



**Department of Energy**  
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Yucca Mountain Site Characterization Office  
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QA: N/A

**NOV 19 1999**

OVERNIGHT MAIL

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**U.S. DEPARTMENT OF ENERGY (DOE) RESPONSE TO U.S. NUCLEAR  
REGULATORY COMMISSION (NRC) REQUEST FOR ADDITIONAL  
INFORMATION ON THE DOE TOPICAL REPORT ON DISPOSAL CRITICALITY  
ANALYSIS METHODOLOGY**

Reference: Ltr, Reamer to Brocoum, dtd 8/18/99

The NRC provided DOE with a Request for Additional Information (RAI) on our Disposal Criticality Analysis Methodology Topical Report (YMP/TR-004Q). We appreciate the NRC's detailed review that resulted in the RAI (reference).

We have developed responses to your questions and are submitting them for your review as Enclosure 1. Draft responses were discussed with your staff at a technical exchange on October 5 and 6, 1999, and during a follow-up teleconference on October 22, 1999. These discussions have helped clarify the information requested in the RAI and have helped ensure our responses will facilitate the issuance of the NRC's Safety Evaluation Report (SER) as we discussed with your staff.

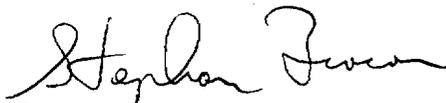
The central issue reflected in many of the RAI items is the demarcation between methodology and application of the methodology. While the Topical Report provides some examples of how the methodology would be applied, we are only seeking acceptance of the methodology (i.e., design criteria and approach to model validation), acceptance of validated models and actual analyses will be sought in the Validation Reports and License Application. In our responses to the RAI, we have attempted to clarify the distinction between methodology and application.

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During the technical exchange, your staff requested clarification on particular aspects of the disposal criticality analysis methodology discussed in DOE's Topical Report for which DOE seeks acceptance. The DOE recognizes that Section 1.2 of the report seeks acceptance of more aspects of the methodology than the NRC can provide in the near term based on information presently available. Therefore, we are providing, in Enclosure 2, a description of aspects for which near-term acceptance is sought. The DOE plans to seek acceptance of additional aspects of the methodology through a revision to the Topical Report planned for submittal late in Fiscal Year 2000.

We stand ready to work with your staff to address any remaining questions requiring resolution prior to issuance of the SER, if needed, and we would be glad to support another technical exchange to help resolve RAI items and expedite the SER process.

Please feel free to contact Paige R. Russell at (702) 794-1315 or April V. Gil at (702) 794-5578 should you have any questions or wish to discuss this matter.



Stephan Brocoum  
Assistant Manager, Office of  
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OL&RC:AVG-0240

Enclosures:  
As stated

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ORIGINAL SIGNED BY

*Stephan Brocoum*

Stephan Brocoum  
Assistant Manager, Office of  
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## ENCLOSURE 1

### **U.S. Department of Energy (DOE) Responses to Requests for Additional Information Developed by the U.S. Nuclear Regulatory Commission (NRC) on DOE's *Disposal Criticality Analysis Methodology Topical Report*, YMP/TR-004Q, Revision 0**

The following are DOE's responses to the NRC's requests for additional information (RAIs) on the *Disposal Criticality Analysis Methodology Topical Report*.

#### **Chapter 1.0 Introduction**

*RAI 1-1 Explain the basis for the following statement: "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 analysis methodology to HLW will be to demonstrate this fact for a few worst-case configurations of moderator and geometry."*

*The sources for the "present information" are not provided. The validity of these statements can only be verified after the indicated information and demonstration analyses have been submitted.*

#### **Response:**

The "present information" referred to that describes the material specifications of the high-level-waste (HLW) glass waste form is preliminary (Stout and Leider 1991, Table 6-14). When the HLW compositions are finalized, the validity of the statement regarding the insufficiency of fissile material will be verified. If, as expected, the content of the HLW material is insufficient to pose a credible risk of criticality (i.e., there is not a sufficient mass of fissionable material in a waste package), DOE plans to use the analysis methodology to demonstrate that fact for a few worst-case configurations of moderator and geometry. If, on the other hand, the content of the HLW material can pose a credible risk of criticality (i.e., there is a sufficient mass of fissionable material in a waste package), the proposed methodology will be applied to the HLW just as it is applied to all other waste forms.

The last two sentences in the footnote were for informational purposes only. They are not significant for justifying the methodology and can be removed. The two sentences will be removed in a revision to the Topical Report.

Stout, R. B. and Leider, H. R. 1991. *Preliminary Waste Form Characterization Report*. Livermore, California: University of California/LLNL. ACC: MOL.19940726.0118.

## **Section 1.2 Objective**

**RAI 1-2** Explain why the Criticality Consequence criterion refers to consequences of only a single criticality event.

*Certain classes of scenarios with common-mode or correlated pathways may lead to criticality of a number of packages over time with a probability that may or may not be much less than that of a single criticality in a single package. Once a certain scenario or pathway is established, criticalities in other similar packages by that pathway or a closely correlated one are not statistically independent. Therefore, in such cases one may need to consider the consequences (and probabilities) of more than one criticality event under this criterion.*

**Response:**

The criticality consequence criterion refers to a single criticality to provide a screening criterion for individual waste forms. This is a coarse criterion intended to identify those design/waste form combinations that can immediately be characterized as requiring a detailed Total System Performance Assessment (TSPA) evaluation. It is expected that most design/waste form combinations will pass this screening. However, criticality consequences may subsequently be identified with an unacceptably large contribution to the overall dose at the accessible environment (the ultimate consequence, determined by the TSPA). DOE plans to add this feed of all criticality consequence results to the overall TSPA to the Overview (Figure 1-1) when the Topical Report is revised. Attachment B shows an updated version of the overview figure.

DOE plans to include consideration of multiple criticality events, including those from common mode failures, in the comprehensive criticality consequence evaluation performed in connection with TSPA. It should be noted, however, that a major source of common mode failure is either a design or manufacturing defect. DOE expects to be able to show that the probability of such a defect is very small (e.g., CRWMS M&O 1999), and that even if such a defect were to occur, it would not lead to a criticality.

CRWMS M&O 1999. *Analysis of Mechanisms for Early Waste Package Failure*. ANL-EBS-MD-000023 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: TBD.

**RAI 1-3** Clarify the range of applicability of the methodology discussed in Item G.2, page 1-5.

*The footnote on page 1-1 states that the methodology and processes are to be applicable to all different waste forms (WFs). Item G.2 is inconsistent with this in requesting consideration of the validation process for a limited class of waste forms (i.e., commercial Spent Nuclear Fuel (SNF)).*

**Response:**

As stated in the Topical Report, the planned range of applicability for the methodology is any waste form. However, some elements of the methodology, such as Item G.2, are applicable to specific waste forms. This is discussed in the first paragraph on the top of page 1-4. DOE recognizes that applicability to any given waste form will need to be demonstrated. Item G.2 was intended only for commercial Spent Nuclear Fuel. DOE plans to discuss the requirements that will make up the isotopic model validation process for specific waste forms in separate addenda (in the case of naval fuel) or validation reports. DOE considers demonstration of applicability to any particular waste form to be an application issue and not a methodology issue, and therefore inappropriate for inclusion in the Topical Report.

DOE will modify Item G as follows:

- “G. The criticality model validation process described in Section 4.1.3 is acceptable in general for model validation. Specifically, 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 process will be followed to calculate CL values for specific waste forms and waste packages as a function of the degradation conditions. The applicability of the CL values for postclosure repository conditions will be demonstrated in validation reports which will be referenced in the License Application. NRC acceptance of CL values and their applicability for postclosure repository conditions will be sought in the License Application.”

*RAI 1-4 Explain why a broader range of configurations is not discussed in Item J.1, page 1-5.*

*The configuration identification process may fail to identify those configurations with the greatest potential consequences, i.e., configurations with potentially positive feedback. Such configurations should be identified using a process, supplementing the existing proposed method, whereby the most significant credible or postulated configurations are first identified and then either eliminated or further considered based on an evaluation of the probabilities of mechanisms that could produce such configurations.*

**Response:**

A “broader range” of configurations was not discussed in J.1 because DOE believes that the range discussed already covers the full spectrum of recognized critical configurations. The process for identifying configurations will trace all recognized movements of fissionable material and, therefore, will fully address credible configurations with the greatest potential consequences. The range of configurations considered includes criticalities inside and outside a waste package (i.e., all locations) and both transient and

steady-state events (i.e., all types). "Configurations with potentially positive feedback" are a subset of the generic transient critical configurations.

The methodology already incorporates the steps asked for in the RAI. Items B and C (page 1-4) describe the process for identifying the credible configuration classes from the standard scenarios. Item C (page 1-4) covers using the potential mechanistic processes to determine which configuration classes can exist, and Item E (page 1-5) covers determining the probability of the potentially critical configuration classes.

The Topical Report does not fully specify the parameter ranges for the standard scenarios or the resulting configuration classes. DOE believes that specification of the parameter ranges is an application issue and not a methodology issue. Nevertheless, DOE intends that they be comprehensive and that they include configurations of the kind suggested by this RAI. For example, DOE intends to evaluate the probability of all configurations that have been identified as potentially autocatalytic in published articles.

### *Section 1.3 Scope*

*RAI 1-5 Explain why the scope of the TR does not correspond to the methodology and processes actually described in the TR.*

*The methodology and processes discussed in the Topical Report were developed primarily with commercial Light Water Reactor (LWR) fuel in mind. In addition, the LWR discussions are mostly restricted to Pressure Water Reactors (PWRs), with little consideration of the Boiling Water Reactors (BWRs). The staff expects to see numerous exceptions and differences in the methodologies ultimately used for naval Spent Nuclear Fuel (SNF), other U.S. Department of Energy (DOE) SNF, other highly-enriched materials, graphite-moderated fuel, and vitrified High-Level Waste (HLW). The acceptability of the methodology described in the Topical Report to the broad variety of waste forms (e.g., all 250 DOE SNF types) cannot be established in this review.*

Response:

The scope of the Topical Report is primarily to describe a methodology for predicting the potential for, and the consequence of, criticality during the postclosure period of the geologic repository. The methodology described in Chapter 3 of the Topical Report is intended to be applied to all types of spent nuclear fuel (SNF) and high-level waste (HLW) expected at the repository. General NRC acceptance is requested for the process (methodology) described in Chapter 3 of the Topical Report. Some of the information presented in Chapter 4 is related to the methodology, as discussed in subsequent RAI responses. Other parts of Chapter 4 are related to application of the methodology and will be addressed in validation activities and future revisions of the Topical Report. The individual RAI responses applicable to Chapter 4 clearly state for which aspects of the chapter acceptance is being sought. PWR fuel data are used throughout the Topical Report as an example spent fuel type to illustrate application of the generalized

methodology. The examples and waste form-specific items will be removed from the main body of the Topical Report, or more clearly labeled, when it is revised. Once this is done, the scope in Section 1.3 will be consistent with the remainder of the report.

It is expected that differences in the details of specific methodology components will occur with application to different spent fuel types. DOE recognizes that applicability to any specific waste form will need to be demonstrated. However, DOE believes demonstration of applicability to a specific waste form is an application issue and not a methodology issue. DOE plans to provide validation of the methodology components for each of the waste forms, with the exception of naval SNF, in validation reports. The planned workscope for a commercial SNF validation report is given in Attachment A to this response. The classified Addendum to the Topical Report which addresses naval fuel, was issued to the NRC on October 29, 1999. This addendum contains both a description of the methodology to be used, as well as information that DOE believes demonstrates that naval fuel can be successfully analyzed within the repository environment. Thus, DOE believes the addendum provides a comprehensive demonstration that the methodology is appropriate for and applicable to analysis of naval SNF in the Yucca Mountain environment.

#### **Section 1.4 Quality Assurance**

*RAI 1-6 Clarify the statement that "the information presented in this topical report is not design information that can be used to support procurement, fabrication, or construction." with respect to Quality Assurance.*

*If the methodology is formulated (e.g., specifying critical limit, dismissing configurations not having potential for criticality, etc.) based on the data presented in this report, and the design of the criticality control systems in the waste packages (WPs) is based on this methodology, it is not clear how these data are not used, directly or indirectly, in the design of the waste package. In particular, some of the references (e.g., CRWMS M&O 1998e) state that "this document will not directly support any DOE Office of Civilian Radioactive Waste Management (OCRWM) construction, fabrication, or procurement activity and therefore is not required to be procedurally controlled as to be verified (TBV)."*

Response:

Development of the Topical Report was subject to DOE Office of Civilian Radioactive Waste Management (OCRWM) Quality Assurance Requirements Description (QARD) controls (DOE/RW-0333P). The purpose of the statement in question was to note that the methodology documented in the Topical Report can not be used directly for procurement, fabrication, or construction activities in accordance with the procedures implementing the OCRWM QARD. The procedures implementing the QARD controls require design information for those activities to be controlled in drawings and specifications supported by design analyses. The Topical Report provides an analysis methodology, but it does not provide drawings or specifications, and so by procedure

does not (directly) support procurement, fabrication, or construction. The Topical Report and its internally developed supporting calculations, analyses, and technical reports were prepared in accordance with the procedures implementing the QARD requirements. The use of the methodology from the Topical Report in design analyses supporting drawings or specifications would be acceptable from the standpoint of the procedures implementing the QARD. DOE plans to use the methodology in the Topical Report, when accepted, in design analyses that will be used to generate drawings and specifications which in turn will be used to support procurement, fabrication, and construction. The statement in the QA Section of the Topical Report was not intended to imply a quality assurance deficiency but rather to reflect limitations on use of a methodology document in accordance with procedures.

*RAI 1-7 Specify what part of the Actinide-Only Burnup Credit Topical report is used in this topical report.*

*The "Topical Report on Actinide-Only Burnup Credit for PWR Spent Nuclear Fuel Packages (DOE 1997)" has not been approved by the NRC Spent Fuel Project Office.*

Response:

This section of the topical report is required per the OCRWM procedures to note interface issues with the development of this report. The burnup credit issue was considered an internal OCRWM interface issue because two organizations of OCRWM (transportation and disposal) were addressing burnup credit issues with the NRC.

As noted in the topical report (last sentence in the third paragraph of Section 1.4), some of the data and parts of the methodology from the *Topical Report on Actinide-Only Burnup Credit for PWR Spent Nuclear Fuel Packages* are referenced in the *Disposal Criticality Analysis Methodology Topical Report*. The data actually come from second- and third-tier references that both reports reference and not from the Actinide-Only Topical Report referenced in the *Disposal Criticality Analysis Methodology Topical Report*. These data include the chemical assay data and the benchmark criticals (laboratory critical experiments). Because this reference is so indirect and not needed to support the description of the methodology in the Topical Report, DOE will remove the statements that reference the Actinide-Only Topical Report.

### ***Section 1.5 Overview of the Methodology***

*RAI 1-8 Justify the approach used to dismiss configuration classes as having the potential for criticality based on an evaluation of a given configuration with parameter values at some selected points for each of the configurations (Figure 1-1).*

*If configuration classes are dismissed based on evaluation of a given configuration with parameter values at several points rather than examination of*

*full range of parameter values, it is possible to dismiss a configuration or even configuration class, which has potential for criticality. It seems it would be more appropriate to perform the criticality analyses for a full range of parameter value for each configuration, examine those results against the Critical Limit criterion, and then decide if that particular configuration or configuration class is acceptable for disposal from a criticality standpoint.*

Response:

Figure 1-1 requires that configurations be evaluated "for a range of parameters and parameter values." This is from the box above the "satisfy Critical Limit (CL) criterion" decision diamond. The intent of the box above the first decision point in Figure 1-1 is to evaluate the full range of parameter values to prevent a potentially critical configuration from being overlooked. In practice this may include examining only bounding values for certain key parameters and the range of values for other parameters. For example, a configuration class of intact commercial fuel in a waste package may be evaluated with 5 wt% U-235 fuel. If the case satisfied the CL criterion, there would be no need to run the same configuration with 4 wt% U-235 fuel and the same or greater burnup. But if the CL criterion was not satisfied, the configuration class would be considered potentially critical, and additional cases would be run to develop regression expressions (the second box to the right of the satisfy CL criterion decision diamond). The justification for acceptance of a specific configuration is considered an application issue and not a methodology issue. Therefore, the justification will be provided in the supporting documents for the License Application to allow NRC review and concurrence.

The referenced box in Figure 1-1 will be modified as follows:

**"Perform Criticality Analysis ( $k_{eff}$ ) of Defined Configurations (for each class)  
Over the Range of Parameters and Parameter Values"**

As part of the NRC staff's review of the supporting documents for the License Application, DOE assumes that the staff will review the documents, developed based on the methodology from the Topical Report, to verify that the range of parameters and parameter values evaluated in the cases is sufficient to justify dismissing configuration classes.

## Chapter 2.0 Regulatory Perspective

*RAI 2-1 Throughout this section, there are references to Regulatory Guide 3.58. However, it, as well as 3.1, 3.4, 3.43, 3.45, 3.47, 3.57, 3.68, 3.70, and 8.12, has been superseded by Regulatory Guide 3.71, published in August 1998. The references should either be updated or an explanation for the choice to use Regulatory Guide 3.58 should be provided.*

**Response:**

DOE will revise Section 2.3.3 of the Topical Report to replace references to Regulatory Guides 3.4 and 3.58 with reference to Regulatory Guide 3.71 as recommended in the RAI. The section will note that Regulatory Guide 3.71 endorses use of ANS/ANS-8.1-1983, ANSI/ANS-8.10-1983, ANSI/ANS-8.15-1981, and ANSI/ANS-8.17-1984, with certain caveats and exceptions discussed in the Regulatory Guide. The section will then refer to DOE's commitment to these standards as stated in the preceding Topical Report section and will describe DOE's commitment to the Regulatory Guide. Neither the Regulatory Guide nor the standards referenced in it are explicitly applicable to disposal, and some of the referenced standards are clearly inapplicable to the postclosure period. The exceptions DOE proposes to take as noted in the Topical Report will remain. In addition, the revised Topical Report section will note that DOE believes the remaining standards referenced in the Regulatory Guide are inapplicable to postclosure disposal, and, therefore, commitment to them via this Topical Report is inappropriate.

In addition, Chapter 2.0 will be revised to reflect the NRC's new Yucca Mountain regulations at 10 CFR Part 63 if these regulations are issued by the time the Topical Report is revised to address the RAI comments.

**Chapter 3.0 Methodology**

**Section 3.1 Standard Criticality Scenarios**

*RAI 3-1 Indicate how the effects of disruptive events will be considered in the evaluation of potential criticality events in the repository.*

*The scenarios listed in Figure 3-1 and 3-2 appear to be comprehensive for an undisturbed repository. However it is not clear whether the potential effects of disruptive events have been adequately considered. Failure to consider all potential scenarios that could result in a criticality event could result in an underestimation in the probability of a critical event occurring within the repository. Some potential effects of disruptive events include:*

- (a) Seismic events could cause the waste packages to rotate on their invert, potentially allowing corrosion products to be released while the hole in the waste package is facing down. Later, the hole could rotate back to the top of the package, allowing the package to fill with water.*
- (b) A volcanic event, although a low probability event, could fail many waste packages and force their contents into a compact configuration encased in lava at the end of the tunnel.*

**Response:**

Disruptive events (e.g., seismic or volcanic events) are not explicitly included in the standard scenario/configuration class scheme given in Section 3.1 of the Topical Report.

Seismic events are included implicitly, because they deal with configurations already considered in the scheme. The principal potential role for seismic events is the rapid transfer between configurations that could be reached by other mechanisms. If the final configuration has a  $k_{eff}$  above the critical limit, while the initial configuration has a  $k_{eff}$  below the critical limit, then the seismic event can provide a rapid reactivity insertion mechanism leading to a transient criticality.

To explain the treatment of seismic disturbance within the standard-scenario/configuration-class scheme, DOE plans to add the following text as Section 3.1.3 of the Topical Report:

### **“3.1.3 Effect of Seismic Events**

Configurations having  $k_{eff}$  above the critical limit will also be evaluated to determine whether they can be reached from a configuration having  $k_{eff}$  below the critical limit by sudden reactivity insertion due to a seismic disturbance. This evaluation will consist of identifying representative configurations (called seismic predecessor configurations) that could be transformed to the subject configuration by a seismic event. A representative configuration is one that is reached from a scenario that has parameter values specified by probability distributions or taken from the conservative end of the possible range (worst case). The predecessor configurations will have significantly higher gravitational potential energy than the subject final configuration. If there are parameters that can have different worst-case values or ranges (e.g., relative corrosion rates of the waste form and potential chemistry-altering material such as stainless steel), then there will be several representative configurations. The probability of any predecessor configurations will be evaluated together with the probability of the seismic event of sufficient magnitude to take such configuration to criticality. The combined probability will then be used with the estimated transient criticality consequences to develop a transient criticality risk. This risk will be summed over a representative set of seismic events to arrive at an expected risk, incorporating the effects of large seismic events, weighted by suitably small probability.

