/mtU Fuel at 25,000 Years in the 33 vol.% Uniform Configuration

% Original Fuel Rod Clearance		Assembly Horizontal Spacing	k_{eff}	2σ
Vertical	Horizontal			
100%	100%	0 cm	0.99309	0.00388
73%	100%	0 cm	0.97300	0.00448
73%	73%	1.1 cm*	0.96998	0.00400
73%	73%	0 cm	0.95799	0.00338
0%	100%	0 cm	0.91239	0.00366
0%	0%	4.9 cm*	0.81261	0.00392
0%	0%	2.45 cm	0.85417	0.00338
0%	0%	0 cm	0.79258	0.00342

*Spacing maintains original assembly center-to-center spacing

A final case run with all of the fuel rods touching and completely settled into a cylinder segment at the bottom of the waste package yielded a k_{eff} of 0.65588 ± 0.00394. Based on these results, it is evident that any degradation of the assembly structure, be it by corrosion of the grid spacers or dynamic loading by rockfall, will result in significantly reduced k_{eff} values.

As the above analyses indicated reduced reactivity with further consolidation, completely degraded fuel with only pellet size and smaller particles of fuel distributed in the oxide was not explicitly evaluated. Previous studies (ORNL 1985, Appendix) of fuel rubble conducted as part of the Three Mile Island Unit 2 defueling examined the k_{eff} of spherical UO_2 particles (evaluated at enrichments of 2.34 weight-percent and 2.96 weight-percent) distributed in borated water, and found an optimum particle size of 3.5 cm in diameter and occupying 66 percent of the total volume. Since a fuel pellet is much smaller than this particle size, an increase in k_{eff} above that shown for fully consolidated rods would not be expected. Additional analyses to confirm this will be performed for License Application.

3.2 CRITICAL LIMIT CRITERION

Based on the information presented in Subsection 4.1.3.4 of the main report, sample critical limits have been chosen for the degraded PWR configuration classes. These critical limits are provided in Table C-7 below. In the absence of specific critical limits for BWR fuel, these critical limits will also be applied to the degraded BWR configuration classes for this example. If a configuration does not fall below the critical limit over the entire parameter range specified for that configuration in Subsection 2.1.3, then the probability of obtaining the conditions necessary to exceed the limit for that configuration, and the resulting consequences, must be estimated.

Table C-7. Sample Critical Limits for Potential Configurations

Configurations	Critical Limit
Moderated intact fuel lattice inside waste package, intact-to-degraded waste package basket array	0.98*
Moderated degraded fuel (non lattice) inside waste package, degraded waste package basket	0.98*

* For this example, the actual critical limit of 0.978 (from Subsection 4.1.3.4 of the main text) was rounded up to 0.98.

3.3 CRITICALITY REGRESSION EXPRESSION

The criticality evaluation in Section 3.1 determined that the partial 21 PWR basket configurations (IP-3b) and the fully degraded 21 PWR basket configuration (IP-3c) have the potential for exceeding the critical limit over a portion of their parameter range. Similarly, the preliminary evaluation of the fully degraded 44 BWR basket configuration (also IP-3c) has the potential for exceeding the example critical limit. This section will discuss the development of k_{eff} regressions for these two degraded configuration classes, for later use in the probabilistic evaluation.

CRWMS M&O 1996g (Section 7.6) developed regressions which relate the k_{eff} for a particular class of degraded 21 PWR waste package configurations (e.g., intact fuel with fully degraded basket and oxide settled to bottom of waste package) to various parameters for that class (e.g., time, burnup, enrichment, assemblies covered by oxide, etc.). Since MCNP is a Monte Carlo code, each result is reported as a mean and a standard deviation (σ). For conservatism, the regressions were fit to $k_{eff}+2\sigma$ (upper bound at 95 percent confidence). The coefficients for the partially degraded 21 PWR basket regressions for both a uniform and settled distribution of oxide corrosion products are provided in Table C-8, and the form of the regression in both cases is as follows:

$$k_{eff}+2\sigma = C_0+C_1b+C_2b^2+C_3a+C_4a^2+C_5Ln(t)+ C_6Ln(t)^2+C_7Ln(t)^3+C_8O+C_9T+C_{10}T^2+C_{11}T^3 \quad \text{Eq. C-1}$$

where b is burnup in GWd/mtU, and a is initial enrichment in weight-percent, t is decay time in years, T is thickness of borated stainless steel remaining in mm, and O is either volume-percent oxide for the uniform oxide configuration, or fuel rod rows covered for the settled cases.

Table C-8. Regression Coefficients for Partially Degraded PWR Basket $k_{eff}+2\sigma$

Regression Coefficients	Uniform Oxide	Settled Oxide
C_0	2.35498	1.72095
C_1	-6.6737e-03	-6.7237e-03
C_2	-1.8096e-05	-1.6667e-05
C_3	1.4180e-01	1.3348e-01
C_4	-7.1354e-03	-6.0497e-03
C_5	-5.1930e-01	-3.1232e-01
C_6	5.9471e-02	3.7442e-02
C_7	-2.2406e-03	-1.4715e-03
C_8	-5.0889e-03	-1.6797e-02
C_9	-7.4906e-02	-6.6316e-02
C_{10}	1.0646e-02	9.4036e-03
C_{11}	-5.2334e-04	-4.6905e-04

The coefficients for the fully degraded 21 PWR basket regressions for both a uniform and settled distribution of oxide corrosion products are provided in Table C-9, and the form of the regression in both cases is as follows:

$$k_{eff}+2\sigma = C_0+C_1Ln(t)+C_2b+C_3a+C_4Ln(t)^2+C_5Ln(t)^3+C_6b^2 +C_7b^3+C_8a^2+C_9a^3+C_{10}Ln(t)b+C_{11}Ln(t)a+C_{12}O \quad \text{Eq. C-2}$$

where b is burnup in GWd/mtU, a is initial enrichment in weight-percent, t is decay time, and O is volume-percent oxide for the uniform oxide configuration and assembly rows covered for the settled cases.

Table C-9. Regression Coefficients for Fully Degraded 21 PWR Basket $k_{eff}+2\sigma$

Regression Coefficients	Uniform Oxide	58% Settled Oxide
C_0	-5.12955	-1.25161
C_1	1.65615	6.83155e-01
C_2	-8.52852e-03	-6.65133e-03
C_3	2.92660e-01	2.66145e-01
C_4	-1.53971e-01	-6.40282e-02
C_5	4.67070e-03	1.92631e-03
C_6	6.89640e-05	-2.67041e-05
C_7	-1.63227e-07	6.12197e-07
C_8	-6.71372e-02	-6.18276e-02
C_9	5.36083e-03	5.20352e-03
C_{10}	-4.08151e-04	-1.36497e-04
C_{11}	7.23708e-03	5.08490e-03
C_{12}	-5.25978e-03	-1.40918e-01

A multivariate regression was also developed by CRWMS M&O 1996g for predicting the $\Delta k_{eff}/k_{eff}$ resulting from various amounts of boron remaining in solution for the partially degraded 21 PWR basket with various amounts of iron oxide settled to the bottom of each assembly, and various borated stainless steel plate thickness remaining. While the amount of boron in solution is generally much smaller than in the basket, this correction is justified because it is still an effective neutron absorber until it is removed from the waste package. The corrected k_{eff} is obtained using:

$$Corrected\ k_{eff} = k_{eff} + \Delta k_{eff} = k_{eff}(1 + \frac{\Delta k_{eff}}{k_{eff}}) \qquad \text{Eq. C-3}$$

The coefficients of the regression are provided in Table C-10, and the form of the regression is as follows:

$$\Delta k_{eff}/k_{eff} = C_0 + C_1 \ln(B) + C_2 \ln(B)^2 + C_3 \ln(B)^3 + C_4 T + C_5 O \qquad \text{Eq. C-4}$$

where B is the total grams of ^{10}B in solution in the fully flooded waste package, T is thickness of borated stainless steel remaining in mm, and O is fuel rod rows covered.

Table C-10. Regression Coefficients for $\Delta k_{eff}/k_{eff}$ as a Function of Dissolved ^{10}B for the 58 vol.%Settled Oxide Partially Degraded 21 PWR Basket Configuration

C_0	6.37971e-03
C_1	-6.07375e-02
C_2	2.08433e-02
C_3	-2.21564e-03
C_4	3.59713e-04
C_5	4.23685e-03

CRWMS M&O 1996g also developed a multivariate regression for predicting the $\Delta k_{eff}/k_{eff}$ resulting from various amounts of boron remaining in solution for the fully degraded basket with 58 volume-percent iron oxide settled to the bottom. The coefficients for this regression are provided in Table C-11, and the form of the regression is as follows:

$$\Delta k_{eff}/k_{eff} = C_0 + C_1 \ln(B) + C_2 \ln(B)^2 + C_3 \ln(B)^3 \qquad \text{Eq. C-5}$$

where B is the total grams of ^{10}B in solution in the fully flooded waste package.

Table C-11. Regression Coefficients for $\Delta k_{eff}/k_{eff}$ as a Function of Dissolved ^{10}B for the 58 vol.% Settled Oxide Fully Degraded 21 PWR Basket Configuration

C_0	2.32558e-02
C_1	-3.56383e-02
C_2	1.42821e-02
C_3	-1.91685e-03

Finally, CRWMS M&O 1996g provided a regression which predicts the peak k_{eff} for the fully degraded 21 PWR basket with settled oxide configuration as a function of fuel assembly burnup and initial enrichment. The regression coefficients are provided in Table C-12, and the form of the regression equation is as follows:

$$Peak\ k_{eff}+2\sigma = C_0+C_1b+C_2E+C_3b^2+C_4E^2+C_5b^3+C_6E^3 \qquad \text{Eq. C-6}$$

where b is burnup in GWd/mtU, and E is initial enrichment in weight-percent. Figure C-27a uses this regression to illustrate burnup and enrichment pairs which would have a peak k_{eff} of 0.98 in PWR configuration IP-3c (fully degraded basket) with settled oxide distribution. For perspective, Figure C-27a also includes the intact loading curve from Figure C-3 (which is based on a preclosure critical limit of 0.93 in an intact flooded package), and the burnup and enrichment distribution of the entire historical and projected PWR waste stream (CRWMS M&O 1998g, Section 5.1.10).

Table C-12. Regression Coefficients for 58 vol.% Settled Peak k_{eff} as a Function of Burnup and Enrichment for the 21 PWR Basket Configuration

C_0	6.40653e-01
C_1	-1.02912e-02
C_2	3.00169e-01
C_3	-2.54581e-05
C_4	-4.90929e-02
C_5	9.92035e-07
C_6	3.64521e-03

A similar type of regression expression was also developed for the worst 44 BWR degraded configuration in CRWMS M&O 1998o (Section 6.2). This regression is:

$$Peak\ k_{eff} = 0.850736 + 0.087294e - 0.007751b \qquad \text{Eq. C-7}$$

where b is burnup in GWd/mtU, and e is initial enrichment in weight-percent. Figure C-27b uses this regression to illustrate burnup and enrichment pairs which would have a peak k_{eff} of 0.98 in the BWR base case fully degraded basket configuration. As these PWR and BWR configurations have been shown to bound the other degraded internal configurations with respect to k_{eff}, Figures C-27a and C-27b could be utilized as loading curves to significantly reduce the potential for postclosure criticality in these waste packages.