For internal criticality, the search for predecessor configurations will be performed according to the following guidelines, which apply individually to each of the six internal criticality configuration classes identified in Section 3.1.1 of this document:

1. Mostly degraded basket, with only partly degraded waste form (principally spent fuel assemblies), reachable from scenarios IP-3a, b, c, d. Two types of configurations will be examined for predecessor configurations. The first type of final configuration reachable from a higher energy predecessor configuration has assemblies stacked in their lowest potential energy configuration with little, or no, basket steel between the assemblies. The potential predecessor configurations to be identified are those that have some assemblies displaced vertically (upward) with support by some still-

uncorroded steel basket material. The evaluation consists of calculating the  $\Delta k_{\text{eff}}$  between the predecessor and final configuration and calculating the probability of occurrence of the predecessor configuration.

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

2. Both basket and waste form, mostly degraded, in a sludge of degradation products at the bottom of the waste packages reachable from all scenarios. Analyses thus far have not identified any configurations in this class having  $k_{\text{eff}}$  greater than the critical limit. If such configurations are identified, the search for predecessor configurations will include two types of configurations. Both types of predecessor configurations would have the same composition of solid degradation products as the final configuration, as determined by the geochemistry calculations. The first type of predecessor configuration would differ from the final configuration by having a void in the sludge. The void could be filled with water and it would be supported by some basket remnant. If the  $k_{\text{eff}}$  were increased significantly by removal of this support, the configuration would be further evaluated as a potential sudden-insertion predecessor, including estimation of the probability of occurrence of the predecessor configuration.

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

3. Mostly degraded waste form, only slightly degraded basket, is reachable from IP-1a, b. Most such configurations would have some neutron absorber in the basket material, and such a configuration could not become critical until much of that basket material had corroded or fallen to a configuration removed from the SNF itself. Analyses thus far have not identified any configurations in this class having  $k_{\text{eff}}$  greater than the critical limit. If such configurations are

identified, the search for predecessor configurations will include configurations for which less basket material had fallen away from the SNF. The disruption would then drop additional basket material away from the SNF. Whether there could be physical implementations of this concept would depend on whether enough absorber plate could be removed from the basket by the breaking and falling processes to cause criticality before much of the SNF itself had also fallen to the bottom of the waste package, thereby reducing the reactivity.

Configuration classes 4 and 5 would be similar to class 3 but would pertain to waste packages containing a large amount of HLW glass, as well as the potentially critical waste form.

Configuration class 6 is similar to class 3 and should be examined for potential rearrangements in the same manner.”

The situation for volcanic events is completely different from that for seismic events. If a volcanic event were to occur in the repository and were to impact the waste package, it would likely lead to a configuration quite different from anything in the standard degradation scheme outlined in the Topical Report. It is, therefore, appropriate to provide a completely separate analysis of the volcanic disturbance. To describe the methodology for this separate analysis, DOE plans to add the following text as Section 3.1.4 of the Topical Report.

#### **“3.1.4 Effect of Volcanic Events**

The analysis for the criticality potential of a volcanic event will consist of the following steps:

1. Evaluate the potential for waste package breach due to a volcanic event as a function of the magma temperature and the degree of existing degradation of the waste package barriers. This will include consideration of the probability distributions of all the determining parameters.
2. Evaluate the potential patterns for transport, by magma, of the fissionable material, including consideration of the probabilities of patterns that confine the magma flow versus patterns that disperse the flow.
3. Evaluate the potential for accumulation of fissionable material from the magma flow, including identification of the required geometries and their probability.
4. Evaluate the criticality of any accumulations identified in the previous step, using silica and/or water moderation, depending on the mechanism of accumulation.

It is expected that when the low probability of the occurrence of the volcanic event is combined with the low probability of the conditions favoring criticality in the four steps to criticality listed above, the resulting probability of criticality will

be well below the TSPA screening threshold of  $10^{-8}$  per year for the entire repository.”

DOE believes that analyses of specific configurations, such as items (a) and (b) from the RAI, are application issues and not methodology issues and therefore are not within the scope of the Topical Report. DOE plans to provide these analyses in the supporting documents for the License Application. The following discussion is provided for informational purposes only. The information provided is preliminary and will be updated as necessary with additional evaluations or experiments prior to the License Application.

a) DOE expects to show that the seismic event ground motion at a 200-meter depth would not be sufficient to cause a significant rotation of a horizontally emplaced waste package. DOE also expects to show that by the time of significant waste package degradation there would likely be significant degradation of the drip shield. This, in turn, would be expected to transfer significant pressure from the backfill directly onto the entire circumference of the waste package, thereby greatly inhibiting any rotation. DOE plans to complete all the supporting calculations for the final engineered barrier system (EBS) design in time for License Application.

b) DOE expects to evaluate the potential for criticality of a volcanic event such as specified in this RAI comment (b), using the four-step methodology outlined above. It is expected, however, that the probability will fall below the TSPA screening threshold for the following reasons: (1) Low enriched uranium (which is most of the fissionable material in the repository) is in its most reactive geometry in the intact assembly configuration; (2) There is not much opportunity for concentrating even the high enriched waste forms because there is so much non-fissionable solid material in the waste package that will be transported by the magma along with the fissionable material; and (3) Silica is a much less efficient moderator than water, and once the waste package barriers are fully degraded, there is little probability of accumulating water.

*RAI 3-2 Justify the scenario selection process used to focus on the degraded modes and phenomena that produce the critical configurations of interest.*

*The process as now proposed may not identify and address some scenarios that should be considered. For example:*

*(a) The internal scenarios do not give adequate consideration to criticality at the less-burned ends of the fuel. Even in scenarios where the basket poison material, or absence thereof, is uniformly distributed over the length of the active fuel material, criticality will occur predominantly at the fuel ends. End-effect criticality is made even more relevant by scenarios where fuel and basket poison material are displaced axially relative to one another. Such displacement or shifting would remove poison from where it is most needed, i.e., at the ends.*

- (b) *For external near-field and far-field criticality, more focused consideration should be given to scenarios with potentially positive neutronic feedback characteristics. This could be done by first identifying hypothetical configurations that produce positive feedback effects and then evaluating the credibility or likelihood of mechanisms that might form such configurations. The methodology as now proposed does not seek and address those criticality scenarios that have the greatest potential consequences. Furthermore, the probability criterion for events with potentially high consequences should be lower than that for events with less consequences.*

Response:

The scenario selection process does not focus on generating critical configurations of interest. Rather, the process evaluates what scenarios are mechanistically possible for a given waste form, waste package, engineered barrier, and repository design system. The process will provide input to the processes described in the Topical Report that will evaluate potentially critical configurations. The response to RAI 3-1 contains more on the comprehensiveness of scenario generation process.

DOE believes that the example configurations (a) and (b) noted in the RAI are application issues and not methodology issues and are therefore not appropriate for inclusion in the Topical Report. The following discussion is provided for informational purposes only. The information provided is preliminary and will be updated as necessary with additional evaluations or experiments prior to the License Application.

- a) DOE plans to include axial effects for commercial SNF fuel in the neutronic models. The consideration of axial or "end-effects" is noted in Section 4.1.3.1.4 (2<sup>nd</sup> paragraph, 2<sup>nd</sup> sentence) of the Topical Report in the requirements of the isotopic model. The example with BWR fuel in Appendix C of the Topical Report included accounting for the axial effect with 10 axial nodes (Section 3.1.1). The exact number of nodes to be used is considered an application issue and not a methodology issue, so the number will be justified in the commercial SNF validation reports and referenced in the License Application. DOE also believes that the detailed description of how a feature of one waste form (axial effects for commercial SNF) will be modeled is an application issue and not a methodology issue. DOE plans to revise the Topical Report to state that the criticality model needs to account for specific waste form features like axial burnup in commercial SNF.

With respect to absorber plate displacement for commercial SNF, there is likely to be no room to displace the borated stainless steel plates axially relative to the fuel in the current designs. The absorber plates extend essentially the full length of the fuel assembly cavity in a waste package. The length of the cavity that the plates do not extend to is less than the length of an end plate of a fuel assembly. Configurations involving relative movement between waste form and absorber are covered as part of degradation analysis. For designs that contain control rods, DOE plans to consider means for holding the control rods in place to prevent significant displacement. Again, DOE plans to consider

degraded configurations involving relative movement between control rods and the waste form in the methodology. The only cases for which significant separation of the control rods and waste form could occur are those for which the waste form has degraded. The preliminary results of those example calculations referenced in Appendix C of the Topical Report (Section 3.1.4) indicate the degraded commercial SNF cases are less reactive than the intact fuel cases, and then the control rods may not necessarily be needed.

The displacement cases do not appear to be of much concern for criticality. Cases that are more likely to have potential for criticality are configurations for which preferential corrosion occurs in the plates at one end of a waste package and cases for which there are problems with construction of a waste package (i.e., use of a non-borated plate in a section). The first case will be addressed as part of the degraded analysis and the second case will be addressed in an extension of the early (juvenile) failure analyses. DOE plans to provide complete evaluations in supporting documents for the License Application.

b) As stated in the response to RAI 1-4 and in Section 4.4.1.2 of the Topical Report, credible critical configurations with positive feedback effects (and those without) will be evaluated. The last sentence of this RAI item suggests the need for a lower probability threshold for events with a greater consequence. The probability threshold is not intended to exclude low-probability events from further consideration, so it is not analogous to probability thresholds applied to preclosure safety analyses. The concept of risk, which is the product of criticality probability multiplied by a measure of the criticality consequence, is designed to accomplish this compensation (of probability against consequence). DOE plans to base its licensing argument on the measure of risk, consistent with the requirements of 10CFR63. Therefore, DOE believes there is no need for a probability criterion that varies with consequence.

*RAI 3-3 Explain why a discussion of the fast-fissionable, non-fissile actinides that by themselves can sustain a critical chain reaction is not included in this section.*

*The discussion of fast criticality scenarios in which little or no moderation is required should be extended to include "minor actinides" (see ANSI/ANS 8.15) that by themselves can sustain a critical chain reaction with fast neutrons only. Such actinides are sometimes called "fissile." The TR should indicate how these actinides have been considered with regard to their abundance over time in various waste forms and should discuss the bases for any conclusions about their significance (or lack thereof) to repository criticality.*

Response:

A discussion of criticality scenarios that include "minor actinides" is included in the methodology as described in Section 3.1 of the Topical Report. The methodology addresses "fissionable" isotopes, which covers the minor actinides of concern in ANSI/ANS-8.15. The examples in the Topical Report, which do not specifically address the minor actinides, are not intended to represent the complete application of the methodology. DOE considers addressing specific configurations with the minor actinides

which are fast-fissionable, non-fissile to be an application issue and not a methodology issue. Therefore, this information will be provided in the supporting documents for the License Application.

DOE also believes that discussions of the specific scenarios as suggested in the RAI are application issues and, therefore, are not part of the methodology or appropriate for inclusion in the Topical Report. The following discussion is preliminary and is provided for informational purposes only.

The minor actinides are not expected to be of concern. These actinides have been considered in the past and dismissed as having too low an abundance to sustain a criticality, and it is considered incredible that they could accumulate in significant quantities (Gore et al. 1981; Brookins 1978; Allen 1978).

With earliest breach of the waste package expected to occur in the 50,000-year to 100,000-year time frame, no minor actinides, other than Np-237, are expected to be present in significant quantities for transport, as is illustrated in Table 3.3-1. In addition, their decay products do not affect the inventories of fissile isotopes present to which they decayed. Oak Ridge National Laboratory (Allen 1978) observed that neptunium oxide and americium oxide have such large minimum critical masses that they probably do not present a potential criticality problem. These configurations will be considered as part of the evaluations of external configuration classes.

Table 3.3-1 Minor Actinide Isotopes

Isotope	Half-life (GE 1989)	Critical Mass (kg) <sup>a</sup>	Fraction Present <sup>b</sup>
Np-237	2.14E6 years	45	0.0201
Am-241	432.7 years	-	-
Am-242m	141 years	-	-
Am-243	7.37E3 years	78.9	0.0002
Cm-242	162.8 days	-	-
Cm-243	29.1 years	-	-
Cm-244	18.1 years	-	-
Cm-245	8.5E3 years	3.03 <sup>c</sup>	0.00002 <sup>c</sup>
Cm-246	4.76E3 years	3.03 <sup>c</sup>	0.00002 <sup>c</sup>

a Critical masses are for a system moderated and reflected by granite at 10,000 years. (Allen 1978)

b The fraction of a critical mass present from a PWR assembly burned to 33 GWd/mtU, at 10,000 Years (assuming granite moderated and reflected cases). (Allen 1978)

c Values from Allen (1978) are on an elemental basis; values shown are for a combination of Cm-245 and Cm-246.

- Indicates that essentially all the isotope has decayed by 10,000 years.

Gore, B. F.; Jenquin, U. P.; and Serne, R. J. 1981. *Factors Affecting Criticality for Spent Fuel Materials in a Geologic Setting*. PNL-3791. Richland, Washington: Pacific Northwest Laboratory, April 1981. TIC: 229686.

Allen, E. J. 1978. *Criticality Analysis of Aggregations of Actinides from Commercial Nuclear Waste in Geological Storage*. ORNL/TM-6458. Oak Ridge, Tennessee: Oak Ridge National Laboratory, August 1978, pages 34, 26, 30. TIC: 229251.

Brookins, D. G. 1978. *Geochemical Constraints on Accumulation of Actinide Critical Masses from Stored Nuclear Waste in Natural Rock Repositories*. ONWI-17. Albuquerque, New Mexico: Office of Nuclear Waste Isolation, Battelle Memorial Institute, December 1978. TIC: 227691.

GE (General Electric) 1989. *Nuclides and Isotopes, Fourteenth Edition, Chart of the Nuclides*. San Jose, California: General Electric Company, Nuclear Energy Operations, 1989. TIC: 201637.

### *Section 3.1.2 External Scenarios*

*RAI 3-4 Confirm that far-field configuration classes FF-3c, 3d, and 3e are located in the saturated zone.*

*The text in item 1 of Section 3.1.2 contradicts figure 3-2b in assigning these configurations to the unsaturated zone. The distinction is important in modeling hydrologic and geochemical processes.*

Response:

FF-3c could be in either saturated or unsaturated zones. FF-3d must be in the saturated zone by definition, and FF-3e implies spending some time in the saturated zone in order to reach the Franklin Lake Playa. Item 1 of Section 3.1.2 was not intended to exclude the saturated zone. DOE plans to reword this item as follows:

“1. Accumulation, by chemical reduction, of fissionable material by a mass of organic material (reducing zone) located beneath the repository, at a narrowing of the tuff aquifer, or at the surface outfall of the saturated zone flow (FF-3c, 3d, 3e, respectively). The combined probability of the existence of such a reducing zone and its being encountered by a flow bearing fissionable material is extremely low (CRWMS M&O 1998i).”

*RAI 3-5 Explain why, in item 3, configuration NF-1b includes only a reducing reaction with tuff as a mechanism for precipitation of fissile solutes in the near-field below the waste package.*

*Other chemical reactions should be considered as causing such precipitation, such as changes in aqueous chemistry related to the presence of concrete and tuff. This comment reflects the desire for completeness in modeling the configurations.*

**Response:**

The language in the Topical Report identifying reducing reactions as the potential source of external accumulation was only intended to represent the typical possibilities. The evaluation of the accumulation from the waste package outflow (source term) will be accomplished by geochemical-transport computational methods that consider all recognized chemical reactions, as discussed in Sections 4.2.2 and 4.2.3 of the Topical Report and in the response to RAI 4-32. Item 3 will be modified as follows to reflect that these are illustrative only:

“...other void space of the near-field, obtained from processes such as adsorption or from a reducing reaction ...”

DOE believes that analyses of specific reactions are an application issue and not a methodology issue, so discussion of such analysis is not appropriate for inclusion in the Topical Report. The following discussion illustrates the additional types of accumulation reactions and mechanisms that will be considered for the License Application. The discussion is provided for informational purposes only. The information provided is preliminary and will be updated as necessary with additional evaluations or experiments prior to submittal of the License Application. DOE plans to evaluate external accumulation by adsorption. This capability is not available in EQ3/6, so DOE plans to use the geochemistry-transport code PHREEQC.

The principal non-reduction mechanism of deposition appears to involve destabilization of aqueous uranium (U) and plutonium (Pu) carbonate complexes, due to lowering of the dissolved  $\text{CO}_3^{2-}$ . The latter mechanism can occur through reaction with calcium (Ca)-silicates in tuff to create calcite or by lowering the system pH against the constraint of fixed  $\text{CO}_2$  fugacity. A preliminary analysis of external accumulation from waste packages containing mixed oxide wastes showed deposition of U was greatest (~20 kg) when pH 4 solutions were reacted with crushed tuff invert. Such a low initial pH is extremely unlikely but could result from oxidation of chromium in the stainless steels. To achieve such a low pH, the corrosion of the stainless steel would have to be so fast that it would all be corroded in 500 years. The likelihood of significant external accumulation by this mechanism is further reduced by the fact that subsequent, neutral pH solutions would be expected to redissolve a significant fraction of any actinide accumulation.

Calculations (CRWMS M&O 1998) for codisposal waste packages (those containing both SNF and HLW) showed that significant external accumulation of fissile material requires (1) in the waste package, extremely rapid degradation of the fissile-containing waste form, along with reasonably rapid degradation of the glass, to produce an alkaline-carbonate solution capable of mobilizing the actinides and (2) in the drift, reaction of the effluent with Ca-containing silicates, which changes the effluent chemistry enough to induce precipitation. So far this model yields significant (sub-critical) precipitation only for Pu and only insignificant accumulations of U. Even when the effluent encounters incompletely oxidized corrosion products (e.g.,  $\text{Fe}_3\text{O}_4$  from degraded steel sets), which have the capability to support reducing reactions, it is difficult to achieve significant

reductive precipitation before the effluent passes out of the invert, or all the material with reductive capability is oxidized by air.

In the accumulation reactions evaluated thus far, the reducing mechanism is the most effective for producing Pu accumulations. One extreme reducing scenario, in which the effluent from the waste package was assumed to encounter plates of unaltered carbon steel, produced up to ~10 kg Pu deposition, spread over a substantial volume below the waste package. However, it is considered unlikely that substantial, unreacted steel fragments could be maintained up to the period of waste package breach. Preliminary in-process calculations suggest the steel drift supports would be heavily corroded within ~1000 years, well before the probable time of waste package breach.

DOE is extending the prior work to consider: (1) a wider range of deposition environments, with more realistic models for  $fO_2$  (oxygen fugacity, idealized partial pressure) control by  $O_2$  diffusion and effluent reaction with Ca-silicates and reduced phases in the tuff, and reaction with partially-corroded (magnetite-rich) steel fragments; (2) greater analysis of U silicates as possible precipitants; and (3) tighter coupling between the evolution of the waste package effluent chemistry and the invert and drift materials. The tighter coupling of waste package effluents and external-package materials will likely decrease the calculated deposition, since the previous analysis picked snapshot waste package solution composition (with high dissolved actinide content). In fully coupled models, such solutions will be followed by fluids that favor re-dissolution of the actinides.

It should be noted that the enhanced design concept for the EBS (called EDA-II) includes very little concrete in the drift liner or invert material. Ground support in this design may include some concrete, but the total amount of concrete in the drifts will be much smaller than in previous designs. DOE plans analyses that will appropriately account for this concrete as well as the possibility that concrete in the design, but outside the emplacement drift, could impact potential criticalities.

CRWMS M&O 1998. *Report on Intact and Degraded Criticality for Selected Plutonium Waste Forms in a Geologic Repository, Volume II: Immobilized In Ceramic*. BBA000000-01717-5705-00020 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981007.0180.

RAI 3-6        *Clarify whether credit will be taken in the criticality analyses for the assumption that there is no mechanism for completely sealing the fractures in the bottom of the drift so any in-drift accumulations of water will only be present for a few weeks.*

*Previous investigations have indicated that thermal alteration of the rock surrounding the repository or microbial growth has the potential to seal fractures, at least in local portions of the repository (Lin and Daily, 1989<sup>1</sup>). Although it appears that the scenarios listed in figure 3-2 include the potential for water to pond on the bottom of the drift, if credit is taken for the short duration of*

*ponding water in the drift, this assertion that fractures cannot become sealed will have to be justified.*

Response:

DOE believes that the specific inputs or assumptions used in an analysis are an application issue and not a methodology issue and not appropriate for inclusion in the Topical Report. The methodology requires taking into account expected and potential conditions in the repository. Justification for the conditions used in evaluations will be provided in the evaluations or supporting documents for the License Application. While preliminary evaluations have indicated short-duration ponding as noted in Topical Report Section 3.1.2, Item 4, the final conditions that will be used for the License Application have not been determined. DOE plans to describe and justify these final output and assumptions in the supporting documents for License Application.