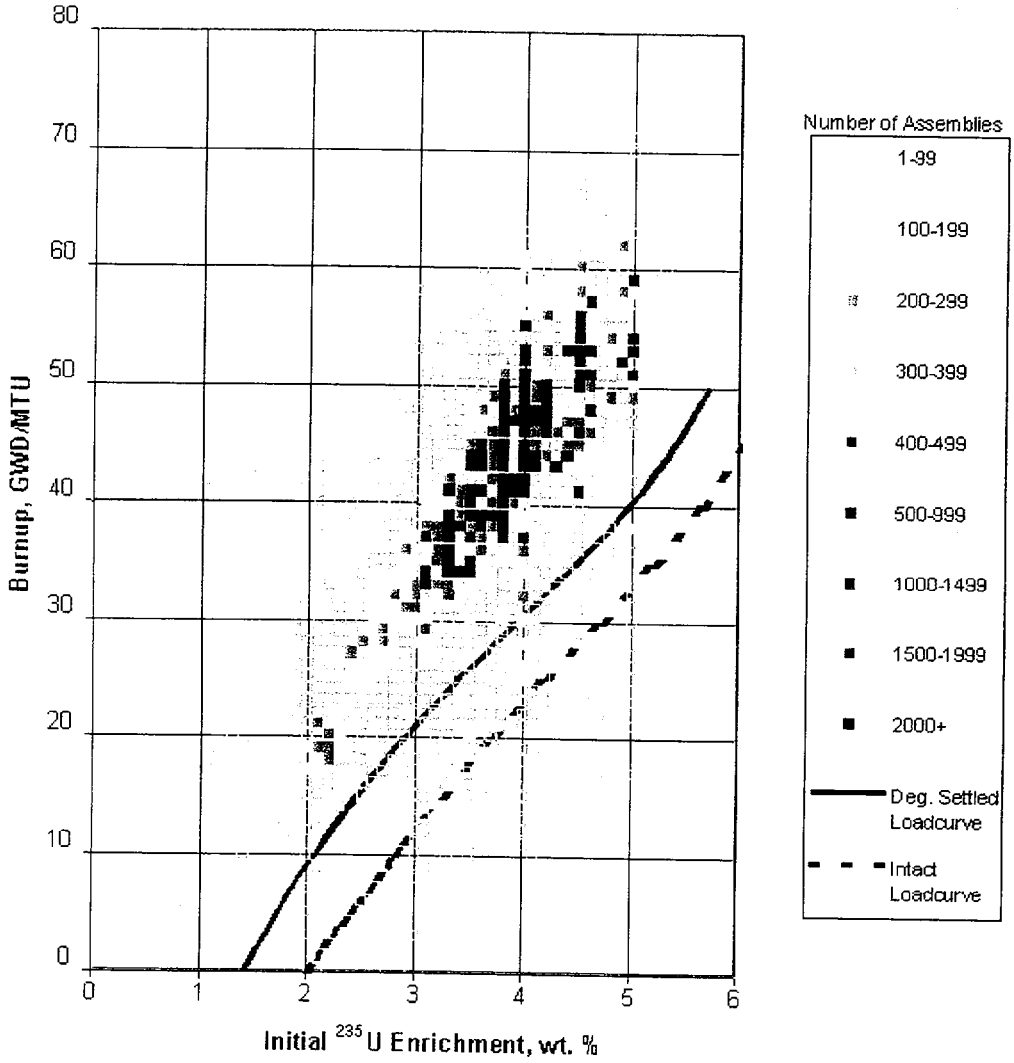

Figure C-27a. Example 21 PWR WP Degraded Loading Curve

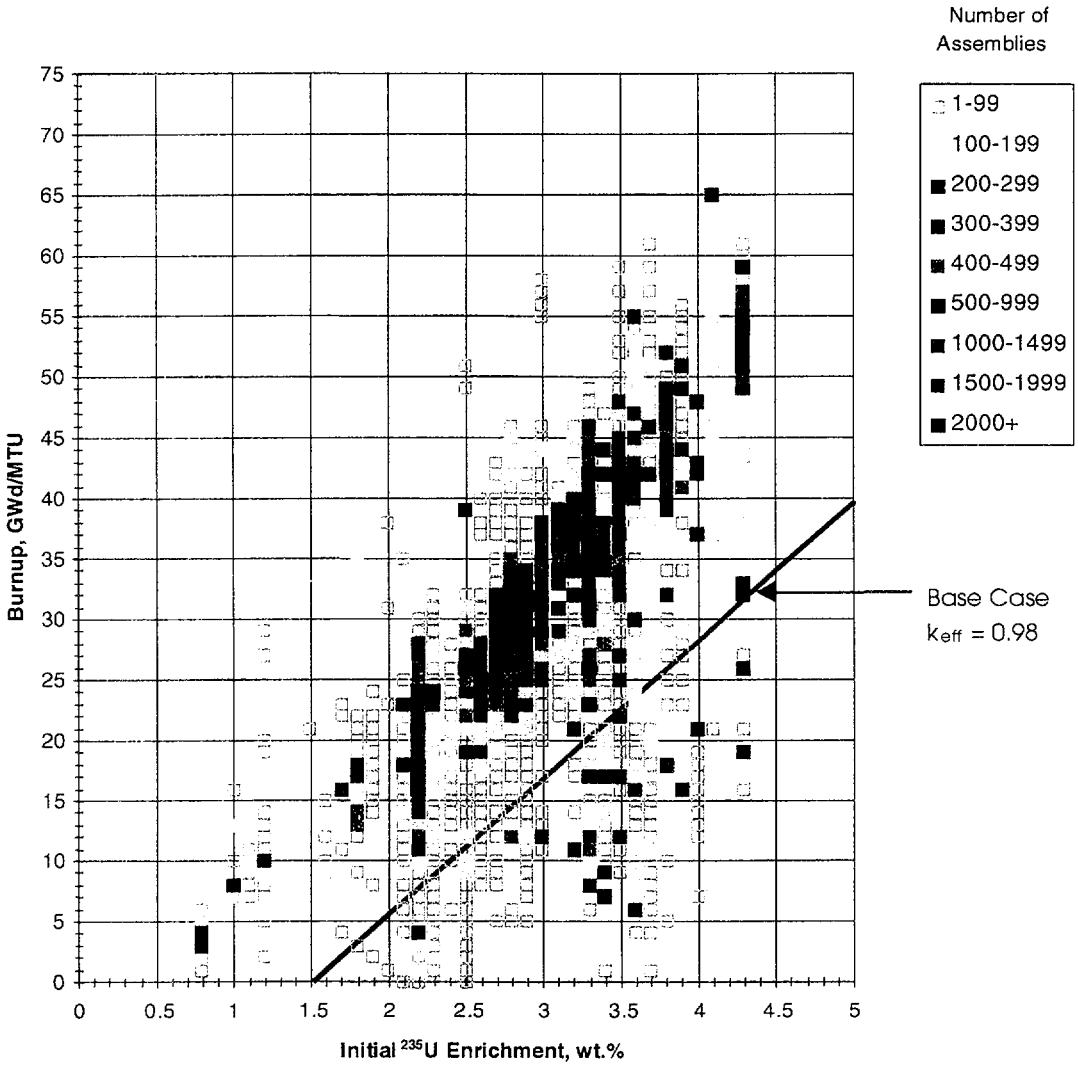

Figure C-27b. Example 44 BWR WP Degraded Loading Curve

4.0 PROBABILITY EVALUATIONS

4.1 PROBABILITY ESTIMATION

The criticality evaluation performed in Section 3 identified that PWR configurations IP-3b and IP-3c could exceed the critical limit over a portion of their parameter range, so an additional evaluation of the probability that this will occur is required. The first step in estimating the probability of exceeding the critical limit for configurations in scenario IP-3 is to develop a configuration generator model that will track the internal degradation of the PWR Absorber Plate waste package. Based on the criticality evaluation, the parameters to be tracked following waste package breach are the thickness of borated stainless steel remaining between the assemblies, the amount and physical distribution of the corrosion products remaining in the package, and the amount of boron in solution (used for the settled case only). A simple mass balance can be used to perform this task given a corrosion rate for the borated stainless steel, and the rate of water dripping into the waste package. The regressions can then be incorporated into the mass-balance to allow the k_{eff} of the waste package to be determined at each step of the degradation process given the burnup and enrichment of the contained assemblies. Using the data on the distribution of assembly burnup and enrichment from the 1995 Energy Information Administration database of historical and projected PWR assembly discharges (CRWMS M&O 1997f), the fraction of the PWR waste stream which would exceed the critical limit can also be determined. Figure C-28 illustrates the results of such a calculation with an example critical limit of 0.98 for a waste package located under a dripping fracture that breaches at 3,000 years, remains continuously flooded, and has a uniform oxide distribution. The results indicate that given the above conditions, a maximum of $\approx$3.5 percent of the PWR waste stream could exceed the critical limit for the uniform corrosion product distribution. These are based on use of the mean borated stainless steel corrosion rate from Section 1.4.

The next step in estimating the probability that the PWR waste package critical limit will actually be exceeded is to factor in the uncertainty associated with the assumed conditions used in the deterministic mass-balance calculation. These conditions are 1) the presence of a dripping fracture above the waste package, 2) the time of waste package breach, 3) the duration of waste package internal flooding (if any), and 4) the corrosion rate of the borated stainless steel. Sections 1.3 and 1.4 provided probability distributions for these conditions based on the abstractions being utilized for TSPA-VA. While the last three items are conditioned on the presence of dripping water, they are considered to be independent with respect to each other and the type of fuel contained within the package. The above mass-balance calculation also assumed that the entire waste stream was loaded into the absorber plate waste package. However, a loading curve is specified in Section 1.2 requiring that some of the most reactive assemblies receive disposal control rods to meet preclosure criticality control requirements. Section 3 demonstrated that these control rods are effective in significantly reducing k_{eff} for configurations involving intact fuel and a fully degraded basket, and are no longer needed once the assembly structure has degraded. Since the use of unirradiated Zircaloy cladding for these control rods assures that they will remain intact at least as long as the fuel, the assemblies in the Energy Information Administration (EIA) database with burnup and enrichment below the loading curve should not be considered as part of the population of PWR fuel capable of exceeding the critical limit in the absorber plate waste package.

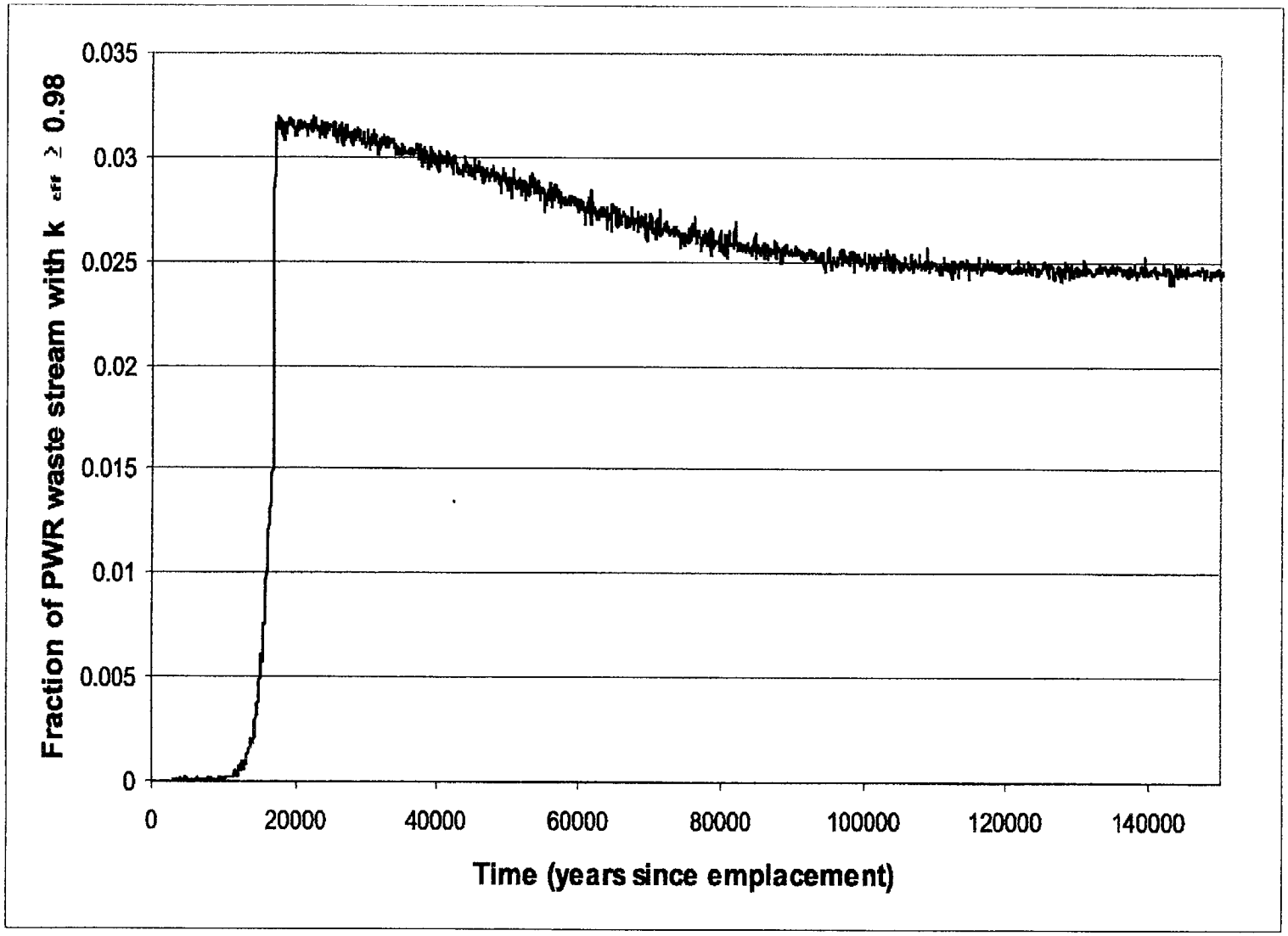

Figure C-28. Time Dependence of the Fraction of the PWR Waste Stream with $k_{eff} \geq 0.98$ Given a Breached 21 PWR Absorber Plate WP Which Remains

As discussed in Section 3.5 of the main report, a simple Monte Carlo sampling technique may be utilized in conjunction with the mass-balance calculation to estimate the probability that a PWR waste package will achieve the required conditions for exceeding the critical limit (CRWMS M&O 1998g). For each realization, the above distributions are sampled to determine if the package is under a drip, accumulates water, and contains fuel within the loading criteria (see Figure C-29). For realizations where all of these criteria are met, the mass balance is performed as before to determine the state of degradation of the waste package (and the resulting fraction of fuel meeting the loading criteria that would exceed the critical limit) at a given time (see Figure C-30). If the fraction of fuel above the critical limit exceeds a randomly determined limit for that realization, then the package is considered to have exceeded the critical limit. The fuel is conservatively assumed to remain intact throughout the degradation process. If the critical limit is exceeded prior to the package breaching on the bottom and draining, the time is recorded before starting the next realization. The total number of waste packages that exceed the critical limit at a given time, divided by the total number of realizations performed, represents the cumulative probability that an absorber plate waste package will exceed the critical limit at that time as a result of internal degradation and flooding.

Figure C-31 shows the cumulative probability of exceeding a critical limit of 0.98 for three types of loading strategies: 1) using the 21 PWR Absorber Plate waste package for the entire PWR waste stream (no loading curve case similar to that evaluated in the deterministic mass-balance), 2) using the intact 21 PWR loading curve shown in Sections 1.2, and 3) using the degraded 21 PWR loading curve defined in Section 3.3. Only the uniform oxide distribution was evaluated based on the expectation in Subsection 3.1.3 that consideration of the corrosion products resulting from the degradation of the aluminum thermal shunts would result in approximately equal criticality potential for both oxide distributions.

Forms of common mode failure other than dripping fractures have not been considered due to their expected low contribution to the overall probability of exceeding the critical limit. Two such potential common mode failures are settling of the corrosion products as a result of seismic shaking of the package, and partial localized flooding as a result of episodes of high dripping flow occurring over a short period of time (as discussed in Assumption TDSS 026 in CRWMS M&O 1998m). The former would not be expected to significantly alter the reactivity of the package based on the Subsection 3.1.3 indication that the uniform and settled oxide distributions would have similar k_{eff} values after consideration of the aluminum corrosion products. The latter event would be expected to be of only limited duration as the repository drifts are designed to drain (CRWMS M&O 1997a, p. 48), and could only affect those packages which had been breached, suffered sufficient basket degradation, and contained fuel which was capable of exceeding the critical limit at the time the flooding occurs.

Cases involving the use of the 21 PWR loading curves in Figure C-31 also include allowance for the potential that a waste package was accidentally loaded with at least one fuel assembly which exceeded the loading criteria during preclosure. A preliminary estimate of the misload probability using human error data and assumed administrative controls is $\approx 5.8 \times 10^{-5}$ per PWR waste package (CRWMS M&O 1998h, Section 6). When the misload probability is multiplied by the cumulative probability that a waste package is under a drip, breached, and floods for any length of time, the cumulative probability of exceeding the critical limit due to misloads may be conservatively estimated.