Item 4 in Section 3.1.2 of the Topical Report will be changed to the following to clarify that the ponding discussion is an example:

- “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. The detailed analyses for the License Application will evaluate the probability of occurrence for a pond of sufficient depth to cover most of the assemblies, while the assemblies are stacked in a geometry favorable to criticality.”

DOE believes that a discussion of the specific ponding assumptions used in the criticality analysis mentioned in the RAI is an application issue and not a methodology issue and, therefore, is not appropriate for inclusion in the Topical Report. The following discussion is provided for informational purposes only. The information provided is preliminary and will be updated as necessary with additional evaluations or experiments prior to the License Application.

Based on the current work summarized below, DOE expects to be able to show that ponding in the drift to a depth of more than a few centimeters is highly unlikely. DOE is presently investigating the possible mechanisms for plugging the fractures (deposition of minerals, clay buildup, and deposits from microbial growth); all indications thus far are that they would be very unlikely to fill all the fracture openings in the drift floor beneath the waste package. In the meantime DOE has performed a simple conservative analysis of the maximum depth that could be sustained under the worst-case (highly unlikely)

conditions that all the fractures are plugged over a certain length of drift (or there happens to be a section of drift that has no fractures in the floor to begin with).

A variant of the pond concept is a groundwater mound inside the invert, which is supported by the flow resistance of a fine-grained backfill and initiated by a large water pulse. It is expected that the DOE Yucca Mountain hydrologic modeling effort will soon produce a realistic value for the largest credible water pulse. In the meantime, the current worst-case estimate of 66 m<sup>3</sup> in one week (1.09E-4 m<sup>3</sup>/s) is used. This value corresponds to an infiltration rate of 165 mm/y focused in a week and from an area of 400 m<sup>2</sup>. It is assumed to be released in the drift over a localized area of 1 m<sup>2</sup>. The mound height is maintained by the porous media resistance to lateral outflow from this source, according to the following formula for flow in a vertical plane through the drift axis:

$$\frac{Q}{4K}L = \int_0^{h_0} A(h)dh$$

where Q is a line source perpendicular to the plane of the flow, K is the invert conductivity, h is the height of water above the bottom of the drift (ponding height), h<sub>0</sub> is the peak height at the center of the mound, and L the maximum horizontal extent of the mound. A(h) is the cross sectional area of the mound perpendicular to the axis of the drift:

$$A(h) = 0.5r^2(\phi - \sin \phi) \text{ with } \phi = 2 \left( a \cos \left( \frac{r-h}{h} \right) \right)$$

where r is the radius of the drift. Assuming it has a conductivity of 0.1 cm/s (reasonable for fine sand of 0.5 mm grain size) and a spacing (L) of 24.6 meters between unplugged fractures (which would have a probability of 1.3E-5 of occurring naturally, according to measured fracture spacing distribution data for the drifts drilled thus far), a mound can form to a height of 59 cm above the drift floor which is 1 cm below the top of the invert.

If ponding by this mechanism would occur it would be of short duration because of the episodic flooding necessary for the mound behavior to reach significant depth. The one-week duration in the present example would not be long enough for any significant radionuclide inventory increment in a steady-state criticality. Considered as a transient criticality, the extremely unlikely one week water pulse of this example would still provide only the very slow reactivity insertion rate considered in the example of Appendix C of the Topical Report. That slow insertion rate transient was shown in Appendix C to produce no significant pressure or temperature pulse.

The profile of the water height as a function of the distance along the drift axis is shown in Figure 3.6-1.

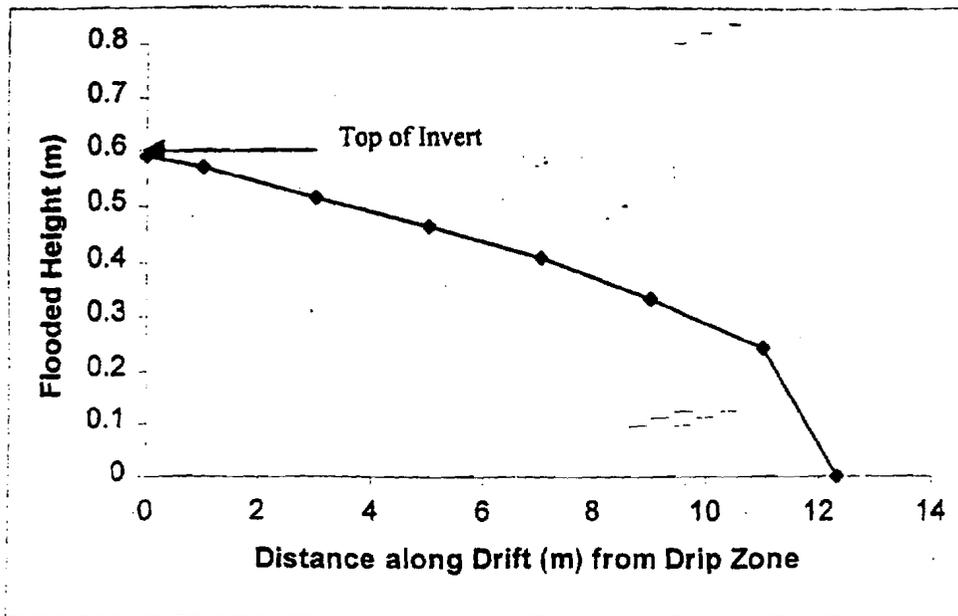


Figure 3.6-1 In-Drift Saturation Profile (0.5 mm sand, episodic flood)

*RAI 3-7 Explain why, in item 3, configuration NF-1b includes only a reducing reaction with tuff as a mechanism for precipitation of fissile solutes in the near-field below the waste package.*

*Other chemical reactions should be considered as causing such precipitation, such as changes in aqueous chemistry related to the presence of concrete and tuff. This comment reflects the desire for completeness in modeling the configurations.*

Response:

See response to RAI 3-5.

*RAI 3-8 Correct item 5 to state that the final two configurations are NF-3b and 3c, rather than FF-3b and 3c.*

*The context of the sentence implies incorrectly that the listed sites of colloidal accumulation are all in the far field. In addition, in the final sentence "open fractures" should be specified as being in concrete to be consistent with Figure 3-2a. These changes will correct the impression from item 5 that all colloidal accumulation sites are far-field.*

Response:

The designation NF (for Near-Field) was inadvertently omitted for 3b and 3c and will be corrected in a revision to the Topical Report. The final sentence of item 5 in Section 3.1.2 will be modified to indicate that the near-field open fracture accumulation would be in concrete and to indicate that there can be open fracture accumulation in the far-field as follows:

"Such transport and accumulation could lead to the far-field configurations FF-2a, 2b, 2c, for final accumulation in dead-end fractures, clay or zeolites, and topographic lows. It could also lead to the near-field configurations NF-3b, 3c, for final accumulation in the invert in open fractures of solid material or porespace of granular material, respectively."

Figure 3-2b, Part 2 will also be modified to indicate this latter fact (by adding to the caption of FF-2a) as follows:

"Filtration and concentration of colloids in granular pore space."

### **Section 3.2 Determining Internal Configurations**

*RAI 3-9 State whether temperature is included among the parameters quantified at this stage of the methodology and describe possible thermal variations.*

*Because equilibrium states and degradation/reaction rates for WP internal components (including WF) are temperature-dependent, all geochemical modeling should include sensitivity to temperature variations, including those caused by repository heating and cooling and by criticality events. With respect to internal configurations, the example analysis of appendix C refers to EQ6 calculations described in CRWM M&O (1998e<sup>2</sup>, appendix C, reference list). The discussion in this reference does not explicitly mention temperature constraints on models. Recent DOE modeling of the near-field (Harbin, 1998<sup>3</sup>) predicts that temperatures of close to 100 ° C may persist at the repository horizon 5000 yr after closure. A more recent repository design, EA-11<sup>4</sup> yields lower drift temperatures, but the waste package would still experience temperatures above 60 ° C for at least 2000 yr. Thermal variations have a strong effect on degradation processes and rates for waste package internal components. Furthermore, high temperatures would affect water chemistry (e.g., see composition of J-13 equilibrated with tuff at 90 ° C in Wronkiewicz et al. (1992)<sup>6</sup>. This comment applies also to discussions of internal and external geochemistry models in topical report sections 3.3, 4.2.2, and 4.2.3.*

Response:

The proposed methodology has the capability to evaluate the temperature sensitivity of geochemistry effects in the computational method (e.g., both EQ3/6 and PHREEQC). Effects of thermal variation on the external and internal geometry models will be documented in supporting reports for the Licensing Application.

DOE believes that a discussion of the specific parameters used in the criticality analysis mentioned in the RAI is an application issue and not a methodology issue and, therefore, is not appropriate for inclusion in the Topical report. The following discussion is provided for informational purposes only. The information provided is preliminary and

will be updated as necessary with additional evaluations or experiments prior to the License Application.

DOE does not expect elevated temperature to play a very significant role in waste package chemistry for the following reasons: (1) Many reactions of interest, which control mobility and precipitation of actinides, show a weak or retrograde temperature dependence in experiments; (2) Below 50°C significant accumulation of water in the waste packages may be impossible, because the rate of evaporation exceeds the drip rate; (3) In the Viability Assessment (DOE 1998) models, the first probable waste package breach is likely to occur only after the average temperature is below 50°C; and (4) In the latest repository design, ventilation will be used to reduce temperature. The following paragraphs provide evidence for the first assertion. The other three assertions are observations of the natural phenomena in the repository, predicted behavior of the waste package design, and a feature of the latest repository design. DOE plans to justify the assertions in the supporting documents for the License Application.

Wilson and Bruton (1989, relevant table is Table 3, page 10) found the temperature-dependence for uranium solubility was weak, and that plutonium solubility actually decreased with temperature. Similar results for plutonium were recently found by Eford et al. (1998, pp. 3893-3900). Thus, it is likely that an increase in temperature will have little effect or may even lower the actinide concentrations leaving the waste packages.

Wruck and Palmer of Lawrence Livermore National Laboratory (1997) proposed a method to extend the current database to include higher-temperature extrapolation for actinide complexes and solids; this method will be considered in upcoming months, but the addition of higher-temperature data will follow development of a QA framework consistent with DOE's and NRC's (NUREG 1298) definitions of "accepted" and "qualified" data.

For calculations of internal criticality, existence of retrograde solubility typically means that use of 25°C data is conservative. In systems with sufficient phosphate, the projected solubility-limiting phase for gadolinium is  $GdPO_4 \cdot H_2O$ , which has a weak retrograde solubility (Firsching and Brune 1991). In low-phosphate systems, the projected solubility-limiting phase is  $GdOHCO_3$  or  $Gd_2(CO_3)_3$ . The temperature dependence for the gadolinium carbonates has not been determined in experiments, but most carbonates are retrograde. Thus, a higher-temperature package may increase the likelihood that the criticality control material will remain with the fissile materials.

DOE plans to include the information discussed in this response, together with other sensitivity studies relating to the uncertainty in configuration parameters, in the validation report for the degradation/geochemistry models. With respect to the issue of temperature sensitivity, it should be noted that the validation of the EQ3/6 code discussed in Section 4.2.4.2 of the Topical Report already includes several cases of elevated temperature. In particular, three out of the four cases in Table 4-3 of the Topical Report have some elevated temperature comparisons.

DOE 1998. *Viability Assessment of a Repository at Yucca Mountain – Total System Performance Assessment – Volume 3*. DOE/RW-0508/V3. North Las Vegas, Nevada: DOE. ACC: MOL.19981007.0030.

Wilson, C.N. and Bruton, C.J. 1989. *Studies on Spent Fuel Dissolution Behavior Under Yucca Mountain Repository Conditions*. PNL-SA-16832 or UCRL-100223. Livermore, California: Lawrence Livermore National Laboratory. ACC: HQX.19891130.0045.

Efurd, D.W.; Runde, W.; Banar, J.C.; Janecky, D.R.; Kazuba, J.P.; Palmer, P.D.; Roensch, F.R. and Tait, C.D. 1998. "Neptunium and Plutonium Solubilities in a Yucca Mountain Groundwater." *Environmental Science and Technology*, 32, 3893-3900. Easton, Pennsylvania: American Chemical Society. TIC: 243857.

Wruck, D.A. and Palmer, C.D. 1997. *Analysis of Elevated Temperature Data for Thermodynamic Properties of Selected Radionuclides*. UCRL-ID-128955. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19980109.0250.

Firsching, F.H. and Brune, S.N. 1991. "Solubility Products of the Trivalent Rare-Earth Phosphates." *Journal of Chemical Engineering Data*, 36, 93-95. Washington, DC: American Chemical Society. TIC: 240863.

### **Section 3.4 Criticality Evaluation of Configurations**

**RAI 3-10** *Justify the use of the fresh fuel assumption in the internal criticality evaluation for waste forms other than commercial and naval SNF.*

*Many types of fuel that contain burnable poisons can be more reactive at moderate levels of burnup than when fresh. For such fuels, analysis of poison depletion and other burnup reactivity effects may be needed, not for burnup credit, but rather as a way of bounding the potential in-package burnup "debit."*

Response:

The "fresh fuel assumption" from the Topical Report is intended to indicate that no reduction in reactivity from burnup will be accounted for in the analyses. The assumption also includes not taking credit for the presence of burnable absorber. DOE intends that the full justification of assumptions for waste forms other than commercial SNF be in the addenda to the Topical Report. This is noted in Section 4.1 of the Topical Report. DOE plans to provide a clear explanation of the "fresh fuel assumption" in the addenda.

Preliminary information on the DOE-owned spent nuclear fuel waste forms has been presented to the NRC staff. From the Appendix 7 meeting at Idaho National Engineering and Environmental Laboratory (INEEL) on June 16, 1999 in the presentation titled "Disposal Criticality Analysis for DOE-Owned Spent Nuclear Fuel," the following conservatisms are planned to be utilized in the analysis of DOE-owned SNF.

- Fresh fuel assumption [which includes a burnup penalty - no burnable absorber credit (the fuel is assumed to not contain burnable poisons)]
- Maximum buildup of fissile isotopes
- Optimum moderation
- Optimum orientation
- Maximum absorber loss from geochemistry calculations using extremes of parameter ranges

In addition to the conservatisms listed above, the effects of isotopic decay are considered (Pu-239 to U-235, Pu-240 to U-236, etc.) to identify the most reactive isotopic composition.

For spent fuel other than breeder SNF, it is not possible for positive reactivity effects to result due to burnup if credit for burnable absorbers is not taken since the fissile inventory decreases. For breeder or plutonium-production SNF, the maximum gross buildup of fissile isotopes will be used to bound all burnup effects. Before SNF acceptance at the repository, verification that the fissile inventories fall below those evaluated will be required. These very conservative approaches will simplify the analyses by bounding the reactivity effects of burnup without requiring extensive calculations or chemical assays. The general discussion in Section 4.1 of the Topical Report will be clarified to address this point. DOE plans to provide detailed information in the appropriate addendum to the Topical Report and/or individual validation reports.

### **Section 3.4.1 Computer Codes**

*RAI 3-11 Justify the use of the fresh fuel assumption in the external criticality evaluations for waste forms other than commercial and naval SNF.*

*Criticality evaluations for near-field and far-field configurations must consider the actual compositions of SNF materials. Using the fresh fuel composition would not be bounding for scenarios where uranium, plutonium, and other fissionable actinides have different potentials for mobilization and reconcentration.*

Response:

DOE plans to justify the fresh fuel and other assumptions in the external criticality evaluations for waste forms other than commercial and naval SNF in addenda and/or validation reports for the waste forms.

As discussed in the response to RAI 3-10, DOE plans to use a conservative representation of the fissile content in the SNF. The burnup of DOE-owned SNF is low compared to commercial SNF, resulting in low production of transuranics. In addition, most of the inventory is medium-to-high-enriched, also leading to low production of transuranics. As

discussed in the response to RAI 3-10, DOE plans to consider the maximum gross buildup of fissile isotopes for breeder or plutonium-production SNF.

Analyses to date (CRWMS M&O 1997; CRWMS M&O 1998) have indicated that tens to hundreds of kilograms of uranium or plutonium are required to accumulate externally in order to create a critical configuration. The tens of grams of transuranics produced in the burnup of DOE-owned SNF are insignificant compared to the isotopes employed in the analyses.

CRWMS M&O 1997. *Criticality Analysis of Pu and U Accumulations in a Tuff Fracture Network*. A00000000-01717-0200-00050 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980216.0260.

CRWMS M&O 1998. *Report on External Criticality of Plutonium Waste Forms in a Geologic Repository*. BBA000000-01717-5705-00018 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980318.0412.

### **Section 3.4.2 Material Composition of Commercial SNF**

*RAI 3-12 Explain how the neutron-induced breeding of fissile and fissionable nuclides over time in the repository has been evaluated.*

*The TR does not indicate whether breeding effects have been evaluated. A scoping analyses of neutron sources, including (a,n) reactions, and associated breeding reactions should be provided or referenced in the TR. The evaluation should consider all fertile nuclides present in the various waste forms (e.g., U-238, Th-232, Pu-240). This RAI also applies to the material in section 3.4.3.*

Response:

DOE agrees that consideration of the neutron-induced breeding of fissionable isotopes in the methodology is appropriate. The DOE plans to revise the Topical Report to note that the neutron-induced breeding of isotopes is to be considered. However, DOE believes that the evaluation of neutron-induced breeding effects is an application issue and not a methodology issue and therefore is not appropriate for inclusion in the Topical Report. The following discussion is provided for informational purposes only and is related to the application of the methodology. The information provided is preliminary and may be updated as necessary with additional evaluations prior to the License Application.

Preliminary considerations have been made on the effect of neutron-induced breeding of fissile and fissionable nuclides over time in the repository. The neutron flux in a waste package is orders of magnitude smaller than that found in an operating reactor core at full power. Thus, the reaction rate required for conversion of fertile to fissionable isotopes is expected to be small in the waste package. During the long time periods that spent fuel would be in the potential repository, significant amounts of fissionable isotopes are not

expected to be generated by this conversion. DOE plans to provide a complete evaluation of this assumption as support documentation for the License Application.

### **Section 3.4.3 Principal Isotopes for Commercial SNF Burnup Credit**

**RAI 3-13** *Explain why the verifiability of the inventory, as part of the isotopic validation, is not one of the criteria considered in selecting the principal isotopes for burnup credit.*

*As indicated in the report, nuclear, physical, and chemical properties of neutron-absorbing isotopes were considered in selecting them for burnup credit. The verifiability of isotopes for pre-closure configuration, in terms of isotopic validation, should also be one of the criteria in selecting the isotopes which can be used in subsequent post-closure isotopic inventory for criticality calculations.*

Response:

DOE is not currently requesting review and acceptance of the method for selecting and verifying the principal isotopes used for burnup credit. DOE agrees that the selection of isotopes for burnup credit is subject to reactivity ranking and verifiability (e.g., comparison to radiochemical assay measurements and other studies). DOE plans to address verifiability of isotopic inventory in validation activities for future revisions of the Topical Report and will seek acceptance of the method for selecting and verifying the principal isotopes to be used for burnup credit at that time. The example principal isotopes selected for burnup credit as listed in the Topical Report are ranked by their expected reactivity contributions (both positive and negative) in discharged commercial SNF as a function of burnup. Inclusion of selected isotopes for burnup credit in intact or degraded waste form configurations will be addressed in detail during validation activities.

DOE plans to address isotopic validation in the commercial SNF validation reports and does not plan to seek NRC acceptance for isotopic validation via the Topical Report. (The planned workscope for these reports is included as Attachment A.) This isotopic validation is expected to rely on comparison of isotopic model calculations to radiochemical assay measurements, on code-to-code comparisons, and on commercial reactor critical integral experiments. Additional validation efforts are expected to include establishing the impact of potential isotopic concentration uncertainties on predictions of criticality. This activity is part of the isotopic model validation requirements noted in Section 4.1.3.1.4 of the Topical Report. These validation efforts include the use of integral experiments (see responses to RAIs 4-4 and 4-5c) and are expected to address the impact of potential compensating effects in these experiments. Components of the isotopic model validation process will be used to confirm the conservative aspects (bounding with respect to  $k_{eff}$ ) of models developed for waste package design. These models will be based upon the required conservative input parameters for integral depletion and reactivity evaluations that minimize waste package criticality potential regardless of waste form configuration.

*RAI 3-14 Provide isotopic importance as a function of time which includes decay and loss of isotopes from spent fuel degradation in the "Principal Isotope Selection Report."*

*The degraded configuration described in CRWMS M&O 1998f indicates intrusion of water into the fuel rods without considering the reduction of isotopes through their dissolution in the water.*

Response:

As noted in the response to RAI 3-13, DOE plans to address isotopic validation in the commercial SNF validation reports and does not plan to seek NRC acceptance via the Topical Report. Isotopic importance as a function of time during time periods of spent-fuel degradation where isotopes can be affected by the presence of water is not addressed in CRWMS M&O 1998f, *Report of External Criticality of Plutonium Waste Forms in a Geologic Repository*, because this information is considered to be part of a degraded-mode configuration. Principal isotope burnup credit including the selected fission products is considered only for configurations in which the fuel is intact. With intact fuel there is no loss of isotopes through spent fuel degraded-mode mechanisms. For configurations in which fuel is partially degraded, combined sets of actinides and fission products may be used depending upon isotope availability and transport within the degraded system, i.e., isotope solubility. For configurations in which the spent fuel is fully degraded, only the appropriate actinides are considered. The presence and removal of actinides during degraded modes are being studied in detail. Isotopic importance as a function of time for actinides and fission products is expected to be quantified in intact and degraded-mode studies during validation activities rather than in the "Principle Isotope Selection Report." Additionally, DOE plans to conduct degraded-mode studies to determine the uncertainties associated with the presence and removal of actinides at extended decay times.

*RAI 3-15 Justify taking credit for the isotopes in Table 3-1 through verification of their quantities predicted by the isotopic model.*

*To assume that the spent fuel is composed of the 29 isotopes listed in Table 3-1, one must verify the quantity of the isotopes predicted by the isotopic models. The isotopic models predict the radionuclide inventory as the function of reactor operating history. This validation must be performed by direct comparison of calculated to the measured isotopic inventory. Under-prediction or over-prediction of an isotope will have a direct effect on predicting the criticality potentials of a waste package accurately.*

Response:

DOE is not currently requesting review and acceptance of the principal isotopes listed in Table 3-1 of the Topical Report. Instead, DOE plans to seek acceptance of the method for selecting and verifying the principal isotopes to be used for burnup credit in a future revision to the Topical Report. Isotopes listed in Table 3-1 are provided as an example of

selected principal isotopes to be used for burnup credit in the general methodology. The establishment of principal isotopes (actinides and fission products) for the methodology described in the Topical Report will occur during validation activities that will be referenced in the license application.

The measured isotopic inventories (radiochemical assay information) and commercial reactor critical (CRC) integral experiment data results are not part of the methodology; therefore, DOE is not requesting NRC acceptance of these results. However, DOE plans to use the results of radiochemical assay and CRC benchmarks, if the methodology is accepted, to perform the validation of isotopic models in accordance with the methodology (see Appendix A for the planned workscope of the commercial SNF validation reports). The following information is provided for informational purposes only.

As noted in the response to RAI 3-13, radiochemical assay data, code-to-code comparisons, and CRC integral experiments will be used in verifying isotopic concentrations predicted by the isotopic model. DOE realizes that under-prediction or over-prediction of an isotope will have a direct effect on predicting the criticality potential of a waste package. DOE plans to perform comparisons of radiochemical assay data with calculated data to establish variations in the isotopic concentrations predicted by the isotopic model. Sensitivity studies of variations in individual isotope concentrations in the model are planned to establish the effect on criticality potential of a waste package. The methodology requires that the isotopic model used for waste package design must produce isotopic concentration values that will ultimately result in conservative  $k_{eff}$  predictions for the waste package.

Additionally, CRC data will be used to further validate the isotopic model. The CRC data provides information on reactor operating histories that include assemblies with strong neutron absorber history effects. This information will be used to supplement the radiochemical assay information that is often collected from "average" assemblies that do not have strong neutron absorber histories.

Thus, the accuracy of predicted isotopic inventory for the selected principal isotopes example listed in Topical Report Table 3-1 will be quantified by isotopic validation activities that include direct comparison of calculated-to-measured isotopic inventory, comparison to CRC data, and code-to-code comparisons. These isotopic validation activities are expected to individually justify taking credit for each principle isotope.

### ***Section 3.5 Estimating Probability of Critical Configurations***

*RAI 3-16 Answer the following questions related to computational feasibility and the discussion on page 3-21:*

- (a) How many repetitions or histories are envisioned for the Monte Carlo simulation?*
- (b) What is the confidence limit on a calculated criticality probability?*

- (c) *How are the probabilities for different configuration classes combined?*
- (d) *What will be done if one of the intermediate steps cannot materialize (i.e., a plausible regression form cannot be obtained)?*

*In order to establish a  $10^{-4}$  probability, a very large number of simulation runs must be generated. Additionally, in calculating criticality probabilities, it is desirable to calculate the associated confidence limit(s) about that probability. Answers to these questions could provide a clearer picture of the described methodology for estimating the probability of critical configurations.*

**Response:**

DOE believes that the questions in this RAI are related mostly to computational convenience and accuracy, and that trade-offs between these considerations are an application issue and not a methodology issue. However, to provide a more complete explanation of the criticality probability methodology, DOE offers the following responses to the questions in the RAI.

a) DOE believes that this question on number of repetitions or histories is an application issue and not a methodology issue. The information that follows is preliminary and provided for information. DOE has used simulations with 50,000 to 1,000,000 repetitions. The latest versions of the Monte Carlo code can execute between 10,000 and 50,000 repetitions per second (on a 300-MHz PC), so a run of several hours could produce  $10^8$  repetitions, if the additional accuracy was required.

b) The probability of criticality will generally be expressed as the expected number of criticalities occurring before some specified time (typically 100,000 years). A confidence limit equal to 0.95 or 0.98 will generally be appropriate for such a parameter estimate. This confidence limit will correspond to a confidence interval of  $\pm 1.98 \cdot \sigma$  or  $\pm 2.33 \cdot \sigma$ , respectively. The value of the standard deviation,  $\sigma$ , will reflect principal uncertainties associated with the Monte Carlo simulation: (1) the random fluctuations due to the limited number of samplings, (2) errors inherent in the regression or table lookup and interpolation process, and (3) uncertainty in the configuration parameters for processes that will take place over long time periods. For the first two uncertainty types, the error can be reduced by increasing the number of repetitions and/or the number of points in the lookup table. The contribution of configuration parameter uncertainty to the overall standard deviation is determined by the probability distribution of such parameters. The standard deviation can be independently estimated from a sample consisting of a series of Monte Carlo simulations with a new random number seed for each simulation and then taking the standard deviation of the sample. For the preliminary simulations run thus far, with from 50,000 to 1,000,000 repetitions per simulation, the standard deviation computed in this manner is only a few percent of the mean (expected number of criticalities).

c) In the Monte Carlo process the probabilities are not really combined; rather, they are expressed by sampling from distributions that characterize the probabilities. If the probabilities are independent, the probability distributions will be functions of a single

variable. If there are dependencies, the probability distribution of one parameter will be a function of one or more other parameters. To properly apply such a conditional probability distribution, care must be taken to sample the independent parameter(s) before the dependent one(s). In this manner the value(s) of the independent parameter(s) can be used when sampling for the dependent parameter from the conditional probability distribution.

d) If there are difficulties with intermediate mathematical steps, there are always alternatives. For example, DOE has already found difficulties in using the concept of a regression (or curve fit) for  $k_{\text{eff}}$  as a function of various degradation parameters. For waste forms with relatively high plutonium concentration, the sensitivities to neutron spectrum were confounding (reducing the determinacy of the regression coefficients) the degradation parameters actually being modeled (e.g., loss of fission products, loss of iron oxide). This problem was detected by DOE's routine, careful comparison of results for different parameter sets. The alternative of table lookup and interpolation was used instead of the regression. For three or more parameters, and a large number of iterations, the table lookup and interpolation have increased the running time for each case. But it is still well under a minute for the scenarios internal to the waste package.

With respect to the question of the number of simulation runs (repetitions) required for a probability of  $10^{-4}$ , it should be noted that the *uncertainty* of a Monte Carlo estimate, expressed as a fraction of the parameter being estimated, will be approximately the reciprocal of the square root of the number of repetitions. The  $10^8$  repetitions that can be accomplished in a few hours [see (a) above] would be sufficient to drive the uncertainty to  $10^{-4}$ .

In order to more explicitly identify the calculation steps used in this process, DOE plans to replace the paragraph of the Topical Report, Section 3.5 that starts at the bottom of page 3-20 and finishes at the top of page 3-21 with the following paragraphs:

"The first step in estimating criticality probability is to identify the configuration classes that are critical, which, in turn, are developed from the standard scenarios. Probability will be estimated for all configuration classes that have a  $k_{\text{eff}}$  exceeding the CL over a portion of their parameter range. Therefore, the first step in applying the methodology is to identify the range of parameters that will result in calculated  $k_{\text{eff}}$  greater than the CL. This screening is applied to each configuration class considered in DOE's comprehensive evaluation. The potentially critical configurations are characterized by a parameters having a range of values, and the individual waste forms will generally have a range of characteristics (e.g., burnup and enrichment, which vary significantly over the family of commercial SNF).

It would be impractical to subject all of the possible combinations of parameter values to MCNP4B (Briesmeister 1997) calculations. Therefore, a table of  $k_{\text{eff}}$  values for representative parameter values is used to determine  $k_{\text{eff}}$  values for any given set of parameters. Either of two techniques is used for this purpose. The

table of  $k_{\text{eff}}$  values can be used to construct a regression for  $k_{\text{eff}}$  as the dependent variable, with the configuration and waste form parameters as independent variables. To get a good fit, the regression must usually be non-linear with terms up to the third power in the individual parameters and cross products of different parameters. If the regression fit is good, it can be used to calculate  $k_{\text{eff}}$  for any values of the parameters that fall within the range of the table. Alternatively, the table can be used directly for a multidimensional lookup and interpolation. The latter technique is more robust, since the regression may introduce anomalous behavior, but it also requires more computation if the number of parameters is large. The number of computations for a regression with cubic cross terms could increase as the third power of the number of parameters while the number of computations for an n-parameter interpolation would increase as  $2^n$ .

An illustration of the regression development and Monte Carlo 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 (called Monte Carlo trials, iterations, repetitions, or realizations) from these distributions and determination of whether the selected set of parameter values satisfies the requirements for criticality. The probability of criticality is then determined by dividing the number of trials, which satisfy the requirements for criticality occurrence, by the total number of trials. The regression example in Appendix C used approximately 1 million trials. Even the slower table lookup and interpolation technique could handle 100 million trials in a reasonable computation time."

DOE also plans to modify the last sentence in the first paragraph of Section 3.5 in the Topical Report to the following:

"Acceptance is also sought for the use of the multivariate regression model, and/or the table lookup and interpolation, as a significant component this methodology."

In addition, DOE plans to modify item E in Section 1.2 of the Topical Report to the following:

"The methodology for estimating the probability of postclosure critical configurations and using multivariate regressions, or table lookup and interpolation, discussed in Section 3.5 is acceptable in general for disposal criticality analysis."

Briesmeister, Judith F., ed. 1997. *MCNP, Version 4B: Monte Carlo N-Particle Transport Code System*. User Manual. LA-12625-M, Version 4B. Los Alamos, New Mexico: Los Alamos National Laboratory. TIC: 241044.

*RAI 3-17 Justify the assumption that  $Fe_2O_3$  is the product that is formed by the corrosion of iron.*

*Credit is being taken for the filling of breached WPs by iron corrosion products, namely  $Fe_2O_3$ , thereby limiting the quantity of water present. It is unclear why the possibility that some of the iron corrosion product may be in the form of  $FeOOH$  was not considered. Justification of why the formation of  $FeOOH$  in lieu of  $Fe_2O_3$  was not considered should be provided or else the effects of  $FeOOH$  formation on criticality control should be determined.*

Response:

The Topical Report does not include an assumption of the presence of  $Fe_2O_3$ . All applications of the methodology have considered both  $Fe_2O_3$  (hematite) and  $FeOOH$  (goethite). The body of the Topical Report uses the generic name, iron oxide, to cover both oxide and oxy-hydroxide. The example given in Appendix C uses only iron oxide because our evaluations have shown that both goethite and hematite have approximately the same  $k_{eff}$  reducing effect for water moderated criticality. Both act primarily by displacing water. The hematite has higher density and, therefore, does not displace as much water as an equal number of moles of goethite. This advantage of goethite is approximately compensated by the moderating effect of the hydrogen in goethite. In the EQ3/6 geochemistry analyses the hematite occurs when the goethite is suppressed and vice-versa. Although criticality evaluations have thus far not detected any significant neutronic difference between hematite and goethite (CRWMS M&O 1998, Tables 6.1-2 and 6.2-3), future evaluations are expected to continue to test for sensitivity between them.

CRWMS M&O 1998. *Criticality Evaluation of Degraded Internal Configurations for a 44 BWR Waste Package*. BBA000000-01717-0210-00020 RE 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19989825.0207.

*RAI 3-18 Indicate whether the criticality calculations will account for neutron interactions between WPs.*

*The calculation of the effective neutron multiplication factor,  $k_{eff}$ , should account for all fissile material that can impact the modeled system. The EDA-11 design places the WPs much closer together in the line-loading formation, which will lead to greater neutronic interaction between the packages. It is not clear from the topical report whether these effects will be accounted for when calculating the  $k_{eff}$  of the fuel both inside the WP and in the near-field.*

Response:

The effects of interactions between adjacent waste packages and between waste packages and adjacent near-field accumulations will be accounted for. Because DOE believes that the details of how this will be done are beyond the appropriate scope of the Topical Report, DOE plans to document those details in the supporting documents for the License Application. DOE expects to show that no significant neutron interaction will occur

between waste packages because of neutron absorption in the thick waste package lids. The worst case, of the lesser burned assembly ends facing each other, will be evaluated, considering the axial dependencies described in the response to RAI 3-2. The validation of the isotopic model to support the axial dependence specification is described in Section 4.1.3.1.4 of the Topical Report.

### **Section 3.6.1 Type of Criticality Event**

#### Slow versus fast reactivity insertion rate.

*RAI 3-19 Explain why the configuration with seismic event causing reshuffling of spent fuel and the spent fuel being fully submerged in the water inside the waste package is not considered as a plausible scenario for the fast reactivity insertion rate.*

*The reference cited in the topical report (CRWMS M&O 1997a) provides earthquake consequence analysis with respect to criticality in terms of iron oxide settling in the bottom of the waste package and providing the transient criticality analysis.*

*With respect to iron oxide, it has not been demonstrated that the iron oxide can remain in the waste package. Secondly, the reshuffling of the spent fuel assemblies during a seismic event is a more plausible scenario than the iron oxide mixing with water and becoming a homogenous solution. Thirdly, if even the iron oxide would remain in the waste package, the settled iron oxide configuration is the initial condition and the uniformly distributed configuration is the condition right after the seismic event. It is not clear how the scenario is postulated with these two conditions being reversed. Therefore, the reshuffling of spent fuel in the*

*time frame of a second or less without the iron oxide is the more realistic scenario than the one presented in CRWMS M&O 1997a.*

Response:

The evaluations referenced in the Topical Report are example evaluations to demonstrate how the methodology would work, not part of the methodology itself. The DOE believes that the specific types of configurations analyzed are application issues and not methodology issues and are, therefore, not appropriate for inclusion in the Topical Report. The following discussion is provided for informational purposes only. The information provided is preliminary and may be updated as necessary with additional evaluations prior to the License Application.

The re-shuffling of the fuel by a seismic event was considered a plausible scenario. However, it was not used as a model for the example transient criticality because preliminary calculations with intact assemblies indicated that there was no physically possible shuffling that could produce a sudden increase in  $k_{eff}$  from below to above the CL. It is still possible that a configuration with one, or a few, collapsed assemblies could

result from such a shuffling. DOE expects to evaluate such configurations, and if any is found to produce a significant increase in  $k_{eff}$  to above the CL, the transient consequences are expected to be evaluated at the higher insertion rate. It is expected that this behavior will only occur for a limited set of collapse patterns (those concentrated in the bottom of one stack of assemblies), so the probability of such a configuration is also expected to be evaluated for inclusion in the overall risk evaluation.

The shift from uniform to settled iron oxide was used as the nominal fast insertion scenario in the Topical Report example (Appendix C) because the latter configuration was significantly more reactive than the former. The question of particulate adherence to surfaces and entrainment in flow is so complex that DOE cannot state with high confidence which configuration would be more stable following a seismic upset. However, subsequent modification of the waste package design, i.e., adding aluminum thermal shunts, has altered the water displacement possibilities so that it appears there is now no longer much difference in reactivity between the two iron oxide distributions.

DOE plans to address the issue of iron oxide solubility and whether iron oxide remains in, or flows out of, a waste package in the degradation analyses and the detailed geochemical analysis. For the License Application, DOE expects to show that most of the iron oxide from steel corrosion remains in solid form. Evidence will be included from archeo-metallurgy, pictures and other records of examinations of sunken steel vessels, and experiments.

#### Steady-state versus transient

*RAI 3-20 Explain why, for transient criticalities, you cannot have conditions 1 and 2 met under a more realistic scenario with seismic event and partially-flooded waste package with no iron oxide.*

*The confining condition stated in the topical report is not needed for an impact of fast reactivity insertion in the waste form. With respect to the second condition, the fast reactivity insertion is plausible under the seismic event with the top row assemblies rolling over and being submerged inside the waste package or fissible materials reshuffling and coming together outside of the waste package. With regard to the third condition, even for the optimistic condition described in the topical report, the  $k_{eff}$  for inside the package is 1.0189 which is super prompt criticality. Therefore, the rate of energy release is very fast.*

Response:

This RAI refers to the conditions stated in the third paragraph of Section 3.6.1 of the Topical Report, for a transient criticality having *significant kinetic energy release*. In this section the phrase *significant kinetic energy release* was intended to refer to a nuclear explosion. This paragraph was only intended to set the issue in perspective and not to screen it out. DOE plans to evaluate all recognized autocatalytic configurations for possibility of explosion, as discussed in the responses to RAI items 1-4, 3-21, 3-22, and 4-50, and in compliance with the direction in the letter from USNRC to DOE (Knapp to

Barrett), August 7, 1995, *Review of Potential for Underground Autocatalytic Criticality*. It was not intended to indicate any diminution of the transient criticality effort using RELAP5, which is given as an example in Appendix C of the Topical Report. The Topical Report will be modified so that this intention is clarified.

With respect to the specific configuration suggestions of this RAI, DOE believes that comprehensive discussion of specific scenarios or configurations is an application issue rather than a methodology issue and, therefore, not appropriate for inclusion in the Topical Report. The following discussion is provided for informational purposes only. The information provided is preliminary and may be updated as necessary with additional evaluations or experiments prior to the License Application.

DOE has not evaluated the possible reactivity insertion rates for configurations having no iron oxide because it is physically impossible to lose all the iron oxide and still retain most of the fissile material in the waste package. This is because most of the iron oxide forms as a hard scale, not as an easily poured or easily entrained fine powder (PNL 1980, page 6.3). As mentioned in the response to RAI 3-19, DOE expects to show, in documents supporting the License Application, that most of the iron oxide from steel corrosion remains in solid form. Nevertheless, in the interest of conservatism, DOE plans to evaluate possible upset conditions with a significant fraction of the iron oxide removed from the waste package.

Pacific Northwest Laboratory 1980. *Durability of Metals from Archeological Objects, Metal Networks, and Native Metals*. PNL-3198. Richland, Washington: Pacific Northwest Laboratory. TIC: 229619.

#### Under-moderated versus over-moderated

*RAI 3-21 Justify why moderation was the only mechanism used to govern the positive or negative feedback characteristics of a critical system.*

*The topical report's current discussion does not recognize, for example, that in certain configurations water is a poison and that other moderators (SiO<sub>2</sub>) more strongly influence the thermal neutron spectrum. Furthermore, particle self-shielding mechanisms for absorbers and fissile materials can have important implications not normally associated with the concept of over/under-moderation. Reflection dynamics likewise may be important in certain scenarios.*

*The concept of under/over-moderation has limited applicability outside LWR cores. For example, the 1986 Chernobyl disaster, by far the worst autocatalytic criticality event in history, was governed by positive void reactivity effects that have nothing to do with the concept of over-moderation. The positive void reactivity effects in CANDU reactors are likewise unrelated to over-moderation.*

*Especially in configurations where positive feedback effects are deemed credible, it is important to analyze the dynamic progression of criticality events using*

*appropriately coupled models of the actual neutronic and thermal-mechanical phenomena in that system. Repository physics can differ fundamentally from LWR core physics. Correct analysis of the criticality dynamics is essential to assessing any potentially disruptive effects in the repository.*

Response:

The methodology mechanistically determines the possible configurations. The feedback mechanisms or conditions associated with each configuration will be accounted for. The examples evaluated in the Topical Report are not intended to be all-inclusive. Their purpose was to demonstrate how the methodology could be applied, not all the conditions to which it would be applied. DOE believes that comprehensive discussion of specific scenarios or configurations is an application issue rather than a methodology issue and therefore is not appropriate for inclusion in the Topical Report. The following discussion is provided for informational purposes only. The information provided is preliminary and may be updated as necessary with additional evaluations or experiments prior to the License Application.