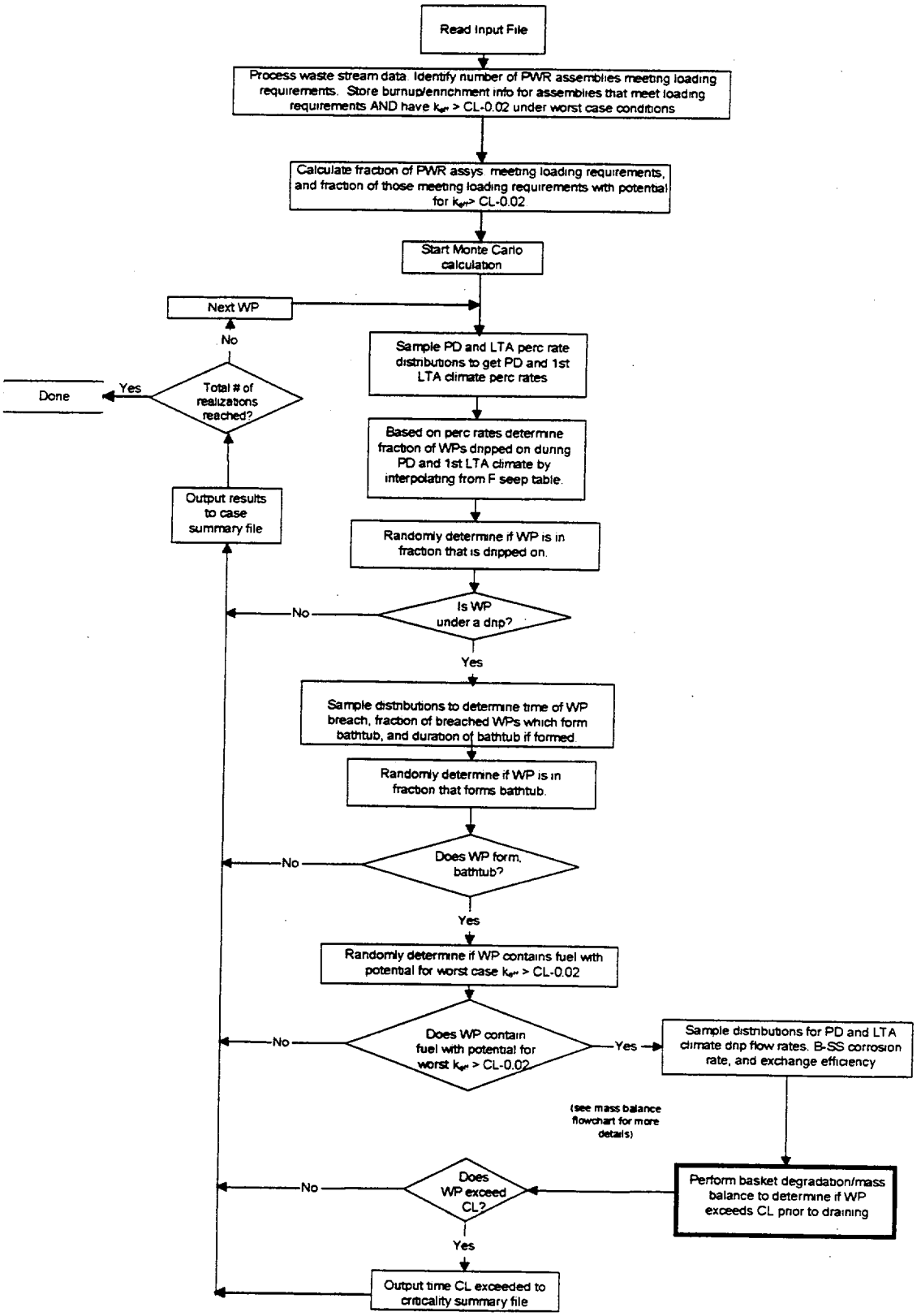

Figure C-29. Flowchart for Monte Carlo Simulation Used to Estimate Probability of Exceeding a Given Critical Limit

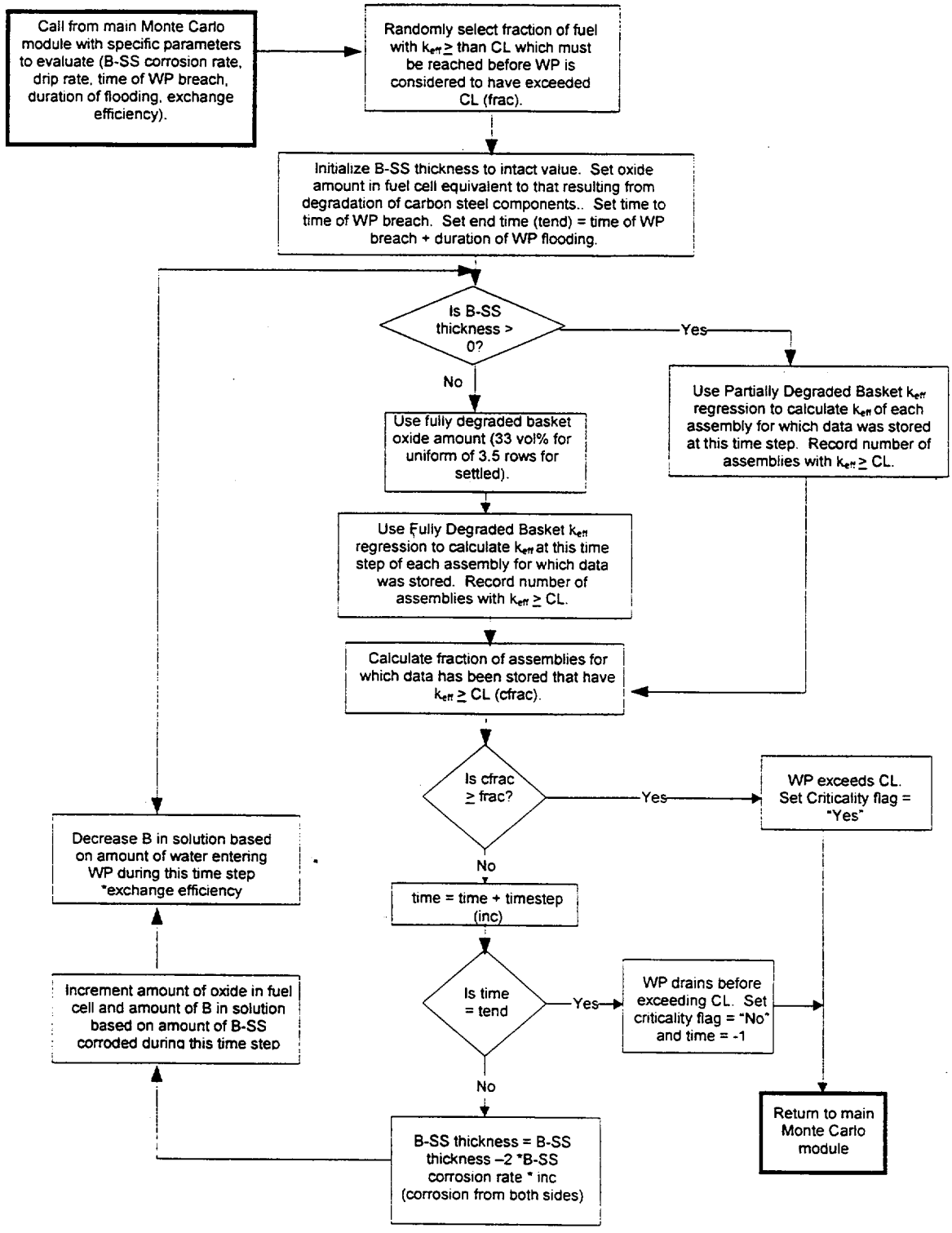

Figure C-30. Flowchart for Mass Balance Portion of Monte Carlo Simulation

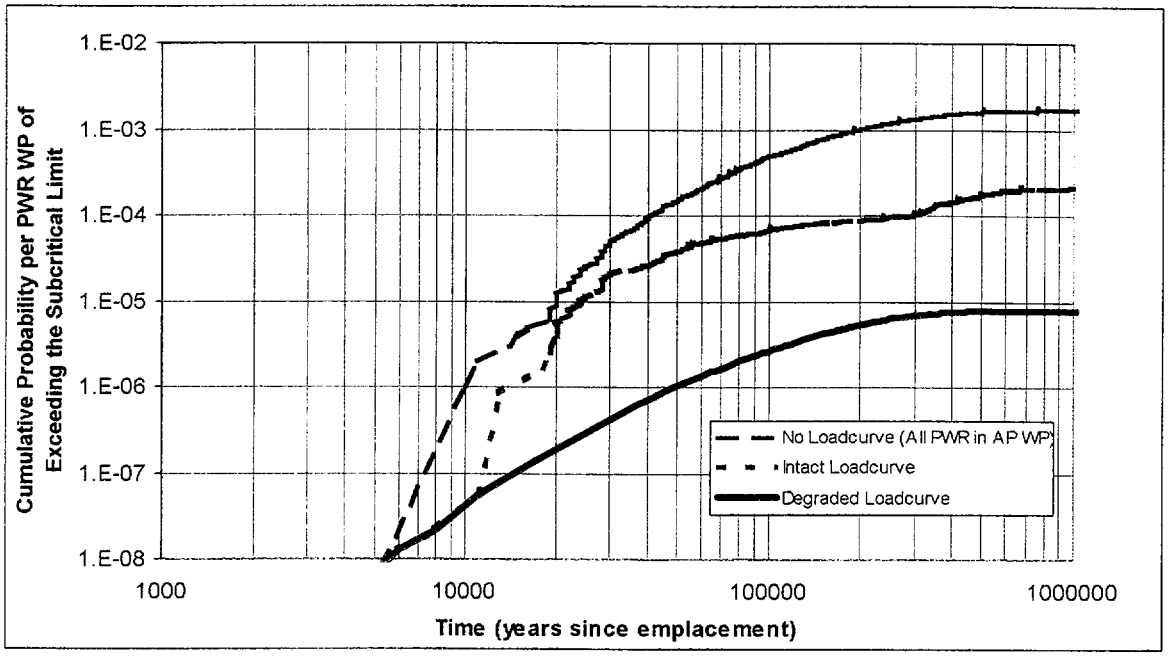

Figure C-31. Cumulative Probability of a PWR WP Exceeding the Critical Limit (k_{eff}=0.98) as a Function of Time

The results of Figure C-31 are best put into perspective by comparison with the expected number of PWR waste packages to be emplaced (4,792 based on Key Assumption 003 from CRWMS M&O 1998m). Based on this number of packages, if all fuel was loaded into the Absorber Plate waste package (no-loading curve case) one package might be expected to have exceeded a critical limit of 0.98 in 60,000 years. However, this is not a realistic case as an intact loading curve has been specified in Section 1.2 in order to meet preclosure criticality control requirements for the intact package. Based on 4,792 packages loaded according to the intact loading curve in Section 1.2, one package might be expected to exceed a critical limit of 0.98 by approximately 700,000 years. If the waste package loading strategy were further augmented by use of the degraded loading curve discussed in Section 3.3, no packages would be expected to exceed the critical limit with 1,000,000 years, even after consideration of potential misloads. Another familiar method is to express likelihood in terms of annual probability of occurrence. Table C-13 provides estimates of the annual probability that a PWR waste package will exceed a critical limit of 0.98 for various time periods. The annual probability never exceeds 10^{-8} per package-year for any of the cases considered.

Table C-13. Annual Probability (pkg-yr^{-1}) of Exceeding a Critical Limit of 0.98 for a PWR Waste Package

Applicable Times (years)	No Loading Curve	Intact Loading Curve	Degraded Loading Curve
0 to 5,000	$< 2.0\times10^{-12}$	1.6×10^{-12}	1.6×10^{-12}
5,000 to 10,000	1.4×10^{-10}	7.3×10^{-12}	7.3×10^{-12}
10,000 to 50,000	3.8×10^{-9}	9.7×10^{-10}	2.5×10^{-11}
50,000 to 100,000	6.7×10^{-9}	6.2×10^{-10}	3.2×10^{-11}
100,000 to 500,000	2.8×10^{-9}	2.6×10^{-10}	1.3×10^{-11}
500,000 to 1,000,000	1.6×10^{-10}	7.8×10^{-11}	3.1×10^{-13}

While a detailed probability calculation has not yet been performed for the 44 BWR waste package, an initial estimate can be made from the preliminary information obtained thus far. CRWMS M&O 1998o utilized the regression expression given in equation C-7, and the BWR waste stream information from CRWMS M&O 1997f, to estimate that a maximum of 6.9 percent of BWR assemblies could exceed a k_{eff} of 0.98 if the worst case fully degraded configuration occurred at the time of peak postclosure k_{eff}. This is compared with 3.2 percent for the 21 PWR waste package with no loading curve (from Figure C-28). This approximate doubling of the maximum fraction capable of exceeding 0.98 k_{eff} would be expected to translate to the cumulative probability as well. Thus, the cumulative probability of a 44 BWR WP exceeding the critical limit would not be expected to be greater than 1×10^{-3} per package at 100,000 years, and 3×10^{-3} per package at 1,000,000 years, if no loading curve were used. It is expected that use of loading curves, and additional degradation scenario and criticality analysis, will further reduce this probability.

4.2 PROBABILITY CRITERION

The Probability Criterion set in the methodology (Section 3.5 of the main report) is that the cumulative probability of a waste package exceeding the CL not exceed 10^{-4} during the first 10,000 years. If this criterion is not met, design options must be investigated for reducing k_{eff}. In the example, it was determined that both of these criteria are met if the loading strategy discussed in Section 1.2 is followed. Therefore, the example PWR waste package design loaded with the example waste form meets the Probability Criterion check. A Criticality Consequence evaluation to estimate the increased source and conditions due to the potential criticality must now be performed. No comparison of the BWR waste package to the Probability Criterion will be made at this time due to the preliminary nature of the analyses.

5.0 CRITICALITY CONSEQUENCE EVALUATIONS

5.1 CRITICALITY CONSEQUENCE ESTIMATION

This section discusses the results of a sample criticality consequence evaluation for the PWR waste package. The scenarios evaluated are based upon the configurations identified in Section 3 of this appendix. The consequence of criticality events was evaluated for systems where k_{eff} exceeded the critical limit. Based on the evaluations performed in Section 3.0, two positive reactivity insertion scenarios are possible: 1) an extremely slow insertion caused by a slow loss of boron from the package interior during degradation of the basket, or 2) a faster insertion resulting from settling of oxide which was initially uniformly distributed. The latter scenario may become incredible if future neutronic calculations demonstrate that consideration of aluminum corrosion products reduces the reactivity of the settled oxide configuration to that of the uniformly distributed oxides. The base results of these consequence evaluations are increments to the radionuclide inventory. The detailed results are shown in CRWMS M&O 1995b (Section 7.5) and CRWMS M&O 1997h (Section 7).

In the slow reactivity insertion scenario, once a waste package achieves criticality, continued small positive reactivity insertions will cause the power output of the waste package to begin to slowly rise (i.e., a long reactor period). If the power exceeds a certain limit, the rate at which water is consequentially removed from the waste package will exceed the rate of input, and the

resulting water level drop will provide a negative reactivity insertion driving the waste package back towards a critical condition. Conversely, if insufficient power is produced, the water level will be maintained and the flushing process will continue to remove dissolved boron, thus providing a continued source of positive reactivity insertions until the point of equilibrium is achieved. The maximum steady-state power can then be estimated by determining the power required to maintain the bulk waste package water temperature at the point where water is removed at the same rate that it drips into the waste package. The waste package must produce sufficient power to raise the temperature of the incoming water to this equilibrium value, as well as account for heat losses to the environment by radiation and/or conduction. Preliminary calculations, which are provided in detail in CRWMS M&O 1995b (Section 7.5.1) have shown that at a water temperature of 57.4°C, the evaporation rate will match a drip rate of 0.19 m3/yr (approximately the mean drip rate associated with the mean percolation rate for the long-term average climate cycle). The thermal power required to raise the water temperature to 57.4°C, while at the same time compensating for heat losses to the environment, is 2.18 kW.