With respect to moderators other than water, the potential for silica moderation has been considered in preliminary analyses. The internal criticality potential is largest in the codisposal waste package because of the large amount of glass. The codisposal criticality evaluations have always included the moderating effects of any silica present, and they have been carefully analyzed for possible autocatalytic effects. None has been found thus far, but this screening is expected to continue. For external accumulations of fissionable material, analyses thus far have found that although the amount of silica in the rock may be large, the moderating effect is still small compared to water (CRWMS M&O 1998).

The transient criticality example in Appendix C of the Topical Report uses RELAP5, which considers the void effects suggested in this RAI. The only type of criticality consequence calculation that considers only moderator feedback is the steady-state criticality, for which it is the dominant feedback mechanism, as is explained in Section 5.1 of Appendix C of the Topical Report. For transient criticality external to the waste package, the Topical Report states that a code with fully coupled thermal, hydraulic and neutronic effects will be used (Section 4.4.1.2). DOE plans to specify the code to be used, when it is determined, in the validation report for the consequence model.

CRWMS M&O 1998. *Report on External Criticality of Plutonium Waste Forms in a Geologic Repository*. BBA000000-01717-5705-00017 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL 19980318.0412.

### ***Section 3.6.2 Evaluating Direct Criticality Event Consequences***

*RAI 3-22 Justify the statement that accumulation and geometry of fissionable mass needed for large disruptive criticality events is expected to be beyond anything physically possible in the repository.*

*It is not clear why the statement is made when another statement in the same paragraph explains that "some theoretical analyses have identified larger, disruptive consequences..."*

Response:

The statement alluded to was intended to convey the fact that all of DOE's analyses thus far (CRWMS M&O 1997, Section 9.1) fail to support the accumulation of the autocatalytic configurations suggested in the literature (either by Bowman or the group at the University of California Berkley Nuclear Engineering Department, cited in Section 4.4.1.2 of the Topical Report). The statement was for informational purposes only and is not important for justifying the methodology. DOE plans to add specific reference to the analyses in a revision to the Topical Report, and to clarify the Topical Report to remove the apparent contradiction.

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

### **Section 3.7 Estimating Criticality Risk**

*RAI 3-23 Justify the assumption that the only detrimental effect of a criticality event on the repository performance is the generation of additional radionuclide inventory.*

*In addition to the increase in radionuclide inventory, other direct and/or indirect potential criticality consequences must be considered. Increase in the waste package heat output affects the near-field environment and the rate of material corrosion and waste form degradation within the waste package. Additionally, large disruptive criticality transients could generate sufficient heat and pressure to degrade the waste package, cladding, or spent fuel. This degradation of the waste form could increase the release rate of radionuclides and the corresponding dose at the critical group location. This comment also applies to Section 12, Section 4.4.1.2, Section 4.4.1.1, Section 4.4.1.2, and Section 4.5.*

Response:

Any statement about increased radionuclide inventory was intended to apply to the steady-state criticality. DOE plans to revise the Topical Report as necessary to correct any unintentional implication that additional inventory is the only effect of criticality determined. The Topical Report devotes considerable attention (Section 4.4.1.2) to the transient criticality consequences of temperature and pressure, which could cause changes in the near-field environment, changes in the corrosion rates of the waste package materials, and damage to the waste form as suggested in this RAI. The peak transient overpressure calculation mentioned in the Topical Report (Section C-5.1) is not compared to a specific criterion for this damage. However, future calculations of these parameters are expected to include such a comparison.

It is recognized that the temperature elevation that may be associated with a steady-state criticality (up to 25°C) could produce an increase in corrosion rates. For example, a suggested model for the temperature dependence of the Zircaloy corrosion rate shows an increase by a factor of 14 for a temperature increase from 25°C to 45°C, which is typical of what could be expected from a steady-state criticality (Hillner et al. 1998). However, the increase still leaves the Zircaloy corrosion rate very small. In fact, recent analysis (CRWMS M&O 1999a) has shown that even at 100°C the cladding is likely to remain intact for over 100,000 years. Nevertheless, in order to be conservative, the steady-state consequence calculation in the Appendix C example assumed that all the commercial fuel cladding was lost during the steady-state criticality, to show that even the most conservative assumption still fails to produce a significant dose increment.

The pressure increase of the steady-state criticality is too small to estimate directly, but it is certainly much smaller than the low insertion rate transient pressure increase, which is less than 0.01 atmosphere (CRWMS M&O 1999b, Figure 6-40).

To clarify the intention of DOE to consider the time dependence of power level and the impact of temperature induced increase in corrosion rates, DOE plans to add the following paragraph to the end of Section 4.4.1.1.

“The variations in the drip rate will be determined probabilistically from the performance assessment climate model and mountain-scale hydrology model. These slow shifts in the drip rate will be reflected in slow shifts in the steady-state temperature. Because the drip rate distribution will be specified, probabilistically, as a function of time, the temperature and power level will also vary with time. When the radionuclide increment and risk are calculated, the time dependencies of temperature and power will be incorporated into the calculations. The time integrated history of temperature increase can be computed, and a temperature-induced accelerated corrosion of Zircaloy can be calculated. This accelerated corrosion will be reflected in a probability of loss of cladding integrity, increasing with time. The resulting radionuclide increment will thus reflect the time-dependent and probabilistic average power level, and the dose at the accessible environment will reflect the probability of cladding integrity loss.”

Hillner, E.; Franklin, D.G.; Snee, J.D. 1998. *The Corrosion of Zircaloy Clad Fuel Assemblies in a Geologic Repository Environment*. WAPD-T-3173. TIC: TBD.

CRWMS M&O 1999a. *Clad Degradation – Local Corrosion of Zirconium and its Alloys under Repository Conditions*, ANL-EBS-MD-000012 REV 00A. Las Vegas, Nevada: CRWMS M&O. ACC: TBD.

CRWMS M&O 1999b. *Waste Package Related Impacts of Plutonium Disposition Waste Forms in a Geologic Repository*, TDR-EBS-MD-000003 REV 00, REV 00, Las Vegas, Nevada: September 1999.

## **Chapter 4.0 Model Description**

### **Section 4.1.1.2 Postclosure Isotopic Concentrations**

*RAI 4-1 Explain how the so-called bounding bias and uncertainty values are derived from a stochastic process.*

*For example, are statistical confidence intervals associated with the uncertainty values? Are these a function of the number of Monte Carlo histories? In which way is the Monte Carlo analysis used to derive these values of bias and uncertainties?*

Response:

At least 1000 trials are run, resulting in a normal distribution of reactivities, which reflect the effects of the decay and branching ratio uncertainties. The exact number will depend on when convergence is shown. Therefore, the uncertainty values have statistical confidence intervals associated with them that are a function of the number of Monte Carlo histories. The mean and standard deviation are calculated for these trials. The bias, standard deviation, and number of trials run are used to determine a one-sided tolerance limit, which characterizes the population. Monte Carlo analysis uses the standard statistical methods for one-sided tolerance limits to calculate the bias and uncertainties.

Bounding bias and uncertainty values for post-irradiation decay times are those values that produce the largest  $\Delta k_{\text{eff}}$  value to be subtracted from the critical limit for a particular waste package loading. This  $\Delta k_{\text{eff}}$  value must be bounding for the SNF enrichments and burnups loaded into the waste package and must be bounding with respect to future decay times.

### **Section 4.1.3 Neutronic Model Validation**

*RAI 4-2 Justify the applicability of Commercial Reactor Criticals (CRC) for validation of MCNP4B in light of the lack of cross section libraries as a function of temperature.*

*It is not clear how well the MCNP4B cross sections can be validated against CRC when the modeling of CRC requires codes with cross sections as a function of temperature.*

Response:

The following is for information and relates to application of the methodology. DOE is not currently requesting review and acceptance of validation activities associated with MCNP4B cross section temperature effects. The effect of temperature limitations in MCNP will be analyzed as part of the waste form-specific validation reports. The critical limit development is expected to consider the effects of temperature-related uncertainties. Quantification of any temperature-related bias is expected to include a code-to-code

comparison between MCNP and KENO, which has cross sections that can easily be processed for temperature. (See Attachment A, Part H.C.)

Although the MCNP cross section library is limited in available temperatures, it does offer a variety of temperatures for many isotopes. Included in the list of isotopes represented at different temperatures are both U-235 and U-238. Both of these isotopes are modeled in the CRCs using the ".53c" suffix. This suffix represents the cross sections at a temperature of 587 K. Also, the moderator cross sections are corrected for temperature using the scattering-law treatment (the  $S_{\alpha,\beta}$  card) provided in MCNP. The cross sections of the structural material are not significantly affected by temperature. DOE plans to demonstrate that the remaining isotopes are either not significantly affected by temperature or are present in such small quantities that the temperature effects on  $k_{eff}$  related to these isotopes are not significant.

Temperature effects on reactivity worth ( $\rho=(k-1)/k$ ) using MCNP4B cross sections for U-238 and U-235 at both 587 K and 300 K have been quantified (CRWMS M&O 1999) in a preliminary analysis. The analysis was performed using typical pressurized water reactor fuel assemblies. For beginning of life (BOL) fresh fuel assemblies in a CRC environment (reactor core configuration), the difference in reactivity worth when changing MCNP4B cross sections from 587 K to 300 K is +0.0108. For a depleted fuel assembly in the CRC environment, the difference in reactivity worth is +0.00842.

References:

CRWMS M&O 1999. *Waste Package, LCE, CRC, and Radiochemical Assay Comparison Evaluation*. B00000000-01717-0210-00107 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990812.0351.

**Section 4.1.3.1.3 Radiochemical Assays**

*RAI 4-3 Provide information on the initial enrichments and burnup for the new Radiochemical assay measurements that are being conducted to supplement the database for commercial SNF isotopic model validation.*

*Staff notes that the existing data are limited to enrichments between 2.45 and 3.87 wt% <sup>235</sup>U. The new data should be for higher initial enrichments and higher burnup.*

Response:

DOE believes that the radiochemical assay information is related to application issues and is not part of the methodology. It is information that will be used, if the methodology is accepted, to perform the validation of the models in accordance with the methodology (see Appendix A for the planned workscope of the Commercial SNF Validation Report). The following discussion is provided for informational purposes only.

Additional isotopic assays are being performed for both PWR and BWR fuel rod samples. The PWR fuel rod samples were obtained from the TMI-1 reactor at the end of cycle 10. The BWR fuel rod samples were obtained from Quad Cities 1 reactor at the end of cycle 12. Both Argonne National Laboratory (ANL) and General Electric Vallecitos (GE) are performing radiochemical assay measurements on the fuel rod samples. The following table summarizes the enrichments and burnups for the fuel rods that were analyzed. DOE believes that with these additional assays, sufficient assay data will be available to support validation of the analysis method.

Reactor Type	Fuel Rod ID	Rod Average Burnup* GWd/mtU	Fuel Rod Enrichment -(wt% U-235)	Number of Samples Analyzed ANL/GE
PWR	O1	28.5	4.65	0/3
PWR	O12	28.0	4.65	0/3
PWR	O13	27.0	4.65	0/2
PWR	H6	48.5	4.00	5/0
BWR	A2	~70.0	3.80	0/2
BWR	B1	~70.0	3.80	2/2
BWR	C7	~70.4	3.00	3/1
BWR	G5	~62.0	3.00/2.00**	2/1

\* Peak rod burnup is approximately 10% greater.

\*\* Rod contained 2.00 wt% gadolinium oxide mixed with fuel.

#### **Section 4.1.3.1.4 Requirements for Isotopic Model Validation**

*RAI 4-4 Justify the use of 45 reactor core state points to bound the spent fuel operating history parameter values of the historical and projected spent fuel discharge for the spent fuel assemblies, which are destined for disposal in the proposed repository.*

*The operating history parameter values of the 45 reactor core state points do not bound the operating history parameter values of the 100,000 or so commercial spent fuel assemblies, which will be placed in the proposed repository at Yucca Mountain. The bounding operating history parameter values must be established based on the operating history parameter values of the historical and projected spent fuel assemblies to be discharged from the reactors.*

Response:

The aspect of the isotopics methodology described in Section 4.1.3.1.4, for which DOE is seeking NRC acceptance, is stated in Section 1.2 (item K) of the topical report. Item K seeks acceptance that the three requirements presented in Section 4.1.3.1.4 will ensure adequate conservatism in the applications model for burnup credit. These requirements provide acceptance criteria for confirming that the applications model to be used for

burnup credit will be bounding. Once a bounding model is defined, it will be confirmed in the commercial SNF validation reports.

The following is for information, and relates to application of the methodology. DOE is not currently requesting review and acceptance of the 45 reactor core statepoint data for activities associated with the development of bounding spent fuel history parameter values. DOE believes that the data associated with the 45 reactor core criticals are not part of the methodology. These data will be used, if the methodology is accepted, to validate the isotopic and criticality models developed in accordance with the methodology. (See Appendix A for the planned workscope of the Commercial SNF Validation Report.) Additionally, these data will be used to confirm the bounding applications model to be used in design activities.

Development of the bounding model (bounding operating history parameter values) to be used for the prediction of waste package criticality potential will draw from many sources of data. These sources include radiochemical assay data, CRC data, utility/vendor databases, numerical experiments, and code-to-code comparisons that describe spent fuel assemblies and will not be limited to 45 reactor core criticals. The bounding model will not solely rely upon core average values drawn from reactor core criticals. Once a bounding model is defined, it will be confirmed in the commercial SNF validation reports.

*RAI 4-5      Justify the method used to determine the isotopic code bias.*

*The purpose of code validation is to quantify the bias and the uncertainty, which may exist within the isotopic code. The main problems with the approach described in 4.1.3.1.4 are:*

- a)      Not using ANSI/ANS 8.1 and 8.17 to establish area and range of applicability .*
- b)      Using CRC operating history, which is insufficient to cover the complete range of operating history parameters of the discharged PWR spent fuel assemblies destined for disposal, to establish the bounding parameter values.*
- c)      Using the integral  $k_{eff}$  approach, which takes advantage of compensating errors in isotopic prediction to validate the isotopic model.*
- d)      Using the established parameter values from Part a to perform calculation-to-calculation comparison, as opposed to comparing calculations to experimental results for the purpose of isotopic model validation.*

*Other approaches such as direct comparison of measured to calculate values would eliminate some of these concerns.*

**Response:**

In Section 1.2 (item K) of the Topical Report, DOE is requesting review and acceptance of certain aspects of the methodology described in Section 4.1.3.1.4 of the Topical Report. Section 4.1.3.1.4 presents three requirements to be considered as acceptance criteria for confirming that the applications model used for burnup credit will be bounding. Confirmation of the bounding applications model (to be used in design) differs from the validation of the isotopic model. The method used to validate the isotopic model and establish isotopic code bias and uncertainty will be documented in the validation reports (see response to RAI 4-5c below). DOE is not seeking acceptance of this method at this time. The Topical Report will be revised as appropriate to clarify the concerns raised by the RAI.

(a) DOE believes its method for establishing area and range of applicability is consistent with ANSI/ANS 8.1 and 8.17. DOE plans to follow Section 4.3.6 of ANSI/ANS-8.1-1998 and Section 4.10 of ANSI/ANS-8.17-1984 for the validation reports. Section 4.10 states:

“Credit may be taken for fuel burnup by establishing a maximum fuel unit reactivity and assuring that each fuel unit has a reactivity no greater than the maximum established reactivity by (1) a reactivity measurement or (2) analysis and verification of the exposure history of each fuel unit. Consideration shall be given to the axial distribution of burnup in the fuel unit.”

DOE plans to establish the range of applicability of the bounding model in the validation reports using radiochemical assay data and CRC integral experiments. The radiochemical assay data and CRC experiments are expected to be used along with numerical experiments and code-to-code comparisons to define and confirm a waste-package design model that will yield a maximum fuel assembly reactivity (i.e., to satisfy Requirements A and B in Section 4.1.3.1.4 of the Topical Report). Also see the response to RAI 4-4.

(b) Bounding operating history parameter values for PWR (and BWR) spent fuel assemblies are expected to be developed using CRCs, radiochemical assay comparisons to calculated isotopic values, code-to-code comparisons, and numerical experiments. The development of this bounding model will not be limited to CRC data only. A range of applicability is expected to be determined for the bounding model, and spent fuel assemblies that are found to be outside that range of applicability are expected to be treated with alternative conservative model parameters (fresh fuel assumption, etc.). See response to RAI 4-4.

(c) DOE is not currently requesting review and acceptance of the method to be used for validation of the isotopic depletion model and establishment of the isotopic code bias. As noted in responses to other RAIs, the isotopic validation method will be demonstrated in the validation reports. The following is for information and relates to the methodology that will be described in the validation reports.

DOE recognizes that using the integral  $k_{eff}$  approach requires investigation of potential compensating errors in isotopic prediction. DOE plans to compare the calculated isotopic concentrations with measured data (radiochemical assays), best-estimate calculations, code-to-code calculations, and application model calculations to relate the observed effect on  $k_{eff}$  to the change in isotopic concentrations. These comparisons are expected to quantify both individual and integral isotopic effects on  $k_{eff}$ .

A systematic process will be followed to quantify bias associated with the isotopic and criticality models. This bias will be applied to the development of the critical limit. DOE plans to establish isotopic model bias using radiochemical assay data and CRC integral experiments during validation activities and plans to document the results in the validation reports. The fuel assembly burnups (exposure) for the CRC analyses are taken from Core Operation Reports and reflect the exposure history of the fuel assembly. The exposure history is reflected with the presence or absence of neutron absorber material [e.g., soluble boron, burnable poison rods, and control rods/blades (including power-shaping rods)], moderator density, and fuel temperature. The exposure history is also reflected in the axial distribution of the burnup. Fuel assembly burnups and exposure history for the radiochemical assay analyses will also be obtained from similar sources of data. The same level of detail in fuel assembly burnups and exposure history for radiochemical assay data is not always available. In addition, most of the radiochemical assay samples are for small segments of a single fuel rod. DOE plans to use a two-dimensional lattice code to transition fuel assembly core operations data to fuel rod data for the assay analysis. DOE plans to establish the isotopic code bias as a  $\Delta k_{eff}$  bias based on radiochemical assays and integral CRC experiments. Establishing the bias includes using the measured and calculated isotopic concentrations in representative criticality calculations. This bias will be appropriately applied in establishing critical limits (with burnup credit). Critical limits will be established, in part, using integral CRC experiments. The integral experiments contain an isotopic bias component. DOE plans to develop a method during model validation to appropriately account for isotopic bias in the critical limit and avoid repeated application of any portion of the isotopic bias.

(d) DOE plans to make calculation-to-calculation comparisons during confirmation of the applications model. However, for all cases where the calculation-to-calculation comparisons are made, measured data (either  $k_{eff}$  or isotopic concentrations) also exists and will be used.

*RAI 4-6 Explain why  $k_{eff}$  adjustment approach, which takes advantage of compensating errors in isotopic inventory, is chosen over the direct adjustment of each isotopic inventory for capturing the isotopic decay and branching ratio uncertainties.*

Response:

DOE is not currently requesting review and acceptance of the method to be used for validation of the isotopic depletion model and establishment of the isotopic code bias. As

noted in responses to other RAIs, the isotopic validation method will be demonstrated in the validation reports. The following is for information, and relates to the methodology that will be described in the validation reports.

The most important parameter governing criticality potential in the waste package will be  $k_{eff}$ . Waste package design and waste package loading at the proposed repository will focus on this parameter. Because of the primary importance of this criticality parameter, the  $k_{eff}$  adjustment approach has been chosen. The effects of compensating errors will be quantified in the validation report for commercial SNF fuel assemblies (see Attachment A). Quantification of compensating errors will include effects on isotopic inventory as predicted by the depletion code and the corresponding effect on  $k_{eff}$  predicted by the integral calculation (CRC).

While some of the time the effect of one error may "compensate" for the effect of another error, these errors are behaving within statistical bounds. The net effect of the errors will be quantified over the range of the enrichments and burnups for each fuel geometry to ensure that the  $k_{eff}$  adjustment is bounding. The alternative approach that applies direct adjustments to each isotope may not reflect the fact that the inventory of an individual isotope can be dependent on the inventory of other isotopes. In addition, other licensing applications, such as core design using statistical methods and the quantification of measurement system errors, have used this accepted technique.

A method could be chosen to adjust the isotopic inventory of each isotope in the conservative direction (increase for fissile and decrease for absorber) by an amount that might potentially bound the reactivity contribution for all fuel configurations and burnups. However, this would require examining the uncertainties in the precursors of each isotope (not limited to the principle isotope set), as well as the uncertainty in the decay of that isotope for all fuel configurations and burnups and could be a source of additional error in calculations of isotopic inventory. The application of the resulting adjustment factors would require separately modifying all calculated isotopic concentrations before they are used in any criticality calculation, including configurations external to the waste package.

Radiochemical assays would be one source of data used to develop these adjustment factors. Errors inherent to radiochemical assay measurements would be introduced into the calculation of criticality potential based on the adjusted isotopic inventories. Additionally, isotopic concentrations determined from radiochemical assay measurements rely upon "micro scale" data (concentrations determined from a small portion of a fuel pellet) and are most often not accompanied by detailed depletion histories for the fuel assembly being sampled. Reliance upon this type of data for developing isotopic inventory adjustment factors would be risky.

Modification of isotopic concentrations during burnup requires a detailed knowledge of isotopic depletion interdependence. Likewise, modification of isotopic concentrations at discharge burnup requires a detailed knowledge of isotopic decay interdependence. The development of adjustment factors to be applied to isotopic inventory at discharge burnup

would require capturing all of the isotopic decay interdependence detail as well as the uncertainties associated with isotopic decay and branching ratios. Development of these factors could prove to be a formidable task because of the complicated decay schemes common to exposed fuel isotopes and would more than likely introduce additional error into the calculation of isotopic inventory to be used in criticality evaluations. A very small error in isotopic inventory introduced at discharge burnups could translate to a very large error in predicted isotopic inventory after thousands of years of decay. Additionally, these adjustment factors would be difficult to relate to physical examples for verification purposes. Therefore, to minimize the introduction of additional error and to focus on the most significant characterizing parameter of waste package criticality potential, DOE chose the  $k_{eff}$  adjustment approach.

As part of the planned validation report effort described in Attachment A, an approach has been chosen to quantify the effects of decay uncertainties, branching ratio uncertainties, and isotopic distribution variations inherent to the depletion model code. DOE expects that this approach will quantify effects of compensating errors in the integral experiment on  $k_{eff}$  calculations. These compensating effects are expected to be well understood and characterized. See response to RAI 4-5 (c).

#### *Section 4.1.3.2 Determination of Critical Limits*

*RAI 4-7 Provide justification for not incorporating the following information into Figure 4-1 for estimating Critical Limit.*

- (a) Identification of subsets of validation experiments which are applicable to the waste form and configuration classes within and outside the waste package.*
- (b) Performance of a normality test prior to applying any of the statistical analyses such as regression analysis, which is based on the normality assumption. Figure 4-1 shows that the normality test is performed after the regression analysis indicates there is no trends. The base assumption for regression analysis is normality which must be verified through some statistical tests.*
- (c) Performance of a regression fit of  $k_{eff}$  on predictor variables for the relevant subset to identify trending parameters.*
- (d) Inclusion of all the parameters, not just the ones with "strongest correlation," which have statistically significant trends as the function of  $k_{eff}$ .*

Response:

DOE believes the topics addressed in this RAI are all related to the methodology for determining the critical limit. DOE seeks acceptance of this methodology.

- (a) The first box on the top of Figure 4-1 incorporates the idea of identifying subsets of the benchmark experiments applicable to the waste form and configuration*

classes ("Define set of validation experiments ... encompassing desired range of applicability"). DOE expects that the waste form-specific validation reports will document the material, waste form, and configuration class-specific benchmark subsets. The subsets are expected to be developed from the total benchmark database for each applicable configuration class from the master scenario list. The configuration class will dictate the geometry type (e.g., lattice versus homogenous) of the applicable benchmarks. For each configuration class (geometry type), there may be multiple material type subsets (e.g., LEU versus MOX). DOE plans to perform statistical equality tests to determine if the material-type specific subsets can be combined. Attachment A, Part II.A, provides some discussion of the benchmark subset development.

(b) The first step in the assessment of a critical limit is to look for a trend of  $k_{eff}$  on a parameter. This involves a regression analysis. When a trend is not significant, the Normal Distribution Tolerance Limit (NDTL) method is applied, if normality of the  $k_{eff}$  values for the set of criticality experiments can be established. The Distribution Free Tolerance Limit (DFTL) is the only option in a non-trending, non-normal result. See the response to RAI 4-14 for more information on the NDTL, and the response to RAI 4-16 for more on DFTL.

For regression methods, several assumptions form the basis for inference analysis, including inference on the significance of the regression.

Normality of the regression residuals is one assumption. (A regression residual is the difference of the observed value of the dependent variable and the calculated value of the dependent variable for the value of the independent variable.) However, it is necessary to assess normality of the residuals after performing the regression fit, by definition of residual. Most statistical software packages include tests of normality of the residuals as standard or optional output for regression calculations. Statistical inferences about the regression model, including assessment of a trend, are reasonably robust with respect to normality.

Figure 4-1 indicates that if the regression is not significant, the recourse is a statistical tolerance limit based on the  $k_{eff}$  values for the set of critical experiments. Here, there is no predictor variable, because the regression is not statistically meaningful, and the critical limit is developed without accounting for any trend of bias. For this situation, the normality test indicated in Figure 4-1 is for these  $k_{eff}$  values (not the residuals), and the result of this normality test determines the method for computing the critical limit that is appropriate.

If the normality test of the  $k_{eff}$  values does not reject the hypothesis of normality of the  $k_{eff}$  values, then the NDTL method is appropriate. If the hypothesis of normality is rejected, DOE plans to use the DFTL method.

DOE seeks acceptance of the approach described of using one of the specified methods to determine the critical limit, the method chosen for any given case to be determined as described.

(c) The third box down from the top of Figure 4-1 incorporates this idea ("Perform regression fits of  $k_{eff}$  on predictor variables to identify the trending parameter"). The trend analyses performed for the waste form-specific validation reports will consider the benchmark data in appropriate material-specific, waste form-specific, and configuration class-specific subsets of the total benchmark database. (See Attachment A, Part II.B.)

(d) DOE expects that the application of statistical methods to biases and uncertainties of  $k_{eff}$  values for a set of benchmark critical experiments will be the basis of establishing critical limits for a waste form. This process involves obtaining data on various neutronic parameters from the criticality code and other parameters from other sources (e.g., burnup) that may be used to model the behavior of deviations of the calculated values for  $k_{eff}$  from the known value that represents criticality. The determination of critical limits is data-dependent, and the set of benchmark critical experiments must be carefully selected to cover the range of applicability expected for the repository conditions. Quantity of data is therefore an important consideration to assure this coverage.

The situation for a single predictor variable that produces a statistically significant trending regression and the most conservative critical limit is discussed in Section 4.1.3.2.1 of the Topical Report. Sections 4.1.3.2.2 and 4.1.3.2.3 address methods to establish critical limits if there is no meaningful trending variable.

A process that identifies the single predictor variable described above begins with multiple regression techniques on a field of candidate trending variables. The multiple regression model can be used as a filter to identify predictor variables that should be examined in detail. Several outputs of multiple regression analyses are important in this process. For example, the coefficient of each predictor variable is tested for statistical significance, which may eliminate some of the trending candidates directly.

Multiple regression software also provides estimations on the correlations of the predictor variables with each other and with the dependent variable,  $k_{eff}$ . Collinearity is the existence of near-linear relationships (strong correlation) between predictor variables. Where strong correlations exist between two or more predictor variables, each of these variables provide essentially the same contribution to the prediction result. This aids in identifying those predictor variables that may not require further investigation.

Predictor variables that have statistically significant coefficients in the multiple regression may not have a statistically significant coefficient in the simple linear regression model. That occurs when one variable is highly correlated with another predictor variable, but not with the dependent variable. Such a variable would not be necessary for trending the bias of the criticality code in its determination of  $k_{eff}$  values for the benchmark set of critical experiments. The variable with which it is highly correlated and which exhibits statistical significance in the simple linear regression model would be considered for further evaluation relative to other possible predictor variables.

DOE plans to use those predictor variables that result in statistically significant simple linear regression models to establish the critical limits for the waste form through a process that investigates each and identifies the most conservative critical limits as the final critical limit function.

A single predictor variable produces a critical limit function that can be plotted in two dimensions, in the fashion of Figure 4-2 in the Topical Report. Knowledge of a single parameter is all that is needed. There is likely to be only a small range of the calculated  $k_{eff}$  values, which supports a simple linear trending model.

The response to RAI 4-11 also addresses this subject.

Extending the number of predictor variables used in combination in determining critical limits would complicate the application of critical limits to waste forms. The disadvantage is that it produces a critical limit function that is a surface, needing a computation of the critical limit for each instance of the predictor variables at the time of application.

*RAI 4-8 Provide the technical bases (other than "commonly used") for using 0.05, instead of 0.01 or 0.001, for the level of significance in identifying linear trends with respect to the trending parameters.*

*Although it is indicated that approval of a specific value for the level of statistical significance will be sought in the License Application, the TR should provide a statistical rationale used for selecting the specific value.*

Response:

As is noted in the Topical Report, DOE is not seeking acceptance for any particular value of level of significance. The following discussion addresses methodology, for which DOE is seeking NRC acceptance.

Bias trend is defined as the rate of change of  $k_{eff}$  with some predictor variable, e.g., burnup. In simple linear regression, this is the slope of the line. This biasing results because the criticality code computes  $k_{eff}$  values in a fashion that varies with a trending variable.

A logical method for assessing the existence or significance of this trend is needed. One such method is statistical hypothesis testing. Another process for addressing the statistical significance of the slope of the regression is the use of confidence limits - a measure of the goodness of an estimate. DOE plans to use the confidence limits method. Note that smaller levels of significance result in more frequent rejection of trends. This translates into higher confidence limits rejecting trending more often.

The method of using confidence limits on the slope coefficient is simply stated. Two-sided confidence limits, established at the  $(1 - \alpha)100\%$  level can be used to assess whether the slope coefficient is zero. If, at the confidence level desired, this interval

includes zero, then the slope is statistically zero, at the  $\alpha$ -level of significance. If the interval does not include zero, then the slope is non-zero. Here the rationale clearly relates to the risk,  $\alpha$ . This is the rationale that will be applied to the choice of level of significance in the validation submittals.

*RAI 4-9 Justify the basis for redefining  $\Delta k_m$ .*

*ANSI/ANS-8.17 defines  $\Delta k_m$  as "an arbitrary margin to ensure the subcriticality  $k_s$ ." The examples provided for  $\Delta k_m$  in the topical report such as "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" are standard biases, which must be included as part of isotopic bias and  $\Delta k_c(x)$ , respectively. The  $\Delta k_m$  in this case must include a subcritical margin. For example, if CL for a particular configuration is established to 0.95, is the value of 0.9499 for  $k_s + \Delta k_s$  considered to be subcritical? If more neutron histories are used, the calculated value could be 0.95 or beyond. Therefore, the need to identify a zone of criticality and incorporate it into the total uncertainty should be considered.*

*This comment also applies to Normal Distribution Tolerance Limits (Section 4.1.3.2.2) and the Distribution Free Tolerance Limit (Section 4.1.3.2.3).*

Response:

DOE agrees that  $\Delta k_m$  was not used consistently with ANSI/ANS-8.17. The Topical Report will be revised to clarify the differences and the reasons for them. However, the risk-informed methodology for disposal is not trying to ensure subcriticality, as did the past applications of ANSI/ANS-8.17. The risk-informed methodology is defining a Critical Limit (CL) which establishes what is and is not critical. The past applications of ANSI/ANS-8.17 defined an upper subcritical limit that ensured an arbitrary subcritical margin. The CL values will not include an arbitrary subcritical margin (i.e.,  $\Delta k_m$  as defined in ANSI/ANS-8.17). Elimination of this arbitrary margin is consistent with the elimination of the requirement to have one in the NRC's proposed 10 CFR Part 63. That proposed regulation, like DOE's planned criticality analysis method, focuses on risk and not on arbitrary margins. Imposition of an arbitrary margin would constitute a subsystem performance objective, which is inconsistent with the NRC's approach in the proposed regulation. DOE's disposal criticality method is intended to address the proposed 10 CFR Part 63, on the assumption that it will ultimately be issued in a form similar to the draft regulation. DOE's planned method will contain appropriate conservatism for a risk-informed, performance-based approach. DOE believes that the method adequately accounts for uncertainties, such that an arbitrary margin is not needed or appropriate.

The disposal methodology is also performing a screening process by identifying which general configuration classes have or do not have the potential for criticality. This screening process is expected to use subcritical margin (see modified Figure 3-3, Attachment C) to ensure there is a zone of subcriticality that will allow a complete

evaluation of configurations that have a potential for criticality. This is done prior to the evaluation of probability or consequence of a criticality event.

With respect to Sections 4.1.3.2.2 and 4.2.3.2.3, the establishment of statistical tolerance limits is based on a single random sample from a population. For the same reasons as discussed above, an arbitrary subcritical margin is not an appropriate part of a risk-informed methodology for postclosure criticality analysis.

For the example given, a value of 0.9499 would not pass the test because statistical errors would be added to the value of the calculated  $k_{eff}$ . The statistical error would account for the number of histories used. After accounting for errors associated with the system analyzed (e.g., fabrication tolerances, errors in half lives and branching fractions), statistical errors, and errors due to biases as well as adjustments for roundoff, the criteria for acceptance or rejection would be strictly based on the numbers obtained and allowance for the uncertainties.

*RAI 4-10 Justify the use of the linear regression model to fit the data presented in Figure 4-2.*

*Considering the data in Figure 4-2, it seems that another model, i.e., exponential or polynomial, could better fit the data than the proposed linear regression model for trending criticality level.*

Response:

This RAI deals with an illustration of methods discussed in the Topical Report, Section 4.1.3.2.1. While the general approach to determining critical limits is part of the methodology for which DOE seeks acceptance, determinations of critical limit functions are data set-dependent.

DOE believes the following information addresses application and not methodology, and it draws on current experience in calculating CL values.

The data in Figure 4-2 are illustrative, and the justification of the appropriateness of a specific model for establishing a critical limit for a range of applicability is expected to be provided in supporting documents for the License Application. The following discussion is preliminary and is provided for informational purposes.

DOE's experience with regression fits of data similar to those in Figure 4-2 for a polynomial of degree two generally provides no practical increase in the coefficient of determination ( $R^2$ ) or decrease in the standard error as compared to use of a simple linear regression. The exponential model [of the form  $y = a * \exp(bx)$ ] can be made a simple linear regression by taking logarithms. The resulting regression does not improve the fit  $R^2$ , and it further complicates the use of the results, since the results are in logarithms that must be transformed back into the original units.

Trending on the  $k_{eff}$  values for neutronics parameters on the basis of simple linear regression is the method illustrated in the Topical Report. The concept of trending is not the discovery of a complex relation of the calculated and observed phenomena. Rather, it addresses the practical issues regarding the ability of the criticality code to match experimental determinations for  $k_{eff}$ . Therefore, DOE believes that a simple linear model will adequately describe system behavior for the data illustrated in Figure 4-2.

*RAI 4-11 Justify why a single predictor is used for the least-square fits, as explained in the discussions. Examine the data to determine whether a combination of factors would yield a better fit.*

*One could argue that a "less sensitive" model (a model that does not include all significant factors and factor combinations, or a model with a nonlinear structure) is more conservative. This argument would be correct with respect to the measure of uncertainty, since a poor fit is associated with larger uncertainty. However, a more refined regression could have a negative trend that may be undetected due to the simplicity of the model. Therefore, the question is whether the failure to detect a negative trend is outweighed by the large measure of uncertainty.*

Response:

The following information relates to the methodology, for which DOE is seeking NRC acceptance. Evaluation of trend in the bias of the criticality code for a set of candidate predictor variables will be the desired method for determining a critical limit for a waste form. The content of Figure 4-1 coincides with the general philosophy of NUREG/CR-6361, and that is the origin of the reference to the "strongest correlation." The method described in the Topical Report for the trending situation is a single predictor. However, the process is expected to consider identified candidate trending variables. If trending is the basis, DOE plans to evaluate the critical limits for the various regressions to provide the final critical limit.

If a trend is negative and significant, the results will likely display this result. If such a negative trend is not statistically different from zero, failure to detect it should have no practical impact on the resulting critical limit that would be determined using NDTL or DFTL methods. If there is a large measure of uncertainty, then it is unlikely that a more complicated model is going to be more useful than one of these two latter approaches. This position is based on the fact that large uncertainties will result in rejection of trending. Note also the response to RAI 4-7.

*RAI 4-12 Explain how parameters other than those used for trending are applied to characterize a system and the benchmark experiments. The extension of the range of applicability (ROA) must be addressed with caution. How would one know of any trending effects outside the experimental ROA?*

Response:

The following information relates to the methodology, for which DOE is seeking NRC acceptance. Parameters, other than those used for trending, will be applied. Parameters are expected to be chosen from each of the fundamental areas of applicability: material (e.g., initial enrichment, cooling time, fuel temperature, fuel type, cladding type, fuel density, absorber type, absorber concentration), geometry (e.g., square lattice, triangular lattice, homogeneous solution, rod diameter, lattice pitch), and spectrum (e.g., ratio of moderator volume to fuel volume, H/X). For each parameter, the anticipated range of conditions and the benchmarked range of conditions will be documented in a single table for easy comparison.

Large extensions of the range of applicability for non-trended parameters are expected to be performed by introducing additional experiments (see Topical Report, Section 4.1.3.3.3, Paragraph E). Small extensions of the benchmarked range may be justifiable with the existing benchmarks.

Although DOE is seeking acceptance of the general approach for extending the range of applicability as described in Section 4.1.3.3.3 of the Topical Report, DOE is not currently requesting review and acceptance of the process for extending the range of applicability for trending any specific parameters. The choice of method between the two presented in the Topical Report is dependent on the parameter and the specifics of any trend. Where a trend exists, DOE will consider the trend itself, the direction of the trend, and the physical explanation of the trend. Short of adding additional benchmark experiments, the extension process may include a code-to-code comparison in addition to physical explanations for the trend and statistical analyses of the trend. The process is also expected to include a method for determining the penalty to be included in the extended range. The two methods discussed in the Topical Report are consistent with the guidance of ANSI/ANS 8.1, Appendix C and are expected to be documented in the validation reports (see Topical Report, Section 4.1.3.3.3, page 4-25). DOE plans to justify any extension of the benchmarked range for trended and non-trended parameters in the validation reports. See the response to RAI 4-22 for additional information regarding the extension of the range of applicability for trended parameters.

#### ***Section 4.1.3.2.1 Lower Uniform Tolerance Band***

*RAI 4-13 Justify why the application of combined Method 1 and 2 in Lichtenwalter et al (1997, pp. 158-162) as referenced in the topical report was not evaluated.*

*As stated in Lichtenwalter et al., "the recommended purpose of method 2," Lower Uniform Tolerance Band (LUTB), "is to apply it in tandem with Method 1..." The term  $\Delta k_m$  must be included in the LUTB approach. However, the value for  $\Delta k_m$  may be determined based on some reasoning as opposed to the traditional 5% administrative margin.*

Response:

The following addresses methodology, for which DOE is seeking NRC acceptance. DOE believes that  $\Delta k_m$  is not relevant to the postclosure criticality analysis methodology for the reasons addressed in the response to RAI 4-9. Additionally, the method described in the Topical Report is more limiting than the Method 1 of NUREG/CR-6361. Method 1 of NUREG/CR-6361 is a prediction limit that bounds a single future observation. The methods described in the Topical Report are based on tolerance limits, which are bound by definition to be more inclusive than a single prediction.

DOE plans to carefully evaluate Lichtenwalter et al. 1997 for applicability and will incorporate additional guidance from it as appropriate. Lichtenwalter et al. 1997 was intended for transportation packages, whereas the Topical Report addresses a geologic repository. The two applications differ in the design approach and regulations involved. Consequently, the application of the combined Method 1 and 2 in Lichtenwalter et al. does not reflect the repository application to populations of waste material.

The repository will hold populations of multiple waste forms, each of which is subject to a critical limit. The Lichtenwalter et al. Method 1 provides a confidence limit on a best estimate prediction. This is not appropriate for the repository application. Tolerance limit-based CL values provide a specified confidence that at least a certain large portion of the population of  $k_{eff}$  values is covered.

The methods discussed in the topical report allow for either trending or non-trending cases, providing a critical limit that has a stated confidence that a stated proportion of the calculated  $k_{eff}$  values will be below that limit. NUREG/CR-6361 does not address situations for which trending is not appropriate.

Lichtenwalter, J.J.; Bowman, S.M.; DeHart, M.D.; Hopper, C.M. 1997. *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages*. NUREG/CR-6361. ORNL/TM-13211. Oak Ridge, Tennessee: ORNL. TIC: 233099.