To evaluate the effects of a criticality on the radionuclide inventory of a waste package, the computer code ORIGEN-S was run using the B&W 15 × 15 PWR assembly with a 3 weight-percent enrichment – 20 GWd/mtU burnup, and the steady-state power of 2.18 kW discussed above. The criticality was assumed to occur after the fuel had decayed for 15,000 years and was maintained at the above mentioned power for three durations: 1,000, 5,000 and 10,000 years. The maximum duration of 10,000 years is based on the assumption that it is the upper bound for the conditions supporting criticality (high infiltration, integrity of the lower part of the barrier, sufficient fissionable material, and void space remaining). The output of these runs was the radionuclide inventory, in curies, at the times corresponding to the end of each criticality, and at fuel ages (time since reactor discharge) of 45,000 and 65,000 years. In addition a fourth, decay-only case was run to determine the radionuclide inventories at the above times for fuel which did not experience a criticality event. The percentage increase in the inventories of the TSPA isotopes is provided in CRWMS M&O 1995b, Subsection 7.5.2. The overall effect of the criticality can be summarized by the percentage increase in the total curies, over that of the decay only case, for the TSPA isotopes as shown in Table C-14. The explicitly stated times are measured from emplacement. Figure C-32 graphically shows that even the 10,000 year duration criticality does not increase the inventory of the 36 isotopes above that at the time the criticality began. In addition, the criticality appears to have no significant long-term effect on the inventory of these isotopes. Within 25,000 years the total inventory of these 36 isotopes in fuel assemblies which experienced a criticality can approach becoming indistinguishable from the inventory in fuel assemblies which did not experience a criticality.

Table C-14. Percentage Increase in Total Curies of the 36 TSPA-95 Isotopes in a Single Waste Package

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

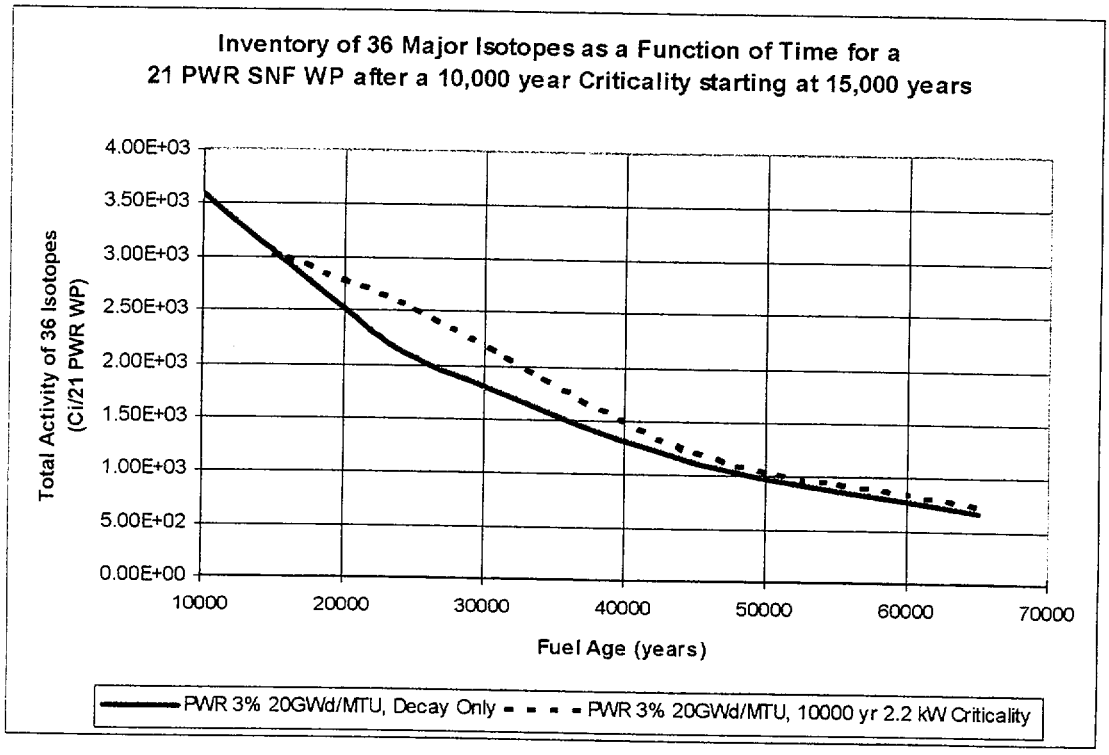

Figure C-32. Increase in Isotopic Inventory from a Slow Reactivity Insertion Leading to a 10,000 year Steady-State Criticality

The consequences of the fast reactivity insertion scenario were investigated with a RELAP5 model (CRWMS M&O 1997h). This scenario involved a constant positive reactivity insertion rate of 23.6 ¢/minute. The rate was based on the difference in k_{eff} between the settled oxide distribution and the uniform oxide distribution for the fully degraded basket configuration with 4.9 weight-percent enriched-34 GWd/mtU burnup fuel. This Δk_{eff} was assumed to be inserted over the ≈1 hour time frame estimated for settling of the oxides following a shaking of the waste package by a seismic event or a rock fall impact (CRWMS M&O 1997h, Section 7.2). The short term (initial power excursion) transient response was dominated by the positive ramp reactivity insertion and negative Doppler feedback reactivity that terminated the initial power rise prior to the introduction of significant negative void reactivity. The transient response of the waste package system following termination of the initial power rise was controlled by the rate of energy addition affecting the rate and magnitude of the void formation and thus the time evolution of the void reactivity component. Ultimately, sufficient fluid inventory was lost from the waste package (>225 kg) to sustain a large negative void reactivity component, keeping the system in a critical condition. Figure C-33 shows the power history for this transient (CRWMS M&O 1997h, p. 44). Maximum pressures in the waste package system remained below 2.55×10^5 Pa and maximum center line fuel rod temperatures remained below 297°C (CRWMS M&O 1997h, p. 44). Sufficient fluid inventory remained in the waste package at the problem termination to redistribute the energy in the system and to reduce the fuel rod temperatures to less than 100°C (CRWMS M&O 1997h, p. 44).

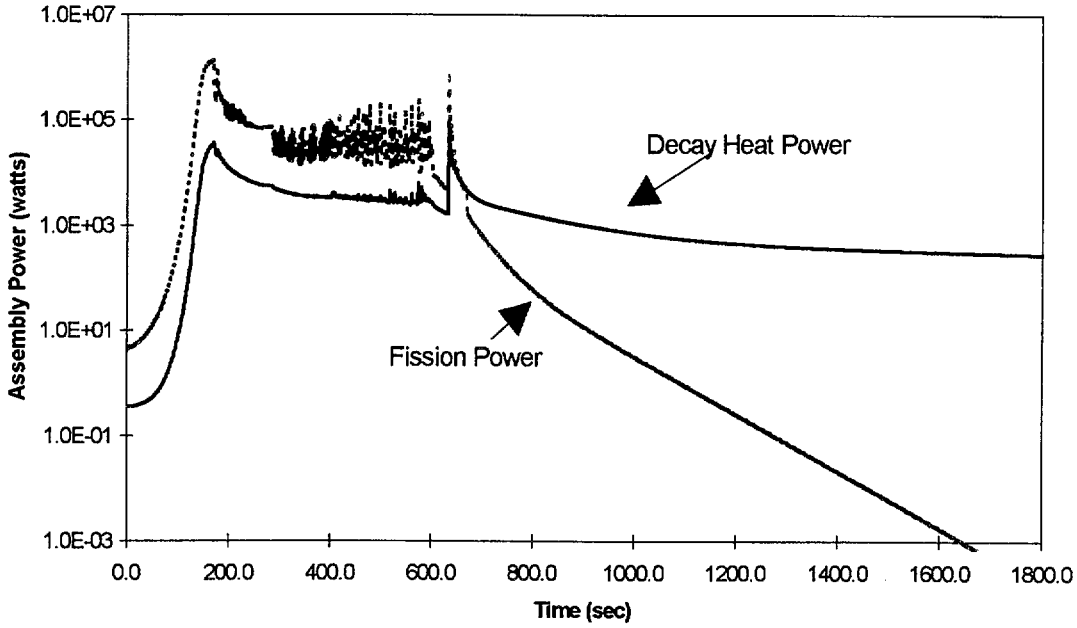

Figure C-33. Dynamic Analysis of a Fast Reactivity Insertion

To evaluate the effects of this transient on the radionuclide inventory of a waste package, SAS2H was run using a 4.9 weight-percent-34 GWd/mtU fuel, power histories from the RELAP5 analyses, and a decay period of one year. The maximum decay period of one year was based on the short operating time of the criticality event which precludes formation of significant inventories of long lived isotopes. The transient fission power history and fuel temperature was approximated by a histogram for the SAS2H input. The burnup calculated from this histogram is only 1.8×10^{-3} MWd/mtU. The change in isotopic inventories due to such low burnups would be expected to be insignificant and this is validated by the SAS2H results. The radionuclide inventory in curies after a one year decay for the transient is compared in Table C-15 to the initial radionuclide inventory for a base 25,000 year decay period (CRWMS M&O 1997h, Table 7.5-2). For this analysis, only those isotopes whose inventories after one year decay differed from the original values by a minimum cutoff value ($\sim10^{-20}$) are listed. As shown, small differences appear in the fission product activity, but the principal radioactivity is due to the actinide decay which is not significantly altered by the criticality events.

Table C-15. Radionuclide Inventory Increase Resulting from a Fast Reactivity Insertion Leading to a Transient Criticality (TSPA isotopes only)

Isotope	Initial Activity (Ci) (CRWMS M&O 1996g)	Transient Increase after 1 yr Decay (Ci)
Actinides	---	
th229	3.71e-02	5.63e-06
th230	2.60e-01	1.17e-05
pa231	9.01e-03	5.20e-07
u233	6.20e-02	-
u234	1.23e+00	-
u235	2.33e-02	-
u236	2.25e-01	-
u238	1.45e-01	-
np237	6.10e-01	-
pu238	0.00	6.27e-04
pu239	9.74e+01	-
pu240	1.56e+01	-
pu241	5.72e-03	-
pu242	5.57e-01	-
am241	5.95e-03	-
am243	5.59e-01	-
cm244	0.00	1.34e-05
Fission Products	---	
tc99	6.02e+00	1.34e-02*
sm151	0.00	1.36e-04

*These values may be significantly overestimated as a result of roundoff to 3 digits in SAS2H.

5.2 RADIONUCLIDE INVENTORY INCREASE CRITERION

The source criterion for criticality set in the methodology is that the increase in the source due to criticality must be less than one percent of the total radionuclide inventory in the repository for the waste form being evaluated (Section 3.6 of the main report). If this criterion is not met, design options must be investigated for reducing k_{eff}.

In the example, the radionuclide source generated by both the postulated single package, long-term, steady-state criticality, and the short-term dynamic transient criticality, is much less than one percent of the total PWR radionuclide inventory in the repository. The example waste package design loaded with the example waste form therefore meets the Radionuclide Inventory Increase Criterion check. A TSPA estimate of dose increment due to the criticality will now be calculated.

6.0 RISK EVALUATION

This section discusses the results of a sample risk evaluation performed for the potential critical events identified in Section 3.0. The probability of the potential critical configuration occurring (from Section 4.0) and the consequence of the resulting criticality (from Section 5.0) are combined into a risk of violating the performance objectives of the facility.

6.1 TOTAL SYSTEM PERFORMANCE ASSESSMENT DOSE ESTIMATION

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

An example calculation was conducted for this report (CRWMS M&O 1998l) using an incremented source term from the long-term, static internal waste package criticality event discussed in the previous section. The results of the example evaluation indicate that, for the example potential criticality event, there was no significant adverse effect to the repository total system performance. The dose to the public was not significantly increased by the inclusion of the potential criticality events identified as part of the example evaluations.

The key isotopes contributing to release and dose to man were determined in TSPA-VA to be ^{99}Tc, ^{129}I, ^{234}U, ^{237}Np, and ^{242}Pu. ^{129}I and ^{99}Tc provided peak release to and doses at the accessible environment at early times and ^{237}Np provided peak, and generally highest release at later times in the base case simulations conducted for TSPA-VA. Gaseous fission products such as ^{85}Kr are ignored because only a small amount are produced even for the longest criticality event (0.186 Ci ^{85}Kr/assembly from CRWMS M&O 1996b (App. X, p. 81), and the estimated travel times for gases to the surface are at least one order of magnitude greater than the half-life for ^{85}Kr (200 to 600 year travel time from CRWMS M&O 1996b, (p. 3-40) versus 10.7 year half-life from General Electric Company 1989 (p. 29). The percent change from the decay only inventory of each of the key radionuclides for each of the three steady-state criticality event durations was reviewed and is presented in Table C-16. These data indicate that the greatest increase in source term inventory occurs for the longest criticality event (10,000 year event).

A TSPA analysis has been performed (CRWMS M&O 1998l) using only the additional source term generated by a 10,000 year duration steady-state criticality event occurring 15,000 years after closure. Based on the cumulative probability of PWR waste package criticality discussed in Section 4.0 of this appendix, criticality was assumed to occur only within a single 21 PWR waste package. Dissolution rate of the source term was assumed to be the same as the initial waste form itself, since the criticality event was assumed to occur within the cladding.

Table C-16. Criticality Effect on Radionuclides Determined to be Important to Total Performance (CRWMS M&O 1995b, pp. 59-61)

Radionuclide	% Difference for 1k Year Criticality	% Difference for 5k Year Criticality	% Difference for 10k Year Criticality
^{129}I	0.45	2.0	4.1
^{99}Tc	0.53	2.2	4.1
^{237}Np	0.26	1.0	2.1
^{234}U	0.90	5.3	11.0
^{242}Pu	-0.37	-1.1	-2.6

Figure C-34 shows the base case dose history at the accessible environment and the additional dose, which would result from the increase in radionuclide inventory due to the 10,000 year criticality. The additional criticality related doses are generally several orders of magnitude below the base case and are inconsequential to performance of the repository.

Figure C-35 shows the dose history at the accessible environment for the radionuclides which are the dominant contributors to additional dose from the criticality event. These radionuclides are the same as those which are dominant contributors to the base case dose, with the exception of ^{242}Pu, which was depleted during the criticality event, and thus did not contribute to additional dose at the accessible environment.

6.2 REPOSITORY PERFORMANCE OBJECTIVES

The total system performance criterion for criticality set in the methodology (main report Section 3.7) is that the risk due to criticality must not significantly affect the total system performance of the repository as measured by the dose at the accessible environment. If this criterion is not met, design options must be investigated for reducing k_{eff}.

In the example, the dose increment due to the criticality was found to be negligible. The example waste package design loaded with the example waste form therefore meets the total system performance criterion check.