#### **Section 4.1.3.2.2      Normal Distribution Tolerance Limits**

*RAI 4-14      Clarify if the Normal Distribution Tolerance Limits (NDTL) are based on the prediction interval or tolerance interval, and justify this approach.*

*The prediction interval is based on predicting, with a predetermined confidence level, a single future value which would be below the critical limit. On the other hand, tolerance limits predicts a percentage of future values which would fall below the critical limit. The latter is a more acceptable approach.*

Response:

The following addresses methodology, for which DOE is seeking NRC acceptance. The NDTL is not a prediction interval. Similarly, the DFTL is not a prediction limit. The NDTL is a statistical tolerance limit for the set of  $k_{eff}$  values that represent a waste form

and is not based on prediction of trending. It is determined by assuming that the set of  $k_{eff}$  values determined via the criticality code provides a random sample of such results from the population of interest. Here the population of interest is a waste form. The specific equation for the calculation is Eq. 4-3 on page 4-16 of the Topical Report.

The NDTL method assesses the capability of the criticality code to predict  $k_{eff}$  values as a single figure of merit encompassing all the evaluations for the set of criticality experiments in which there is no identified trending parameter.

To determine the NDTL, the  $k_{eff}$  values for the critical experiments representing that waste type are tested for normality. If normality is found to be reasonable, the usual method for establishing a statistical, one-sided tolerance limit is applied to determine the critical limit (CL). This calculation is of the general form:

$$CL = k_{ave} - k(\text{confidence, coverage, sample size}) S_{combined}$$

where  $k_{ave}$  is the average value of the  $k_{eff}$  for the set of critical experiments,  $k(\text{confidence, coverage, sample size})$  is a multiplier that provides the desired confidence for the coverage of the population based on the sampled size, normality, and  $S_{combined}$ . The quantity  $S_{combined}$  includes the variability within the sample and the variability of the determination of the  $k_{eff}$  by the criticality code, i.e., the standard deviations that are provided with the individual  $k_{eff}$  values as output of the criticality calculation via the Monte Carlo code.

If normality is rejected, then the distribution-free tolerance limit must be applied. The result applies to that waste type represented by that set of critical experiments.

For NDTL situations not covered by the range of applicability of the set of critical experiments used to derive a CL, there are two cases. If the extension of the ROA is small and the understanding of the performance of the criticality code for these critical experiments is also understood, it would be appropriate to use the established CL and an appropriate margin. If the extension is not small, then more data, covering the ROA, will be necessary. If more data is obtained, the entire process of Figure 4-1 must be applied to the new data set.

*RAI 4-15 Justify the elimination of  $\Delta k_m$  in the Critical Limit for Normal Distribution Tolerance Limits (NDTL).*

*Same argument provided for LUTB with respect to  $\Delta k_m$  can be applied to NDTL.*

Response:

Please see the response to RAI 4-9 for DOE's position on  $\Delta k_m$ .

### **Section 4.1.3.2.3      Distribution Free Tolerance Limit**

**RAI 4-16      Demonstrate that the Distribution Free Tolerance Limit (DFTL) approach is at least as bounding as the lowest  $k_{eff}$  approach.**

*It appears that the selection of the  $l$ th  $k_{eff}$ , which is based on the  $l$  number of samples needed to provide the desired tolerance limit (e.g., 95/95) does not result in a low  $k_{eff}$  value for the critical limit. For example, based on the explanation provided by Natrella (1966, pp. 2-15), referenced in the topical report, using 95 critical benchmarks and 95% confidence,  $k_{eff}$  for 95% of the waste packages under a specific configuration for specific waste type will be below the third largest  $k_{eff}$  for the 95 critical benchmarks. What is needed is that with 99% confidence, 95% of the population (e.g.,  $k_{eff}$ ) fall below the smallest  $k_{eff}$  for the benchmark set.*

Response:

The following information addresses methodology, for which DOE is seeking NRC acceptance. The DFTL provides a Critical Limit (CL) such that for the waste form of interest, based on a sample of calculated  $k_{eff}$  values, there is a specified confidence that a stated proportion of the calculated  $k_{eff}$  values for that population for which the waste form will be critical will be greater than the CL. The CL on this basis is the value that calculated  $k_{eff}$  can not exceed without consideration of the possibility of criticality. There is high confidence that only a small portion of the population of calculated  $k_{eff}$  values for a waste form for which the waste form will be critical will be below the CL. The CL is the value that divides potentially critical and non-critical classifications. In the example values of the RAI, this CL is the value such that there would be 99% confidence that 5% of the population of calculated  $k_{eff}$  values for a critical configuration would be below this limit, which is an upper limit for application to assess potential criticality.

For the confidence and coverage cited in RAI 4-16, a sample of at least 90 values of  $k_{eff}$  values would be required to set a 99%/95% tolerance limit, using the smallest observation as the CL. A sample of about 135 critical experiments evaluated for  $k_{eff}$  would be required to allow use of the second smallest  $k_{eff}$  as the 99%/95% CL. In the example calculations described in the topical report, the confidence used is 95%, and the portion of the population covered is 99.5%. Under these conditions, a minimum sample of 600  $k_{eff}$  values would be required to set a 95%/99.5% tolerance limit, using the smallest observation as the CL. About 1000  $k_{eff}$  values would be required to set a 95%/99.5% tolerance limit, using the second smallest observation as the CL.

Choosing the smallest value of  $k_{eff}$  in a sample of  $n$  will provide, at a given confidence level, a proportion of the population that is above that value. If confidence and proportion of the population are chosen in advance, as in general applications, then, depending on sample size, the smallest observed  $k_{eff}$  may be more conservative than necessary.

As stated in the Topical Report, the sample size may restrict the confidence and/or the proportion of the population values that can be stated for the waste type when using the DFTL to determine the CL. If this is the case, there may be a need to obtain more  $k_{eff}$  data to provide the desired confidence and population coverage. DOE plans to reprocess any situation in which more data are obtained using the logic of Figure 4-1 for completeness.

RAI 4-17 Justify the elimination of  $\Delta k_m$  in the DFTL approach.

*Same argument provided for LUTB with respect to  $\Delta k_m$  can be applied to DFTL.*

Response:

Please see the response to RAI 4-9 for DOE's position on  $\Delta k_m$ .

RAI 4-18 Explain the use of the "3 standard deviations ( $3\sigma$ )" limit in a distribution-free mode.

*It is not clear why the "3 standard deviations ( $3\sigma$ )" is used. Is  $3\sigma$  enough to capture all possible scenarios?*

Response:

The following addresses methodology, for which DOE is seeking NRC acceptance.

Consider the following:

Reported Multiplication Factor	Reported Variability of Multiplication Factor	Value of Multiplication Factor Used to Determine the Critical Limit
$k_{eff, 1}$	$S_{mcnp, 1}$	$k_{eff, 1} - 3 * S_{mcnp, 1} = k^*_1$
$k_{eff, 2}$	$S_{mcnp, 2}$	$k_{eff, 2} - 3 * S_{mcnp, 2} = k^*_2$
$k_{eff, 3}$	$S_{mcnp, 3}$	$k_{eff, 3} - 3 * S_{mcnp, 3} = k^*_3$
.	.	.
.	.	.
.	.	.
$k_{eff, n}$	$S_{mcnp, n}$	$k_{eff, n} - 3 * S_{mcnp, n} = k^*_n$

These data ( $k_{eff, j}, S_{mcnp, j}$  for  $j= 1, 2, \dots n$ ), represent the results of criticality code evaluations of  $k_{eff}$  for a data set of  $n$  critical experiments applicable to a waste form. The individual values of  $k_{eff, j}$  are summary values of many trials, with an associated variability that is estimated by the MCNP standard deviation,  $S_{mcnp, j}$ . It is assumed that the many histories that result in  $k_{eff, j}$  as a summary parameter are normally distributed. The reduction of the individual values of  $k_{eff}$  by  $3 S_{mcnp, j}$  is made to account for this variability in a conservative fashion.

The choice of a multiplier of 3 is because, for a normal distribution, use of three standard deviations accounts for about 99.86% of the distribution. DOE believes this provides adequate confidence. The values of  $s_{mcnp,j}$  are generally small, which reflects the goodness of the estimate of the multiplication factor  $k_{eff,j}$ . This is the degree of conservatism offered. It cannot include all situations, and this method quantifies what is not covered.

In this situation, if the value of a specific  $k_{eff}$  is greater than 1.0, then the 3  $s_{mcnp,j}$  is deducted from 1.0, respecting the "non-positive bias" treatment. These modified values of  $k_{eff}$  are sorted to obtain the tolerance limit value that is the critical limit.

For the table shown, the values  $k^*_1, k^*_2, \dots, k^*_n$  would be sorted to determine the critical limit by the DFTL method.

#### **Section 4.1.3.3.1 Range of Neutronic Parameters**

*RAI 4-19 Provide a justification for not using a systematic approach used to identify the area and range of applicability with respect to criticality model validation for each configuration class and waste form.*

*The approach outlined in Section 4.1.3.3.1 is neither fully consistent with the approach in Lichtenwalter et al., nor is it comprehensive and complete with respect to identifying those parameters which may exhibit a trend in the criticality code bias.*

*Material concentrations, geometry, and spectrum are the areas (i.e., area of applicability [AOA]) within which the benchmarks must be evaluated for their applicability to the specific configuration class and waste form. Furthermore, there are sub-areas, if you will, within each of these AOAs which categorize the substantial variances within each of these AOAs, some of which are indicated in Page 4-18. Then, subsets of benchmarks which are based on waste package configuration class, waste form, and/or benchmark classes (e.g., Table 4.1 in Lichtenwalter et al.) need to be identified. After that, specific variables which can represent each of those categories and presence or absence of any associated statistically significant trends must be identified.*

Response:

DOE intends to use a systematic, comprehensive, and complete approach to identify the area and range of applicability with respect to criticality model validation for each configuration class and waste form. The general approach to identifying the range of applicability for each configuration and waste form is methodology for which DOE is seeking acceptance. The general approach is presented in Section 4.1.3.3.1 of the Topical Report. The specific parameters to be used are expected to be presented in the validation reports. A planned description of the validation report is provided with this response package. In particular, Part II.A of Attachment A addresses the planned development of

subsets. DOE plans to provide a basic description of the method to be used in a revision to the Topical Report.

DOE agrees that the approach in the Topical Report is not identical with the approach in the Lichtenwalter et al., nor is it comprehensive or complete without the information to be contained in the validation reports. It is intended that the approach used for identifying a range of applicability would be consistent with Lichtenwalter et al. 1997, although not necessarily identical. DOE plans to carefully evaluate Lichtenwalter et al. 1997 for applicability and will incorporate additional guidance from it as appropriate. Lichtenwalter et al. 1997 was intended for transportation packages, whereas the Topical Report addresses a geologic repository. The two applications differ in the design approach and regulations involved.

Lichtenwalter, J.J.; Bowman, S.M.; DeHart, M.D.; Hopper, C.M. 1997. *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages*. NUREG/CR-6361. ORNL/TM-13211. Oak Ridge, Tennessee: ORNL. TIC: 233099.

*RAI 4-20 Clarify why the values for AENCF in CRWMS M&O 1998n are in mega electron volt (MEV) range as opposed to fractional or single digit electron volt.*

*Staff notes that AENCF inappropriately weights higher energy neutrons, resulting in thermal systems having an AENCF in the 10 keV range, whereas the predominant fission rate spectrum is actually centered in the 0.1 eV range of neutron energies. Use of Energy of Average Lethargy of neutrons causing Fission (EALF) will correct this problem. SCALE4.4 now includes the EALF parameter in its output. A corresponding Type 4 tally specification for MCNP4B can be designed by the code user.*

Response:

DOE believes that discussions of specific spectrum parameters for characterizing configurations or the value ranges of the spectrum parameters are application issues and not methodology issues and are, therefore, not appropriate for inclusion in the Topical Report except as examples. The following discussion is provided for informational purposes only.

AENCF is an energy-times-weight tally divided by a weight tally. Therefore, the average energy calculated will be in the MeV range, even in a thermal system. Lethargy, on the other hand, is the log of the inverse of energy ( $\ln(10/E)$ , where E is in MeV.). Therefore, the units of EALF will be much lower, in the fractional or single digit electron volt range and can be obtained using a type 4 tally specification using MCNP4B.

DOE agrees that the equivalent of the EALF parameter can be obtained using a type 4 tally specification using MCNP4B. For thermal systems the EALF seems intuitively more appropriate than the AENCF parameter. Both of these parameters will be considered. The one that is appropriate for the configurations and waste form analyzed will be

chosen, assuming that either one shows the most meaningful trend when compared to other parameters investigated.

The Topical Report used AENCF as an example since a significant trend was found when using all of the laboratory critical experiments that were described in the appropriate references supplied with the Topical Report. The use of this example gives the impression that AENCF is the only spectral parameter that will be analyzed and further that it is an appropriate parameter for intact commercial fuel. Because NRC's review is not covering the additional requests made in the Topical Report, such as approval of models or the specific benchmark experiments, DOE plans to remove those parts that imply AENCF is a trending parameter or is fundamental for any waste form. This includes removal of Figure 4-3 from the Topical Report and any other information that implies a parameter has been selected for trending.

#### *Section 4.1.3.3.3 Extension of the Range of Applicability*

*RAI 4-21 Provide the rationale for switching from LUTB method to NDTL method for extending the range of applicability.*

*The method for determining  $\Delta k_c$  must be based on the 99.5% of future calculations as opposed to single future calculation on which NDTL may be based. Furthermore, the margin or zone of criticality must be included in  $\Delta k_m$ .*

Response:

The following addresses methodology, for which DOE is seeking NRC acceptance. The context of this response is for extension of the range of applicability for the situation in which there are no new data. The method described in Section 4.1.3.3.3 of the Topical Report does not change the method for determining the critical limit from the LUTB method to the NDTL method, if the LUTB is the basis for the critical limit. The extension is subject to other conditions, discussed in paragraph D.2 in this section of the Topical Report.

The LUTB critical limit is based on the extreme values on the range of the predictor variable and would not be correct for the extension beyond that range. However, the use of standard regression tolerance limits will provide a lower critical limit than would be obtained by simply extending the LUTB results. This extension follows the original trend line, but the tolerance limit will be calculated using a method that accounts for the extension distance, which makes the critical limit lower than the extension of the original LUTB line. This is what is meant in the Topical Report.

The  $\Delta k_m$  concern is addressed in the response to RAI 4-9.

*RAI 4-22 Describe the approach in establishing an additional margin when performing extrapolation beyond the range of applicability.*

*The report indicates that an additional margin will be added when extrapolation is extended beyond the range of applicability. However, it does not discuss the approach in establishing or quantifying this additional margin. Discussion with regard to the approach in establishing additional margin beyond the range of applicability is needed.*

Response:

Acceptance of the general approach for extending the range of applicability in Section 4.1.3.3.3 of the Topical Report is requested, except for the following modification. Item D.2 in that section discusses use of an additional margin defined as  $\Delta k_m$ . This additional margin is not part of  $\Delta k_m$ . The Topical Report will be modified by removing the phrase " $(\Delta k_m)$  as defined in subsection 4.1.3.2."

The approach to establishing additional margin when extrapolation is made beyond the range of applicability will depend on the nature of the bias and the applicable experiments used to establish the bias. Thus, the approach is dependent upon the waste form and its configuration, as well as various aspects of the applicable experiments. The specific approach is, therefore, an application issue for which acceptance is not being sought. DOE expects to document the methodology and justification of the specific approach in the appropriate model validation report (see Attachment A). The following discussion is provided for informational purposes only.

In general, there are several approaches, some or all of which may be used to perform this extrapolation. The following approach relies heavily on Appendix C of ANS-8.1-1998 and is not necessarily definitive. That is, variations of the approach given below or even other approaches not presented here may be appropriate.

"The area (or areas) of applicability of a calculation method may be extended beyond the range of experimental conditions over which the bias is established by making use of correlated trends in the bias." (ANS-8.1-1998, Appendix C)

As stated in the Topical Report, the first step is to understand the nature of the bias. For this reason, the calculation method should be "subjected to a study of the bias and potentially compensating biases associated with individual changes in materials, geometries, or neutron spectra." This process will allow changes that can affect the extension to be independently validated. In practice, this can be accomplished in a step-wise approach. That is, benchmarks for the validation should be chosen (where possible) such that the selected experiments differ from previous experiments by the addition of one new parameter so the effect of only the new parameter on the bias can be observed (ANS-8.1-1998; Appendix C). In practice, this may be difficult or prove to be prohibitively expensive. However, one can analyze a subset of a series of experiments and subsequently add the data from the remainder of the set of experiments to verify that indeed the bias continues to change in a systematic matter as discussed above. This is a standard technique of regression analysis that is used to test the validity of a trend. An understanding of the bias may also be obtained by an analysis of the physics of the series of experiments to determine if there are reasonable effects that may be causing these

biases. The overall effect of these suspected parameters then may be tested by sensitivity studies that vary these parameters. If it can be shown that the sensitivity studies alter the bias, these may provide some reasonable assurance that extension of the area of applicability is reasonable and may point to a justification for the additional margin to be used.

In addition to the technique above, the calculation method should be "supplemented by alternative calculation methods to provide an independent estimate of the bias (or biases) in the extended area (or areas) of applicability." (ANS-8.1-1998, Appendix C) DOE expects that this alternative method will, to the extent feasible, be one that has been similarly benchmarked against experimental data and is established by industry practices for its intended use. To the extent feasible, it will use techniques that have been previously approved by the Nuclear Regulatory Commission for its use or that have been widely used and accepted in the industry. Further, DOE expects to choose this method to compensate for some of the known weaknesses in the primary method. The secondary method may also be more efficient, or more appropriate for sensitivity studies than a Monte Carlo method. After this analysis is performed and with an understanding of the nature of the bias, a qualified analyst can determine a reasonable additional margin to be used for the application by a comparing the results of each method and choosing a bounding value for the additional margin.

As a supplement to or in place of the sensitivity studies described above, DOE may use stochastic analysis similar to the one used for the additional margin provided for the uncertainty of decay constants and branching fractions of radionuclides. This latter approach is preferable if there is some doubt that an analysis is bounding over the entire range of application of the added margin.

The application of a margin could also consider other margins that are being used as a result of a particular design approach used for a specific waste form, if these margins can be defined. An arbitrary margin could also be used. This additional margin may be arbitrarily large (e.g., 0.05) if any of the above stated approaches are unable to produce a reasonable assignment of the additional margin. DOE expects to document the specific methodology and rationale for determining the additional margin in the appropriate validation report.

An example of an approach to extend the range of applicability for a particular application is given below.

Figure 4-6 of the Topical Report shows a trend of  $k_{\text{eff}}$  versus Burnup, up to a burnup of approximately 33 GWd/mtU. This information was taken from a scoping assessment of the trend shown in Figure 4-6.

In the scoping assessment, a code-to-code comparison was made using the computer codes CASMO and NEMO to calculate  $k_{\text{eff}}$  versus burnup for over 30 statepoints from a particular nuclear plant.

CASMO is a multi-group two-dimensional transport theory computer code for burnup calculations on boiling water reactor and pressurized water reactor assemblies or simple fuel pin cells. The code handles a geometry consisting of a cylindrical fuel rod of varying composition in a square pitch array with allowance for fuel rods loaded with gadolinium, burnable absorber rods, cluster control rods, in-core instrument channels, water gaps, boron steel curtains, and cruciform control rods in the regions separating fuel assemblies. Typical fuel storage rack geometries can also be handled. The CASMO computer code has been approved by the NRC for use in obtaining burnup credit for fuel storage rack licensing. Further, the use of the CASMO computer code has been accepted by the NRC for use in a reactor reload licensing analyses. It is widely used in the nuclear industry and has hundreds of years of reactor experience to support its use.

NEMO is a computer program that allows the user to model the distribution and magnitude of neutrons within a pressurized water reactor in either steady state or transient conditions. The input to the computer code describes a physical size of the reactor core, the location of materials (fuel assemblies, reflector regions) within the reactor core, and the neutronic properties of the materials (cross-sections). NEMO uses a nodal expansion method to solve the two-group, multi-dimensional neutron diffusion equations. The NEMO computer code also performs a multi-dimensional depletion of major isotopes or groups of isotopes present in the reactor core. It also accounts for thermal-hydraulic feedback in performing its assessment of reactivity and calculates the spectral variations occurring in the core of a pressurized water reactor. The NEMO computer code has also been approved by the NRC for use in reload licensing of Pressurized Water Reactors. NEMO and its predecessor codes, also approved by the NRC, have hundreds of years of reactor experience to validate their accuracy.