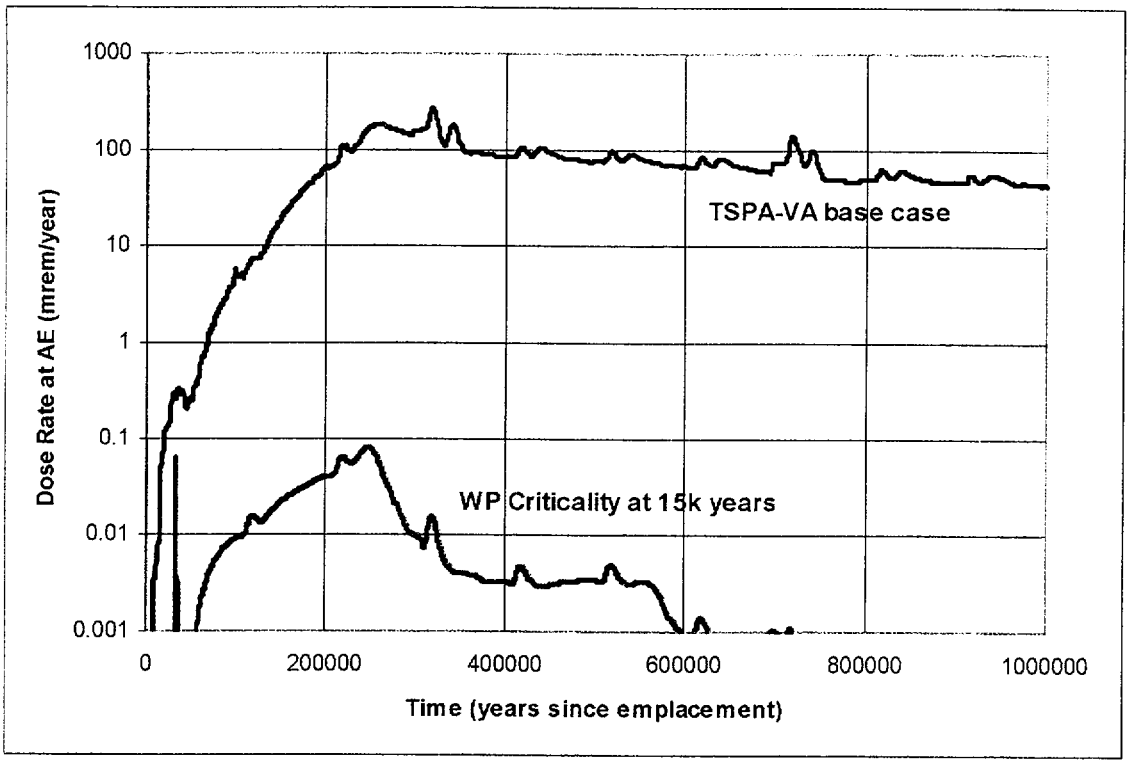

Figure C-34. Expected-Value Dose History at Assessable Environment for TSPA-VA Base Case and for Additional Criticality Source Term

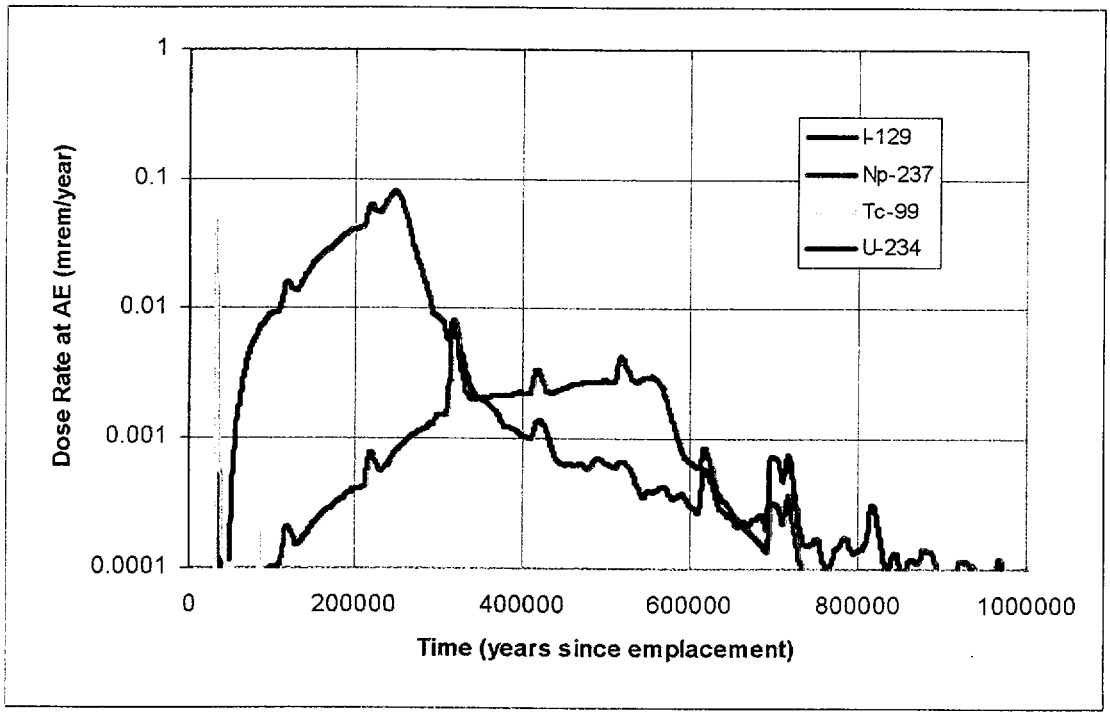

Figure C-35. Expected-Value Dose History at Accessible Environment by Radionuclide for Additional Criticality Source Term

7.0 CONCLUSIONS

7.1 ACCEPTABLE REPOSITORY SYSTEMS

The combination of commercial SNF waste form, 21 PWR UCF waste package design, and engineered barrier design at the proposed Yucca Mountain Site evaluated in the example was determined to be acceptable for postclosure criticality control.

7.2 AUGMENTING CRITICALITY CONTROLS

No augmentations were determined to be necessary for the waste package/engineered barriers system designs evaluated in the example. However, the criticality evaluation identified that increases in carbon steel component thickness above that necessary for structural purposes will also act to reduce k_{eff} in the degraded mode by displacing moderator.

7.3 LOADING CURVES

The intact waste package loading curves developed for the 21 PWR UCF waste package design for preclosure safety analyses were determined to be acceptable using the disposal criticality analysis methodology. However, for defense-in-depth, they may be supplemented with the degraded waste package loading curve developed in Section 3.3.

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APPENDIX D

EXAMPLE APPLICATION OF THE METHODOLOGY FOR DOE SPENT NUCLEAR FUEL

APPENDIX D

EXAMPLE APPLICATION OF THE METHODOLOGY FOR DOE SPENT NUCLEAR FUEL

This appendix demonstrates the application of the disposal criticality analysis methodology to waste forms other than commercial spent nuclear fuel (SNF). The aluminum-clad DOE-owned research reactor fuel has been evaluated for repository disposal. The DOE has performed an evaluation of the potential for criticality and developed a preliminary criticality control design for two specific fuels of this type (CRWMS M&O 1998a). This appendix summarizes the results of that analysis for the fuel type having the higher potential for criticality (partly because of its higher enrichment): the research reactor fuel burned in the Massachusetts Institute of Technology (MIT) research reactor, hereinafter designated as MIT SNF.

This appendix demonstrates only a limited application of the full risk-informed methodology, and that only for internal criticality. The range of parameters evaluated for the internal configuration classes met the Critical Limit (CL) criterion test used for this example, so additional analyses were not required. It is expected that the external criticality evaluation will require a more complete application of the risk-informed methodology.

1.0 INITIAL INPUTS

1.1 WASTE FORM CHARACTERISTICS

1.1.1 General

The waste form and waste package characteristics are a summary of those given in the degraded mode criticality evaluation for this waste package type (CRWMS M&O 1998a). The MIT assembly is constructed from a collection of 15 flat plates tilted at a 60-degree angle so that the resulting assembly has a parallelogram cross section instead of the more common square or hexagon shape. The MIT fuel length values used in these analyses are shorter than the original as-built length of the MIT assembly because the top and bottom ends of the assembly, which do not contain uranium materials, have been removed by cutting. The fuel plates consist of an aluminum cladding over an aluminum/uranium alloy. The maximum fuel mass for the MIT assemblies is 514.25 grams of ^{235}U with an enrichment of 93.5 weight percent. The amount of aluminum present in the U-Al_x alloy is 30.5 weight percent.

1.1.2 Fuel Plates

The flat plates are 2.552 +0.000, -0.002 inches wide, and 23 inches long. All 15 plates are the same size and have a finned cladding surface with a thickness of 0.080 ±0.003 inches and a fin height of 0.010 ± 0.002 inches. The fuel alloy is 0.030 +0.000, -0.002 inches thick, 2.177 +0.000, -0.1875 inches wide, and 22.375 ±0.375 inches long.

1.1.3 Fuel Element

The aluminum outer shroud which encloses the 15 fuel plates on four sides is an equal sided parallelogram structure with a 2.405 inch outside dimension perpendicular to the parallelogram sides (not along the parallogram edges) having two 0.044 inch thick walls parallel with the fuel

plates and two 0.188 inch thick comb plates into which the fuel plates fit. The length (after cutting) is 23.368 inches. The fuel plates are evenly spaced within this rhomboid and angled 60 degrees off the comb plate at a center-to-center spacing of 0.158 inches.

1.2 WASTE PACKAGE/ENGINEERED BARRIER DESIGN

1.2.1 Codisposal Waste Package

The codisposal waste package containing 5 HLW canisters surrounding a DOE SNF codisposal canister is shown in Figure D-1. The barrier materials are typical of those used for commercial SNF waste packages. The inner barrier is composed of 20 mm of Alloy 625 serving as a corrosion resistant material, and the outer barrier is composed of 100 mm of carbon steel serving as a corrosion allowance barrier. During the course of the analysis for this waste form, the nominal design of the waste package was modified by replacing the Alloy 625 inner barrier with Alloy ASTM B 575. The impact of this change was evaluated, and it was found that the slower corrosion of the inner barrier provided by ASTM B 575 would have made criticality less likely. Hence the analysis with Alloy 625 was considered to be more conservative. Therefore, the analysis for this revision was completed with the continued use of Alloy 625.

1.2.2 HLW Glass Pour Canisters

The Savannah River Site (SRS) Defense Waste Processing Facility (DWPF) HLW canister is a cylindrical stainless steel (Type 304L) shell with an outer diameter of approximately 610 mm (24.00 inch), a 9.525 mm wall thickness, and a nominal length of 3 m. The canister inside volume is 0.736 m^3 and the glass weight is 1682 kg. HLW glass occupies 85 percent of the canister's volume. The nominal dimensions of the canister are used for these analyses.

1.2.3 DOE SNF Canister

The following information is from CRWMS M&O 1998a. The canister is a right circular cylinder of stainless steel XM-19 that contains a stainless steel 316L basket. DOE SNF is to be loaded into the basket. The dimensions for the DOE SNF canister are 439.3 mm outer diameter with 15 mm wall thickness. The DOE SNF canister contains basket locations for 16 MIT SNF assemblies in four layers as illustrated in Figures D-2 and D-3, for a total of 64 assemblies/canisters. In the initial design, stainless steel boron alloy (10 mm thick) is used to separate each layer from the adjacent layer within the canister as criticality control material; there were also additional plates of this material placed in the basket between each assembly. It was found that boron is too soluble to be an effective criticality control material for long term disposal, and the final analysis recommended gadolinium, instead (Sections 3 and 4). The MIT SNF canister length is nominally 2628 mm long. The MIT SNF canister with 64 fuel elements has a ^{235}U loading of 32.9 kg (35.2 kg of U).

The MIT SNF codisposal canister basket consists of plates formed into parallelogram slots that fit into a steel disk to provide structural support for the SNF as shown in Figure D-3. Panels of stainless steel boron 2.54 mm thick are attached to one side of each slot to provide neutron attenuation between the slots. Stainless steel boron in-row separator plates, 2.13 mm thick, are provided between adjacent pairs of MIT SNF assemblies to reduce neutronic interaction between adjacent assemblies. The use of gadolinium as a supplemental neutron absorber is discussed in Subsection 2.1.3 of this appendix. The rhomboidal slots provide a 1.72 mm nominal clearance around the MIT assembly. The inner diameter of the codisposal canister is 409.3 mm.

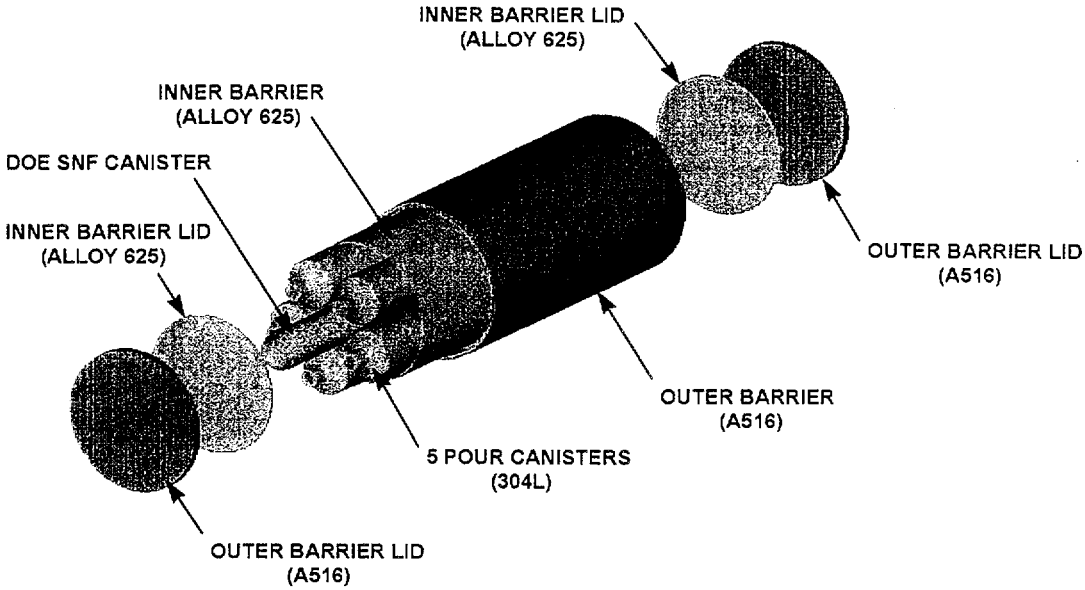

Figure D-1. Codisposal Waste Package Assembly

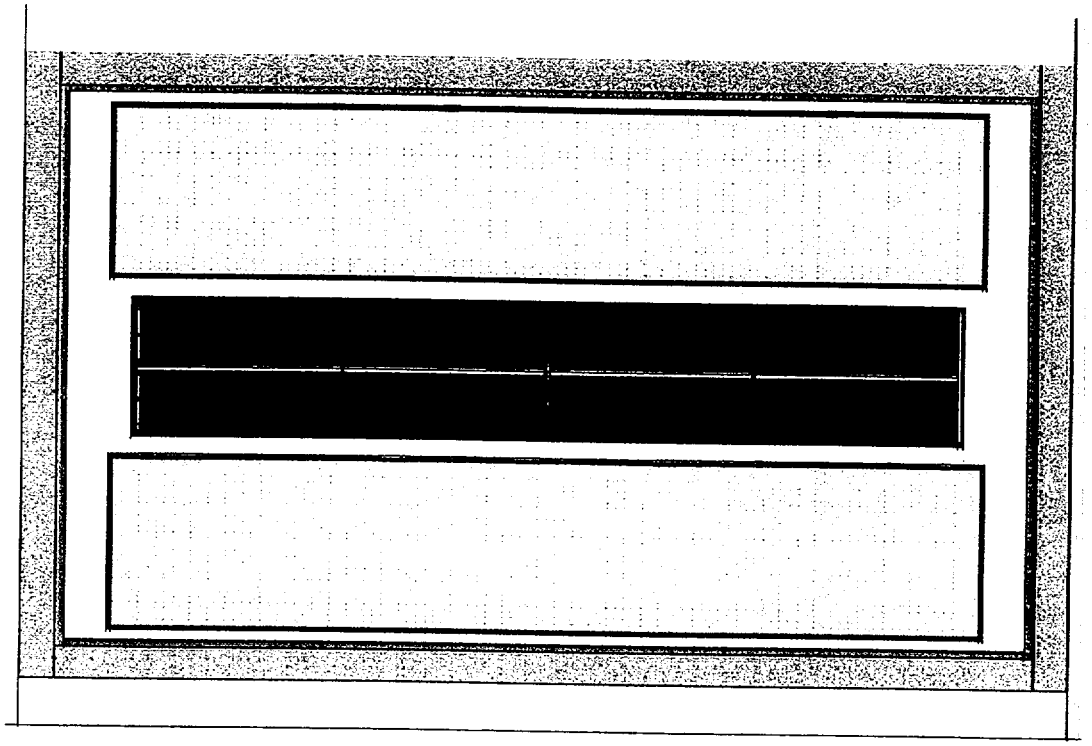

Figure D-2. Longitudinal Cross Sectional View of the Codisposal Waste Package

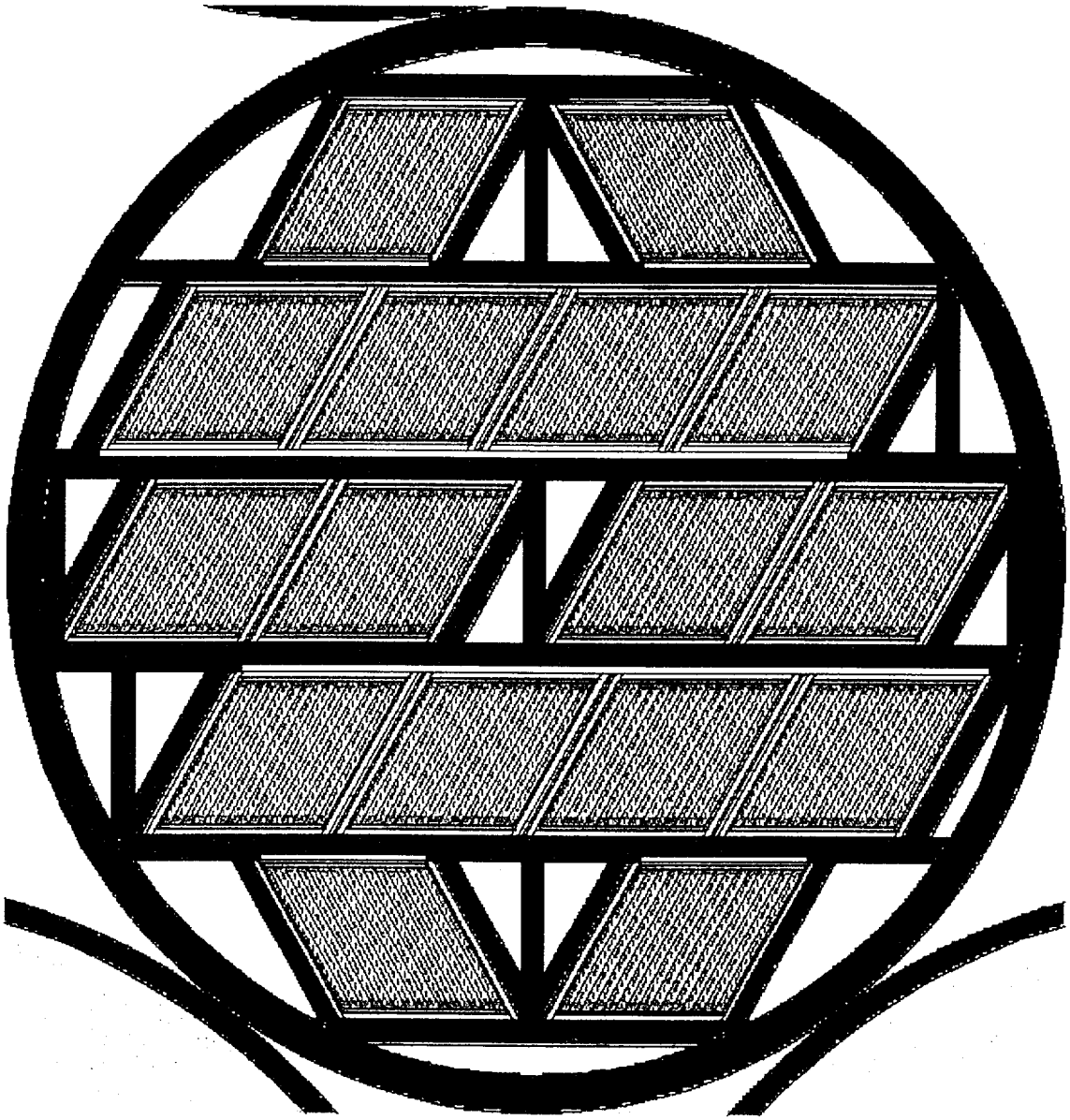

Figure D-3. MIT SNF Canister Radial Cross Sectional

2.0 DEVELOP CONFIGURATION CLASS DEFINITIONS

2.1 INTERNAL CONFIGURATIONS

The degraded mode internal criticality analyses for MIT SNF have covered the range of possibilities, so it is possible to identify those scenarios/configurations which can lead to criticality.

2.1.1 Identify Applicable Scenarios

The degradation scenarios start with the intact configuration; the cross section is shown in Figure D-4. The codisposal waste package for this waste form contains a significant amount of glass; the principal degradation product of glass is silica, which can produce a clay with enough hydration to provide the moderator necessary for criticality. Therefore, standing water is not necessary for criticality, and any of the standard internal scenarios, shown in Figure 3-1 in the main report, could lead to a criticality. However, this waste form will degrade faster than the basket in the DOE SNF canister, so scenarios IP-2 and IP-3 should be removed from further consideration.

2.1.2 Identification of Configuration Classes

The following are the configuration classes that could lead to criticality for the MIT SNF waste form in the codisposal waste package CRWMS M&O 1998a (with references to the configuration class designations in Figure 3-1 in the main report):

1. Degraded SNF, intact basket, and flooded DOE SNF canister. This is the third configuration class listed in Subsection 3.1.1. This is an example of configuration IP-1a, and it is shown in Figure D-5 for the MIT SNF codisposal waste package.

2. Fully degraded with most of the U settled to the bottom of the waste package. This is the fourth configuration class listed in Subsection 3.1.1; it consists of configurations IP-5a, 6a. The scenario leading to this configuration is represented by the sequence of Figures D-6, D-7, and D-8. In this sequence Figure D-6 shows the DHLW glass mostly degraded, but some of the DHLW canisters sufficiently intact to support the largely intact DOE SNF canister near the top of the clay layer, and Figure D-7 shows the DHLW canister shells having sufficiently degraded that they can no longer support the DOE SNF canister, which is still largely intact, and which has sunk to the bottom of the waste package. Figure D-8 is a representation of configurations IP-5a, 6a.

3. Fully degraded with most of the U in a layer on top of the clay filling most of the waste package. This is the fifth configuration class listed in Subsection 3.1.1. It consists of configuration IP-4b. As with the previous configuration, the scenario leading to this configuration starts with Figure D-6. It is followed by the configurations shown in Figures D-9 and D-10. In this sequence Figure D-9 shows the DOE SNF canister mostly degraded, but still supported by steel shells of DHLW canisters. Some of the uranium from the degraded SNF has spread across the top of the clay. Holes in the bottom of the waste package have drained some clay which, therefore, has a lower level than in the previous figures.

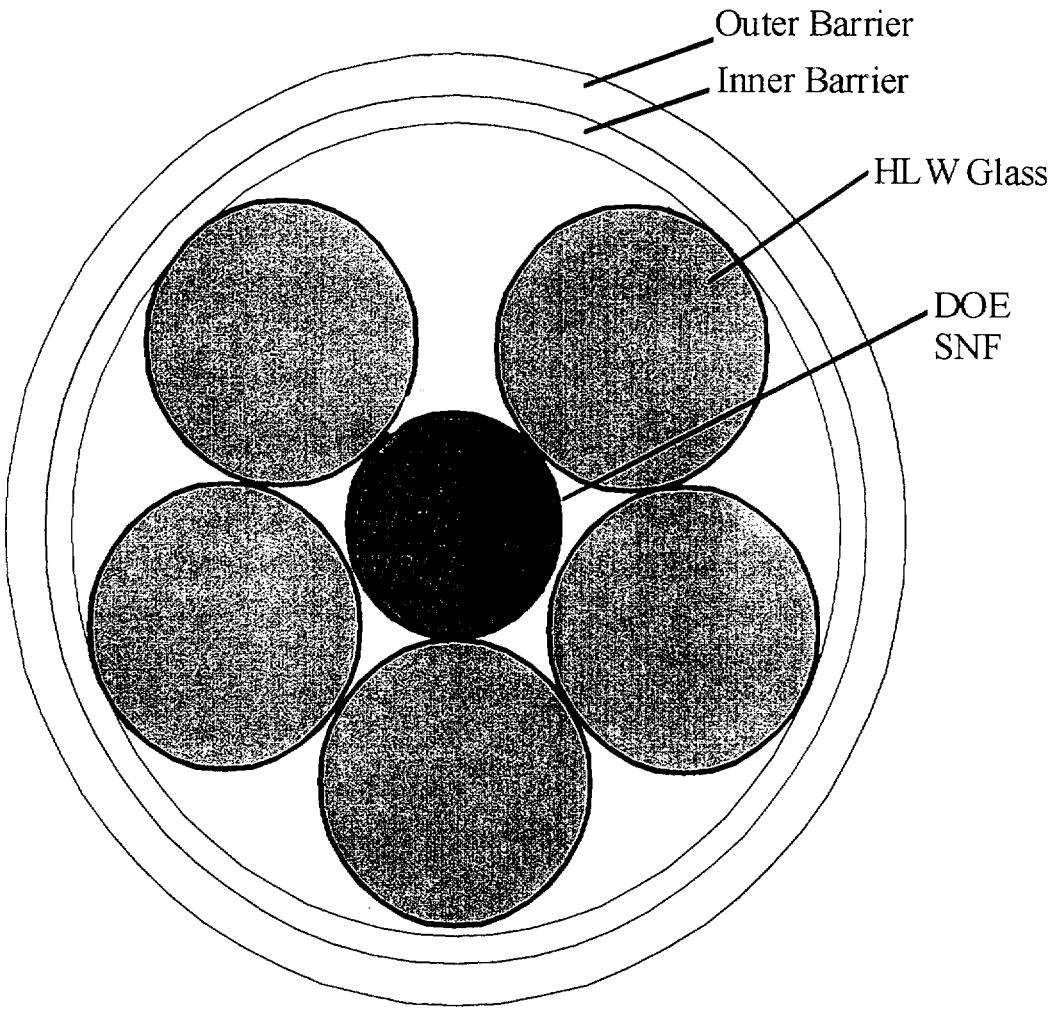

Figure D-4. Intact Codisposal Waste Package with MIT SNF Canister, Radial Cross Sectional View

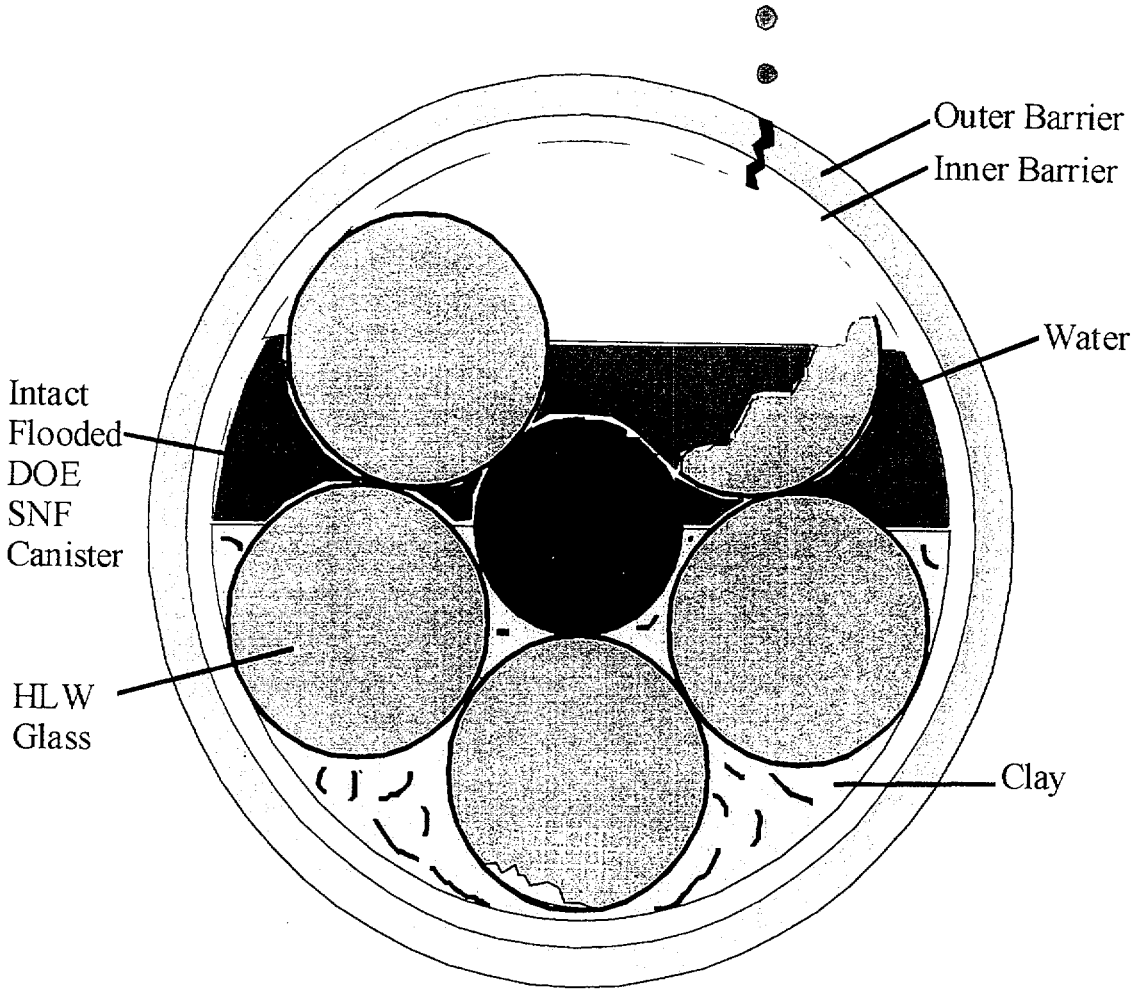

Figure D-5. Water Covering the DOE SNF Canister, Which is Penetrated but Still Largely Intact, so that it is Filled with Water

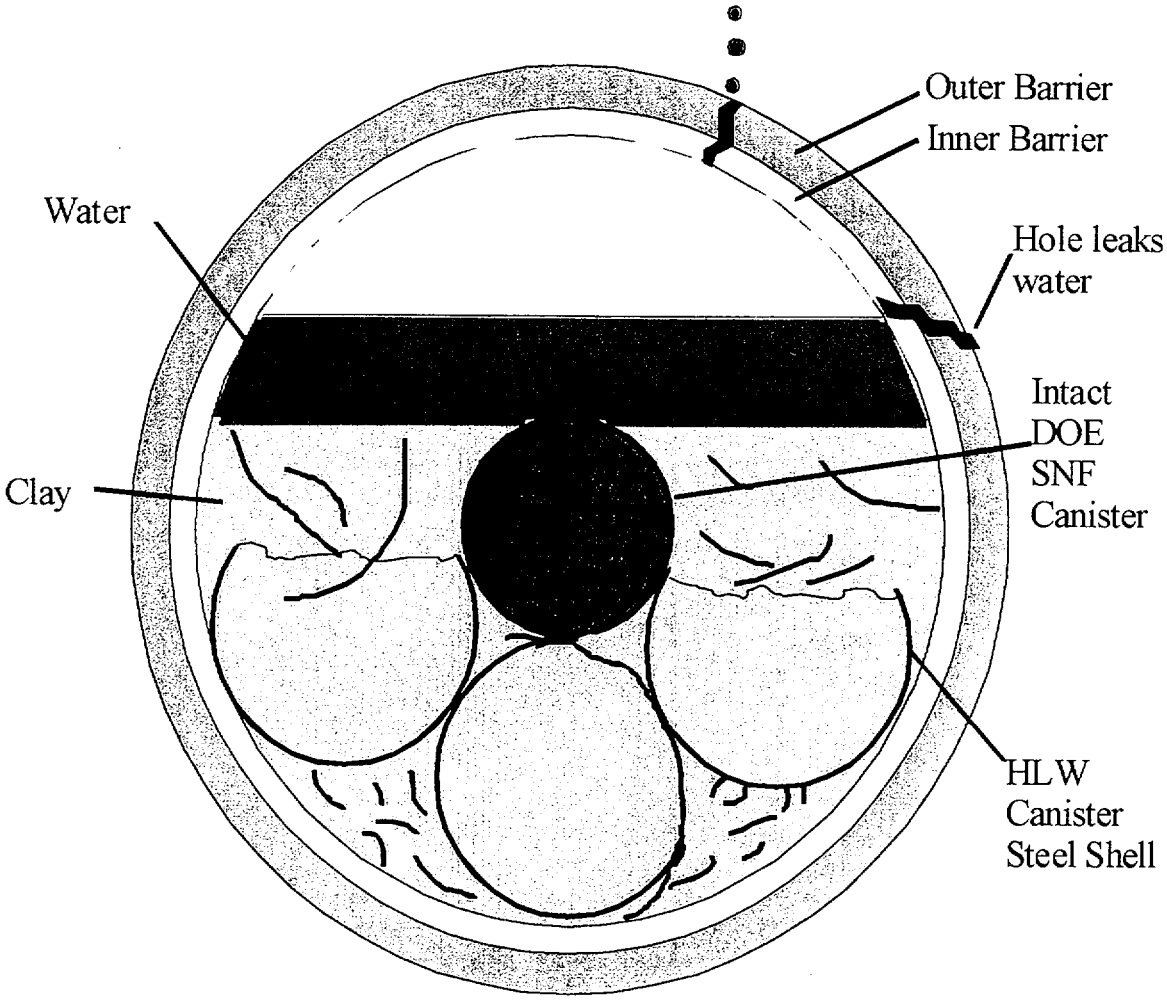

Figure D-6. Departure Point for the Ending Configurations that will have the Fissionable Material in a Layer (Top or Bottom)

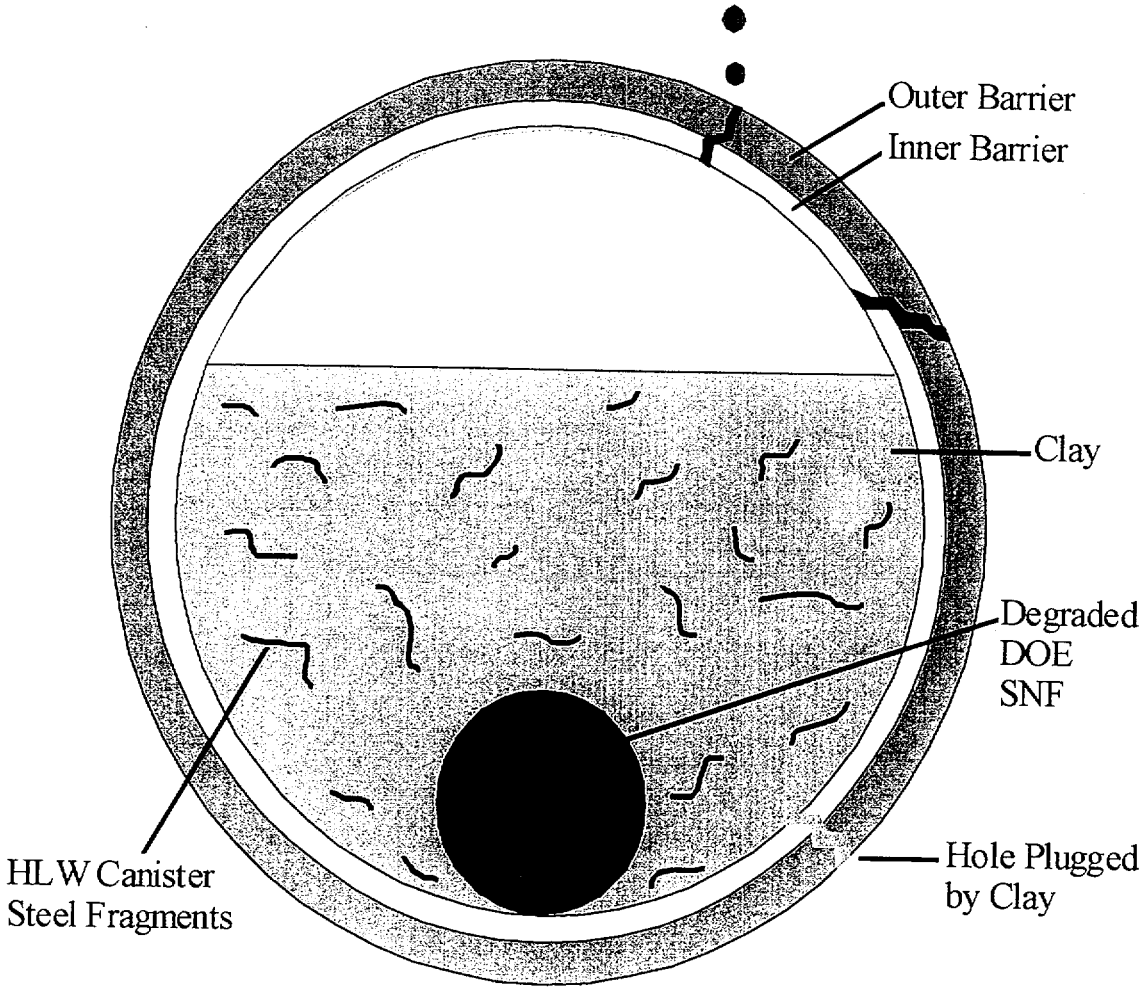

Figure D-7. Intermediate Configuration Leading to Fissionable Layer at Package Bottom

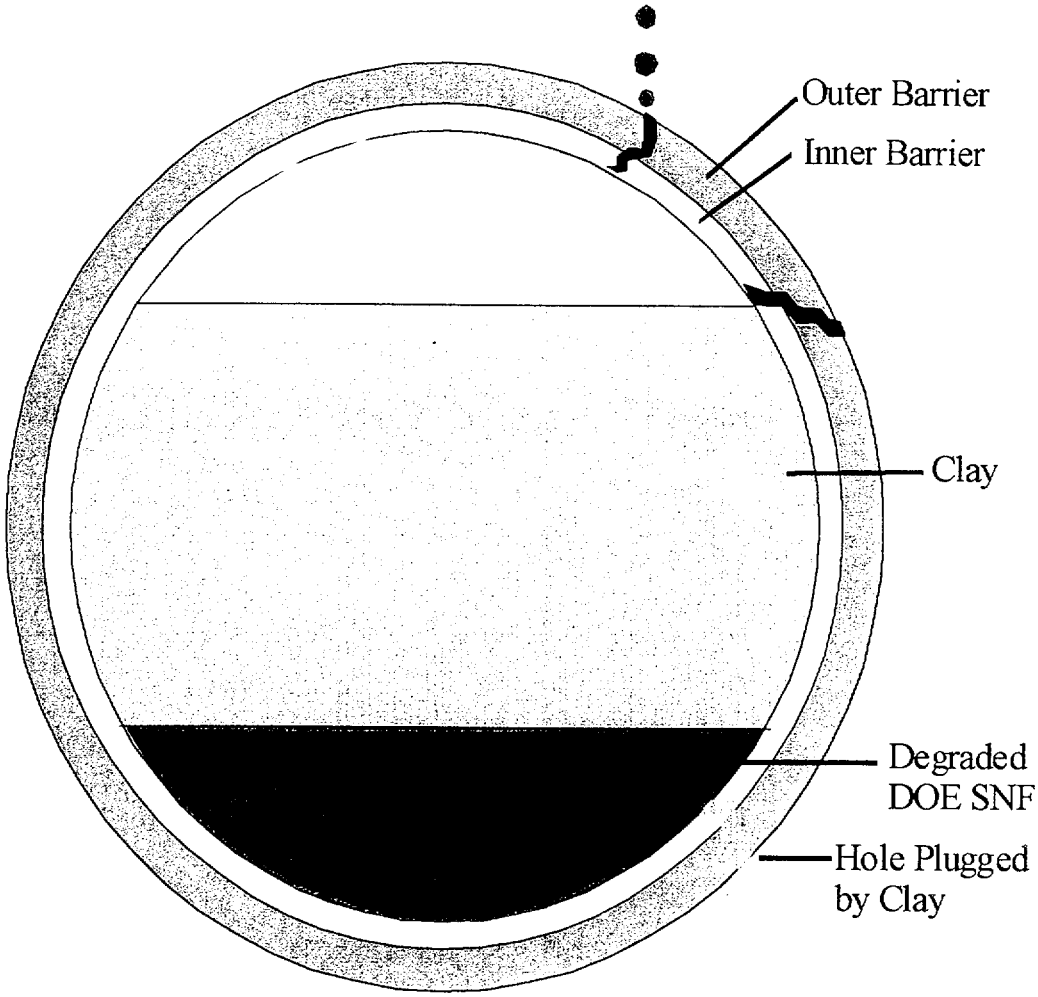

Figure D-8. Uranium from the Degraded SNF is Mixed with Clay and Spread Across the Bottom of the Waste Package

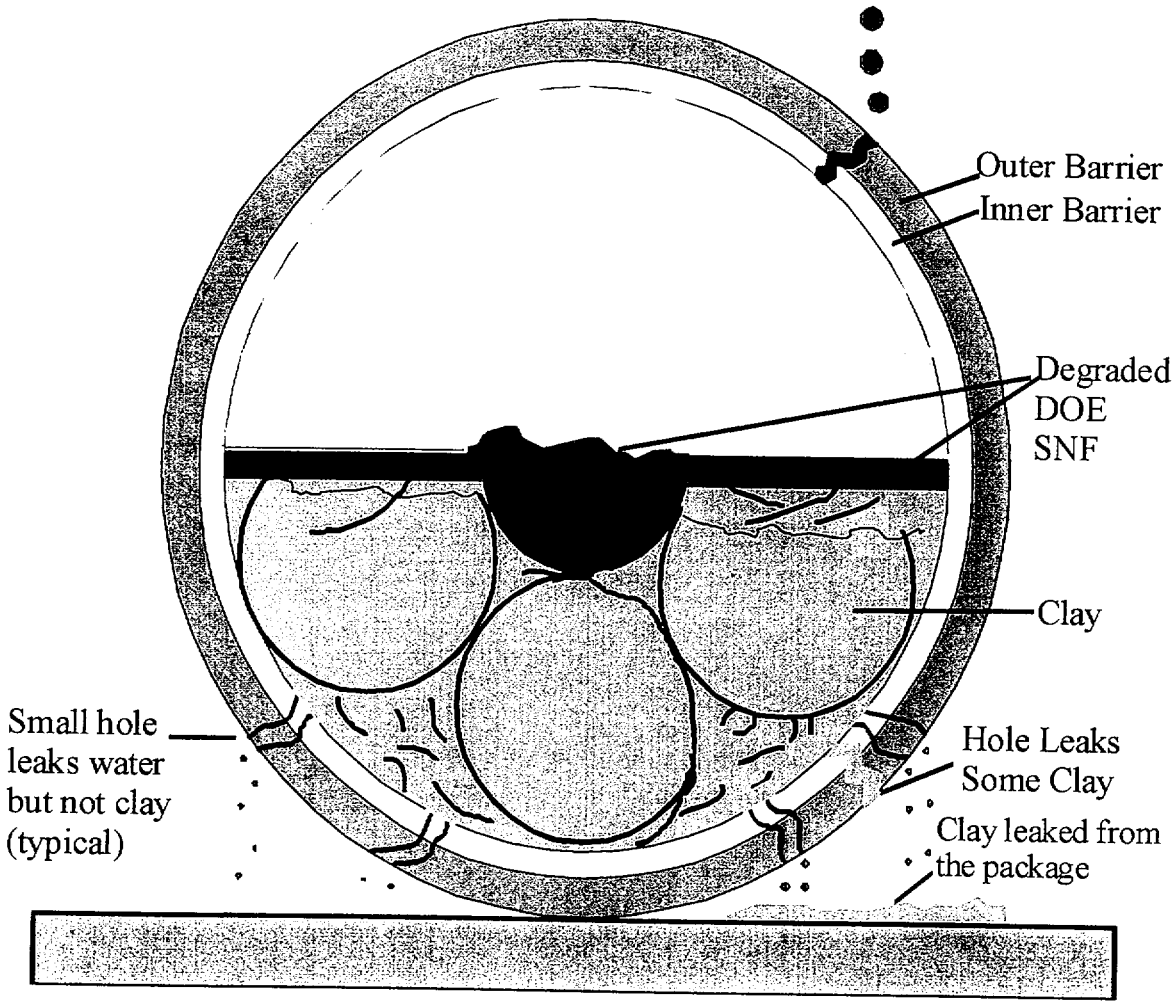

Figure D-9. Intermediate Configuration Leading to Fissionable Layer on Top

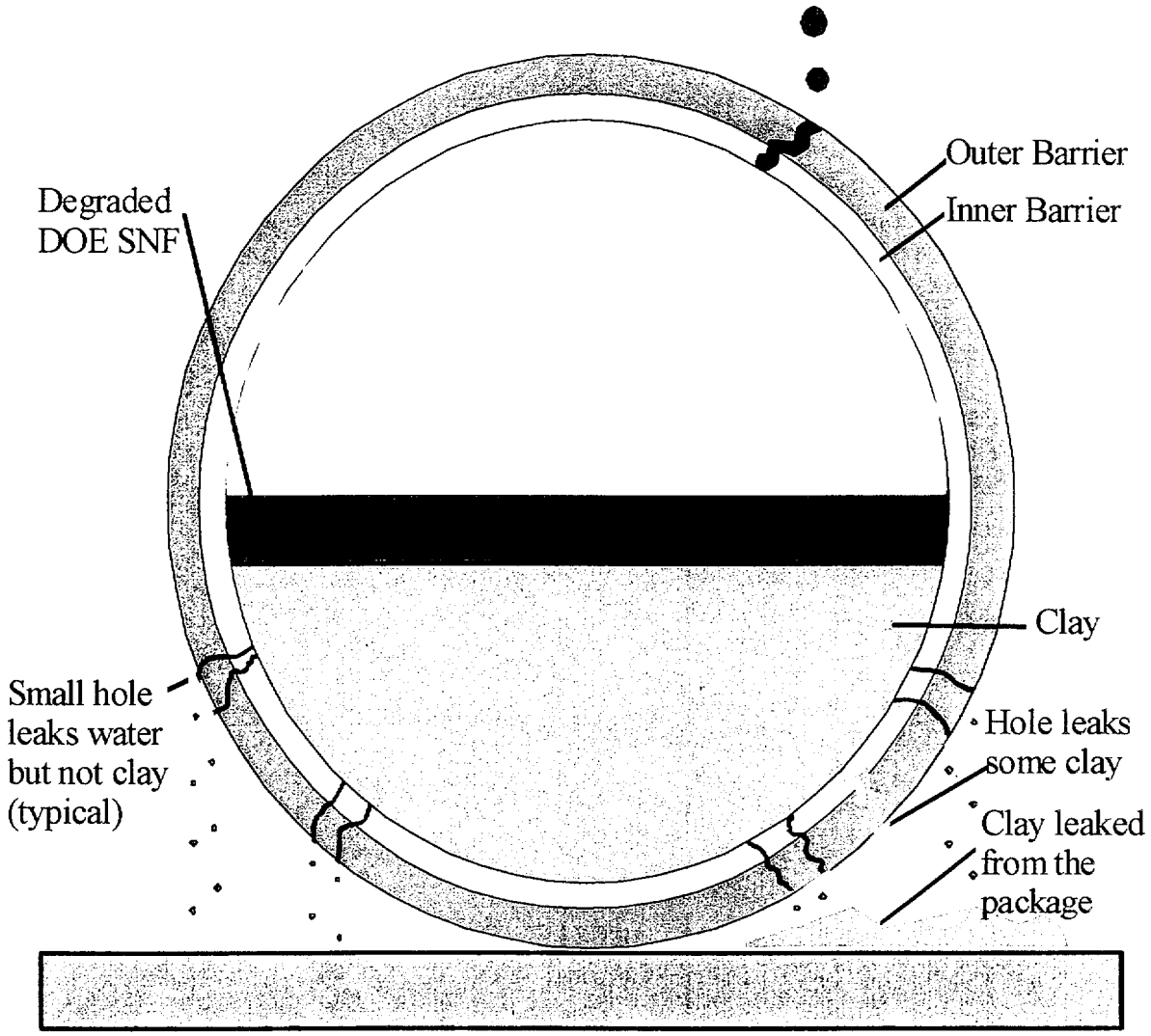

Figure D-10. DOE SNF Canister Has Completely Degraded and all the Uranium Spread Across the Top of the Clay

2.1.3 Configuration Specification: Parameter Ranges

The principal parameter for configuration IP-1a is the amount of neutron absorber. The cases evaluated for the recommended absorber, gadolinium (Gd), cover the range from 0 to 1.5 kg (CRWMS M&O 1998a). Since the canister is assumed to be fully flooded in this configuration, the amount of water is not a significant parameter.

The principal parameters for the remaining configurations, fully degraded with the uranium in a mixture with clay, are the amount of neutron absorber, the amount of iron oxide, and the amount of water in the uranium-clay mixture. For the configurations having most of the uranium settled to the bottom of the waste package (IP-4b, 5a, 6a), criticality can occur for Gd concentrations below 0.05 kg at water fractions ranging from 0.2 to 0.33. For the configuration with most of the U distributed throughout the clay (IP-4a) there is no range of these parameters that is critical.

2.2 EXTERNAL CONFIGURATIONS

There has not yet been any external criticality evaluation for MIT SNF. The external criticality evaluation for this waste form will be done as part of the license application. It will include configurations similar to those discussed in Appendix C, for commercial SNF.

3.0 CRITICALITY ANALYSIS

3.1 EVALUATION OF CRITICAL CONFIGURATIONS

The information presented in this section is a summary of the criticality evaluation of degraded mode configurations (CRWMS M&O 1998a).

3.1.1 Degraded SNF, Intact Basket, and Flooded DOE SNF Canister

Extensive criticality evaluations of this configuration (IP-1a) showed that it was most reactive with no corrosion of the basket at all. Corrosion of the basket would release iron oxide, which would displace water and reduce the reactivity. Since the corrosion of the aluminum matrix of the fuel will expand on corrosion (oxidation), it is possible that the ^{235}U will be dispersed with it. The worst case of this configuration then becomes that with the ^{235}U being uniformly distributed throughout the volume of the DOE SNF canister, while the basket remains intact. The resulting criticality for various amounts of the neutron absorber distributed in the basket is given by Table D-1.

Table D-1. Degraded MIT SNF in an Intact Stainless Steel Basket with Gd Absorber

Mass Gd (kg)	$H/^{235}U$	$k_{eff} \pm 2\sigma$
0.25	113	0.9763 ± 0.0027
0.50	113	0.9458 ± 0.0032
0.75	113	0.9294 ± 0.0027
1.00	113	0.9195 ± 0.0030
1.50	113	0.9020 ± 0.0024

The variation in the mass of Gd shown in Table D-1 was modeled as different initial loadings of Gd, but it could also approximate the loss of some initial Gd by some corrosion of the part of the basket that would be carrying it. These results indicate that criticality will be prevented by loading at least 0.75 kg of Gd.

3.1.2 Fully Degraded with U in the Bottom Layer

This general configuration has two layers. The bottom layer contains uranium oxide mixed with clay (or in the form of a clay mineral) while the upper layer contains only clay. The concentration of clay in the bottom layer was characterized by the percent of the total clay contained in that layer. This percent was varied from 0 to 100 percent, and the maximum k_{eff} was found to occur for 15 percent. The relative effects of gadolinium and iron oxide were then evaluated for this configuration containing 15 percent of the total clay in the bottom layer. Some of the more interesting results are summarized in Table D-2.

Table D-2. Gd and Fe_2O_3 Masses in the Bottom Layer Permitting Near Criticality

Gd Mass (kg)	Fe_2O_3 Mass	$H/^{235}U$	$k_{eff} \pm 2\sigma$
0.05	0	313	0.9621 ± 0.0025
0.10	0	313	0.8959 ± 0.0025
0.02	295	312	0.9537 ± 0.0022
0.04	295	312	0.9257 ± 0.0023
0.00	590.5	312	0.9257 ± 0.0023

Comparing the first and second lines of this table, or third and fourth, it is seen that for low masses of iron oxide even small amounts of gadolinium are very effective in reducing k_{eff}. However, the fifth line shows that with a large enough iron oxide mass, criticality can be prevented, without any gadolinium at all. It should be noted that Table D-2 does not suggest that the degraded waste package will become critical; it is extremely unlikely that gadolinium and iron oxide loss from the waste package, or segregation out of the bottom layer would be so large as to leave such small masses in the bottom layer.

The extensive criticality evaluations also included the influence of water fraction in the uranium-clay mixture (CRWMS M&O 1998b, Subsection 7.3.1.3). The peak k_{eff} has been found to occur when the water content of the uranium-clay mixture is 25 percent by volume.

3.2 CRITICAL LIMIT

The critical limit will be determined by the same methodology and policy as is currently being developed for commercial SNF. The complete analysis has not yet been performed for this waste form, but an estimate of 0.93 has been made, based on evaluation of 47 criticality calculations compared with benchmark experiments for the intact SNF, and based on 119 high enriched uranium nitrate experiments for the degraded SNF (CRWMS M&O 1998a). Since there will be no burnup credit request for MIT SNF, the bias and uncertainty will be no greater than that for commercial SNF.

3.3 CRITICALITY REGRESSION

Because the maximum fissile loading is used (no blending of low burnup with high burnup) in the MIT SNF study, and because the internal configuration classes for the design met the

CL criterion test used in the example, there was no regression developed to refine the criticality evaluation. It may be necessary to develop a regression for the external criticality evaluation.

4.0 PROBABILITY EVALUATIONS

4.1 PROBABILITY ESTIMATION

Since this study was able to identify a criticality control material, $GdPO_4$, which was determined to be insoluble over all chemical conditions of interest, it was not necessary to perform a probabilistic analysis. Nevertheless, an estimate of criticality probability is of interest to be able to assess the benefit of this material compared more common, but more soluble, neutron absorbers.

This comparison is given in Table D-3 for criticality occurrence during a 60,000 year period, most likely near the end of the period. The first line of this table gives the conditional probabilities for the occurrence of a geometry and geochemistry which removes the neutron absorber which was calculated in CRWMS M&O 1998a, Subsections 6.4.3 and 6.4.4.1. For purposes of illustration, the time period covered by these probabilities is taken to be 40,000 to 60,000 years. As explained in CRWMS M&O 1998a, Subsection 6.4.3, for times greater than 8,600 years, the conditional probability of boron loss, given the required dripping and collection of water in the DOE SNF canister, is conservatively estimated as 1. For Gd_2O_3, however, the 60,000 years coincides with the shortest time to achieve low pH and high Gd solubility, as given by the analysis in CRWMS M&O 1998a, Subsection 6.4.4.1, and the probability that the low pH solution will contact the gadolinium remains as calculated in that section. The conditional probability of zero (within the precision of this analysis) in the third column ($GdPO_4$) reflects the geochemistry analysis that indicates that $GdPO_4$ will be almost completely insoluble over the pH range of interest (CRWMS M&O 1998a, Subsection 6.3.4.2), so that it remains in the waste package providing criticality control. This zero probability also reflects the limitation on the amount of physical separation between absorber material and fissionable material which is shown by the analysis of CRWMS M&O 1998a, Subsection 6.4.4.2.

The probability used in all three cells of the second line of Table D-3 is the product of three probabilities: (1) the probability that a particular waste package will be dripped on (0.3), (2) the conditional probability that the waste package will not be penetrated from the bottom before it is penetrated from the top, given that it is dripped on (0.5), and (3) that the bottom will not be penetrated for at least 8,600 years, the time required to corrode the borated stainless steel and flush out the dissolved boron, (0.93). These probability numbers are based on a simplified approximation to the more elaborate analysis used in Appendix C, Subsection 1.3.2 (particularly Figure C-10 with the conservative assumption of twice the current percolation rate of 6 mm/yr) and Section 1.4.1 (particularly Figure C-13).

The combined probabilities of criticality, in the third line of Table D-3 are the products of the first two lines. It should be noted that the probabilistic analysis given here is greatly simplified from that used in Appendix C; the only intention here is to show the relative effectiveness of the alternative criticality control materials.

Table D-3. Probabilities (per Waste Package) of the Occurrence of Potentially Critical Configurations for Alternative Criticality Control Materials

Description of System Element	Probabilities for Alternative Criticality Control Materials [1]		
	Boron	Gd_2O_3	$GdPO_4$
Conditional probability of a geometry and geochemistry which removes the indicated neutron absorber (given the required drip rate)	1.0	0.0725	0
Probability of required drip rate (on any given package) and retention of sufficient water for moderator (same for all alternatives)	0.14	0.14	0.14
Combined probability of criticality (per waste package of this type)	0.14	0.01	0

[1] These are very conservative estimates and should be used for comparison of alternatives only.

4.2 PROBABILITY CRITERION

Since $GdPO_4$ has been determined to be satisfactory for a deterministic demonstration of criticality control, there is no need for a probability threshold screening. A threshold may be needed for the external criticality evaluation.

5.0 CRITICALITY CONSEQUENCE EVALUATION

Since $GdPO_4$ has been determined to be satisfactory for a deterministic demonstration of criticality control, there is no need for a criticality consequence evaluation. Such an evaluation may be needed for external criticality.

6.0 RISK EVALUATION

Since there was no consequence evaluation, there can be no risk evaluation.

7.0 CONCLUSIONS

7.1 ACCEPTABLE REPOSITORY SYSTEMS

Since 1.25 kg of $GdPO_4$ was shown to prevent criticality under the worst case circumstances (CRWMS M&O 1998a, Subsection 6.5.1.3), the proposed disposal scheme is acceptable.

7.2 AUGMENTING CRITICALITY CONTROLS

The analyses of CRWMS M&O 1998a considered the suitability of boron and Gd_2O_3 as well, since they are more common and less expensive materials. It was found that gadolinium is preferred over boron, as the neutron absorber for criticality control, because it is much less soluble over the expected range of pH values. Furthermore, Gd-phosphate is preferred over Gd-oxide because it is less soluble, particularly in the mildly acidic regime which could result from the corrosion of stainless steel.

7.3 LOADING CURVES

Although the individual assemblies of this fuel type may have somewhat different burnups, there is no intention to seek burnup credit for the following reasons: (1) the records relating to individual assembly history have not been accurately kept for some SNF in this category; and (2) the burnup is small compared to the initial reactivity. Since all assemblies will be assumed to have the same initial enrichment and burnup, there is no need for a loading curve for the MIT SNF.

8.0 REFERENCES

CRWMS M&O (Civilian Radioactive Waste Management System Management and Operating Contractor) 1998a. *Evaluation of Codisposal Viability for Aluminum-Clad DOE-Owned Spent Fuel: Phase II Degraded Codisposal Waste Package Internal Criticality.* BBA000000-01717-5705-00017 REV 01. Las Vegas, Nevada: Author. MOL.19980616.0098.

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