Both of the codes cited above, because of their acceptance by the NRC and the hundreds of years of reactor experience, are examples of computer codes that are established in the industry and have been accepted by the NRC. Therefore they are candidates for performing reactivity analysis on the specific benchmark experiments DOE chooses to use for validation of the computer code systems SAS2H and MCNP.

A comparison of the SAS2H/MCNP method with the CASMO/NEMO method showed a negative bias with burnup similar to that shown in Figure 4-6. The slope on the bias using the CASMO/NEMO method was not as large as the slope using the SAS2H/MCNP method. This is evidence that most of the bias is independent of the analytical method and is, therefore, experimental. (The method chosen to determine bias cannot separate experimental bias from calculated bias.)

These biases are most likely caused by one or more of the following:

1. The method used for measuring core power (and hence burnup) is biased such that the actual power in the reactor is less than the measured value.
2. The measured value of the boron-10 concentration may have a bias since the boron content (boron-10 and boron-11) is measured and the naturally

occurring isotopic abundance is assumed. This means of measuring the boron-10 content can be biased if the same boron is used for a long time in a reactor. This allows a significant portion of the boron-10 to be depleted.

3. There may be biases and errors in cross-sections, geometry specifications or material concentrations.

To assess the effects of the three items, sensitivity calculations could be performed to determine the reactivity effects of biasing the phenomenon within reasonable ranges. Additional margins could be estimated by assuming reasonable but bounding extremes for these effects (e.g., assume that the boron used in a given cycle is continuously recycled without the addition of fresh boron for a whole cycle). The difference between the mathematically extrapolated value of the bias and the bias obtained with the bounding assumptions could be used as the extra margin. This extra margin or bias would be in addition to extra bias that was needed due to the mathematical effects inherent in the method chosen to determine the bias at the extreme end of the range of the trended parameter. In some cases additional measurements may be needed to verify the bounding assumptions (e.g., measurements of boron-10 content in the coolant of operating nuclear plants).

The techniques and example described above are applicable to a particular waste form configuration. The causes of the bias for other waste forms (e.g., high-level waste) will be different. It should be further emphasized that this is an example since the range of applicability where burnup is the trending parameter can be extended by adding more commercial reactor critical benchmark experiments to the database. Under any circumstances, the use of code-to-code comparisons and sensitivity studies to understand the physical processes producing these biases (either experimental or analytical) would be used along with an engineering evaluation of the potential causes of a bias.

Since this approach is waste form dependent, approval of the approach in the example is not sought in the methodology Topical Report. It would be subject to NRC review as part of the License Application. Acceptance of the general approach in Section 4.1.3.3.3 of the Topical Report is requested.

#### ***Section 4.1.3.4 Discussion of Results***

*RAI 4-23 Present the results in terms of their applicability to the waste package configurations under repository conditions with respect to material, geometry, and spectrum.*

*Table 4-1 presents only the results of modeling and calculating  $k_{eff}$  for the Laboratory Critical Experiments (LCE) and CRC without making any connection to their applicability to the different waste package configurations in the repository with respect to specific ranges of parameters covering material, geometry, and spectrum.*

Response:

DOE believes that the example results presented in Table 4-1 are application information and not part of the methodology. The following discussion is preliminary and for informational purposes only.

DOE plans to provide the type of information from Table 4-1 and the presentation of the results in the manner requested in the RAI in the validation reports. Until the designs are established, the results presented in Table 4-1 cannot be presented in terms of their applicability to waste packages or repository conditions. Table 4-1 was shown to give a sense of the accuracy of the chosen method by showing average values of  $k_{eff}$  calculated and its standard deviation. It will be removed from the Topical Report, as will the requests for acceptance made in the Topical Report related to specific applications such as specific benchmark experiments.

#### **Section 4.1.3.4.1 Trending Results for Commercial Spent Nuclear Fuel**

RAI 4-24 *Demonstrate the applicability of CRCs to the waste package configuration with the intact waste form with respect to the following areas:*

- (a) *Material (e.g., plate boron concentration, soluble boron concentration, reflector composition, fuel material properties, etc...)*
- (b) *Geometry (e.g., assembly separation distance, poison plate thickness, reflector wall separation distance, etc...)*
- (c) *Spectrum (e.g., Average Energy for Neutrons Causing Fission (AENCF) compared to AENCF for intact waste form)*

*CRWMS M&O 1998n does not establish the applicability of CRCs to the waste package with the intact waste form as requested in this topical report. For example, Table 2.4-1 on Page 60 of CRWMS M&O 1998n shows the AENCF range for CRCs are only between 0.2475 MEV and 0.2643 MEV. However, the same table shows the AENCF range for all the configurations in the repository is between 0.0016 MEV and 0.3311 MEV. Assuming the AENCF range for the waste package configuration with intact spent fuel assemblies is somewhere between 0.0016 and 0.3311 (the report should specify the AENCF along with all the relevant benchmarking parameter ranges for the intact spent fuel assemblies), at least the CRC range with respect to AENCF spectral index must cover the waste package configuration with the intact waste form.*

Response:

DOE will remove the request in the Topical Report for approval of application of the methodology to commercial fuel in an intact form and those parts that imply AENCF is the chosen trending parameter or is fundamental for any other waste form. DOE plans to demonstrate commercial reactor critical (CRC) applicability in the model validation reports. (Attachment A provides the proposed planned workscope for these reports.)

However, a brief response to the questions, for informational purposes only, is provided below. The source of this information is CRWMS M&O 1999.

DOE expects to apply many parameters, in addition to those used as trending parameters, to characterize both the expected repository configurations and the experiments in the waste form- and configuration class-specific subsets. These parameters may include, but are not limited to: cooling time, fuel temperature, fuel type, cladding type, fuel density, geometry type (e.g., square lattice, triangular lattice, homogeneous solution), absorber types, and absorber concentrations. In addition to these, DOE expects to trend against selected spectral, material, and geometry specific parameters. The trending parameters may include, but are not limited to: neutron spectrum ratios, enrichment, burnup, actinide ratios, plutonium concentrations, boron concentrations, fuel pellet diameter, fuel rod spacing, and fuel rod pitch to fuel pellet diameter ratios. The trending parameters may also include parameters that consider the absorption, fission, and leakage spectra. (See Attachment A, Parts II.B.2 and II.D.)

Page 179 of Lichtenwalter et al. (NUREG/CR-6361) states that three fundamental parameters should be considered in the selection of suitable experiments for use in the evaluation of transportation and storage package designs. They are as follows: (1) geometry of construction, (2) materials of construction (including fissionable material), and (3) the inherent neutron energy spectrum affecting the fissionable material. The following discussion provides a general qualitative description of the characteristic ranges that influence the neutronic behavior in the CRCs and waste package, and the applicability of the CRCs to a waste package. It should be noted that the CRCs are included as part of the establishment of bias and uncertainty for a critical limit, which is used in the generation of a loading curve. As stated in the Topical Report, laboratory critical experiments and radiochemical assays will also be used. The CRCs are not assumed to fully correspond with the waste package configuration, which is why the LCEs are analyzed (e.g., to consider absorber plate effects and reflector materials). Figure 4.24-1 is a representative comparison of the relative neutron spectrum in the waste package and in a CRC. This waste package configuration was composed of burned fuel ranging in assembly average burnup from 16.358 GWd/mtU through 34.416 GWd/mtU, with an essentially infinite water reflector.

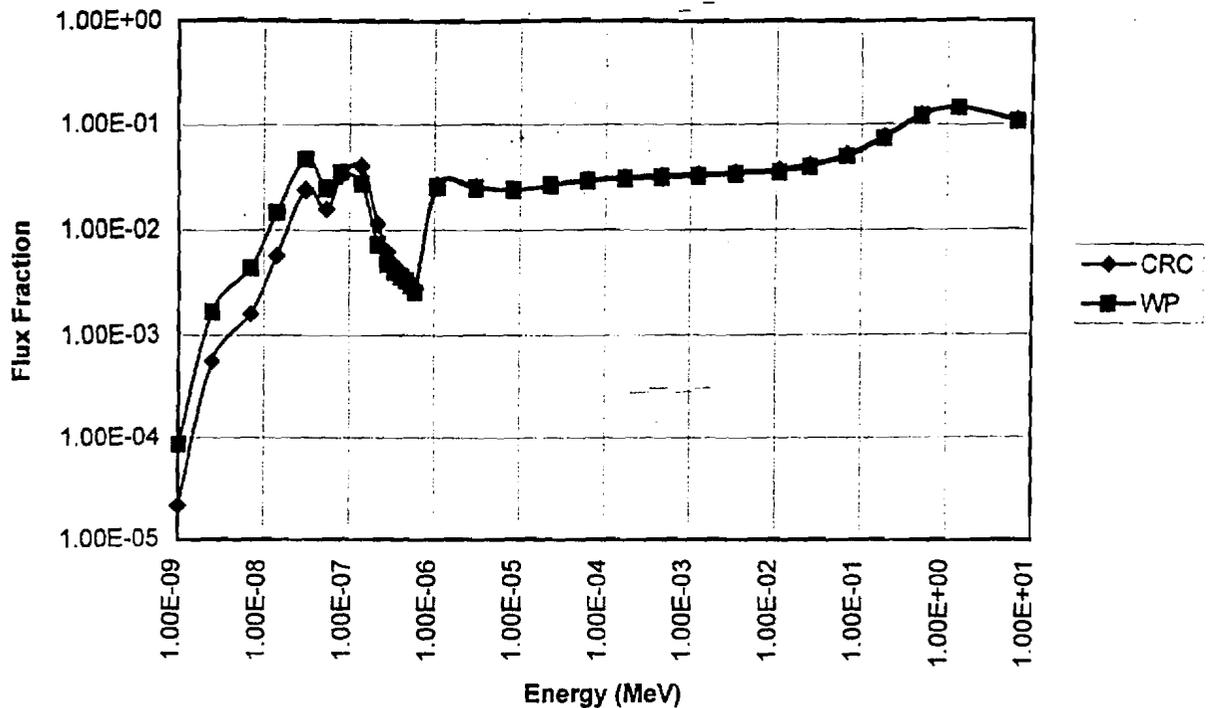


Figure 4.24-1. Neutron Spectra for CRC Core and Inner Cavity of waste package

As can be seen in Figure 4.24-1, the relative flux spectra are essentially identical in the CRCs and waste packages above 4 eV. Figure 4.24-1 shows that the CRC relative flux spectrum is lower at energies below 0.1 eV than the comparable waste package. This behavior is expected from the differences in temperature and fuel-to-moderator ratios. This slight shift in spectrum has a small effect on the fission reaction rate. The effect of this shift in neutron spectrum is expected to be accounted for by the waste package design (e.g., use of neutron absorbers). Thus, the neutron spectra in the waste package and in the CRC are very similar.

CRWMS M&O 1999. *Waste Package, LCE, CRC, and Radiochemical Assay Comparison Evaluation*. B00000000-01717-0210-00107 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990812.0351.

Lichtenwalter, J.J.; Bowman, S.M.; DeHart, M.D.; Hopper, C.M. 1997. *Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages*. NUREG/CR-6361. ORNL/TM-13211. Oak Ridge, Tennessee: ORNL. TIC: 233099.

### **Section 4.2.1 Corrosion Model**

*RAI 4-25 Justify the extensive reliance on the wide range of corrosion rates utilized to determine the probability and location of a WP breach.*

*Given sufficient criticality control in the as-fabricated WP, a breach in the WP is necessary for a criticality event to occur. The model used to determine the probability of a WP breach and its location was the WAPDEG code using the Total System Performance Assessment (TSPA)-Viability Assessment (VA) base case. The primary limitation of this case is that the input parameters for corrosion rate rely extensively on expert elicitation, with nearly five orders of magnitude variance in the corrosion rate utilized. Thus, the possibility exists for a wide range of WP failure times and a commensurately wide range of times in which criticality control becomes important. The wide range of corrosion rates resulting from the heavy reliance on expert elicitation is considered a limitation to the utility and validity of the subsequent criticality analysis, since it leads to dilution of the probability of occurrence and resulting risks.*

Response:

The expert elicitation process for estimating corrosion rates for the more corrosion-resistant steels was only a temporary expedient, caused by the lack of corrosion test data, for preliminary analyses. The range of possible corrosion rates is expected to be considerably narrowed by using data from the extensive corrosion testing program underway at Lawrence Livermore National Laboratory and the University of Virginia. DOE plans to revise the Topical Report to state that corrosion rates are expected to be determined primarily from corrosion testing data.

*RAI 4-26 Provide justification for the long-term credit being taken for the presence of fuel cladding in the degradation analysis.*

*It appears that credit is being taken for the presence of Zircaloy-4 cladding in terms of its corrosion resistance. Although Zircaloy-4 does have good corrosion resistance, it is known to suffer from localized corrosion under reasonably attainable conditions inside breached WPs. Additionally, the cladding can be degraded prior to disposal due to the effects of irradiation, reactor water chemistry, and predisposal storage conditions. Commercial SNF exhibits a wide range of Zircaloy material characteristics, including large variations in the degree of hydriding, oxidation, erosion thinning, embrittlement, crack formation, pellet-cladding interactions, and crud depositions. Further information is requested on the technical basis that this degree of credit can be claimed for the Zircaloy-4 cladding and the effect on criticality control if no credit is taken.*

Response:

DOE believes that the inputs used in the degradation models fall in the application area as opposed to the methodology area and are inappropriate for inclusion in the Topical Report.

However, to provide further information, it is expected that future TSPAs and criticality evaluations used to support the License Application will have a common approach to Zircaloy cladding credit for commercial SNF based on extensive testing, carefully reviewed modeling, and appropriate conservative assumptions.

#### **Section 4.2.2 Internal Geochemistry Models**

*RAI 4-27 Clarify the internal geochemistry model treatment of Uranium (U) produced from WF degradation.*

*WF U is input into solution (along with other degradation products) according to fixed degradation rates and solution evolution modeled in EQ6. What is not clear is if U secondary phases are allowed to precipitate, in effect lowering the U release rate and perhaps lowering the probability for potentially critical external accumulations. References cited in the topical report suggest that secondary U phases will be included in internal degradation models. These references include CRWMS M&O (1998e)<sup>7</sup> and CRWMS M&O (1998q)<sup>8</sup>, the latter being cited in the former. For example, in section 6.3.2 of CRWMS M&O (1998e), EQ6 models of SNF degradation are said to lead to precipitation of the hydrated uranyl silicate soddyite. In contrast, retention by secondary U phases are not modeled in the TSPA-VA. Clarify whether these differing approaches will be reconciled in future work.*

#### **Response:**

The observations of the staff are correct. The references cited in the Topical Report consider the precipitation of secondary phases, while TSPA-VA does not. There are two reasons for the difference in approach. First, there is a difference between the conservative objectives. For criticality internal to the waste package, the conservative approach allows the most neutron absorber to be removed from the waste package, while keeping the most fissile material in the waste package, hence the precipitation of uranium minerals. In contrast, TSPA is concerned with the release of radionuclides such as actinides, which include uranium. Of course, most of the uranium has very low radioactivity, so its precipitation in the waste package would have little effect on dose at the accessible environment.

This leads to the second reason for the difference in approach. Because of the strong concern with the fissile material remaining in the waste package after waste form dissolution, a steady-state flow-through capability (described in Section 3.1.1 of the Topical Report) has been added to EQ3/6 for use in the studies cited in the Topical Report. This capability was not available in 1997, when all the inputs to TSPA-VA were finalized. The geochemistry treatment of waste form uranium and other materials will be similar in the future for both types of evaluations. DOE plans to explain any differences in the appropriate License Application reference document.

*RAI 4-28 Compare and contrast the approach to modeling to be used for release and internal geochemistry in the criticality analysis with that employed in present and future TSPA models (which may or may not use EQ3/6).*

*It was stated in topical report section 4.2.1 that WF degradation modeling in the criticality analysis will employ TSPA model approaches, but it is not clear if this extends to modeling release from WPs. TSPA-VA did not explicitly employ EQ3/6 geochemical modeling of WF alteration, RN release, and secondary solid phase formation. Any deviations from the TSPA-VA approach in the criticality analysis should be demonstrably more conservative or supportable.*

Response:

As stated in the response to the previous RAI, all future geochemistry calculations for performance assessment and criticality evaluations will be consistent as appropriate. They are both expected to use the most up-to-date computer codes available. The current up-to-date geochemistry code is EQ3/6, which is expected to soon be supplemented by the geochemistry-transport code PHREEQC, for external accumulation of fissionable material. DOE plans to include information about PHREEQC in any revision to the Topical Report.

*RAI 4-29 Specify what kinetic models will be used in the internal geochemistry models and clarify whether default EQ6 values will be used.*

*Selection of kinetic models profoundly influences model results regarding degradation products and water chemistry. Cited documents discussing EQ6 degradation models (CRWMS M&O, 1998e, 1998q, and Appendix C reference 1998e) do not address kinetic models affecting the rates at which WP and WF degradation products precipitate. It appears that either default EQ6 kinetic parameters are utilized or kinetics are not included. Because degradation products are integral to criticality models, calculations predicting their formation should rely on supportable or conservative kinetic data. This comment applies also to the external geochemistry models discussed in section 4.2.3 of the topical report.*

Response:

EQ6 calculations are run in kinetic mode (i.e., not in the reaction progress mode). Most calculations use constant rates (EQ6 input parameter nrk=3) for the degradation of initial solid components, with the rate specified in the input file parameter rk1, in moles/(cm<sup>2</sup>·sec). The constant rate is used because (1) limited rate data are available for corrosion of most package materials, and (2) most waste package reactants are grossly out of equilibrium with the aqueous component of the system, and there is no benefit to tracking the affinity of the waste package "reactants." In calculations currently underway, true transition state theory (TST) rates, taken from the literature, are used for modeling silicate reactions with package effluents.

To ensure conservatism, many rate combinations are used for models of waste package degradation. In current calculations, the  $k_1$  of each package material may take two to three values, covering a range of 1 to 3 orders of magnitude. Each EQ6 run combines average-high or low-high-average rates for glass, fissile material, and steels, with drip rates (water influx rates) ranging from 0.0015 to 0.5 m<sup>3</sup>/year. Combinations of low rates from one material, and high rates from another, may produce the most "conservative" results, e.g., a low glass rate may allow acidity to build from rapid steel degradation, increasing loss of gadolinium. While this "rate matrix" approach requires large numbers of runs, it is expected to uncover unusual conditions that may enhance solubility or precipitation of fissile materials.

For most of the degradation products, the kinetic rule is instant equilibrium. However, for those phases for which a kinetic model is controlling (particularly silica bearing minerals), the transition state theory kinetic model is used.

RAI 4-30      *Justify the use of J-13 well water as representative of the solution that would be present within the WP.*

*Once the WP is breached, corrosion and degradation of WP internals play important roles in criticality control. Although some testing data has been obtained, the results are based on experiments conducted in variants of simulated J-13 well water. It seems unlikely that the chemistry of the solution inside a WP would be a J-13. Furthermore, it is unclear if the testing program and the subsequent analysis has considered the possibility of chemistry changes resulting from evaporative processes and dissolution products from WP components (e.g., acidification due to metal cation hydrolysis, alkalization from dissolution of HLW glass, etc.). Because of possible chemistry change, the corrosion mode and corrosion rates could be altered from the general corrosion case considered. For example, alkalization could lead to the formation of a passive film on carbon steel components that could then experience localized corrosion in the form of pitting or crevice corrosion in the presence of chloride. Similarly, the corrosion mode of stainless steel components could change from relatively slow passive dissolution to more rapid localized corrosion, which could lead to unanticipated, catastrophic failure of WP internal components. These accelerated corrosion modes could make conditions for criticality more favorable by allowing fuel materials to coalesce. Further information justifying the environments chosen and any further work examining likely alternate chemistries and their effects on material degradation is requested.*

Response:

J-13 water has been used for the composition of water entering the waste package but never for the composition of the water in the waste package. A principal objective of the geochemistry code calculations is to determine what aqueous composition is expected to result from the various degradation processes. The composition of the solution in the waste package is a function of the volume of standing water in the waste package and the

rate of flow into (and out of) the waste package. The geochemistry calculations cover a range of values for these parameters (CRWMS M&O 1998a).

DOE believes that the inputs used in the geochemistry and degradation models are application issues and not methodology issues and, therefore, are not appropriate for inclusion in the Topical Report. The following information is preliminary and is provided for informational purposes.

The sensitivity of geochemistry results to the composition of the *incoming* J-13 water is being tested by varying the principal parameters over a set of likely ranges. These parameters are determined by DOE's geochemistry experts. In general, the waste package degradation calculations (CRWMS M&O 1998a) predicted that the greatest release of uranium, plutonium, and gadolinium (which is very important because it is an added neutron absorber for disposal of several of the more highly reactive waste forms) occurs when there is rapid degradation of one or more waste package components. Rapid degradation of waste package components has a larger effect on the waste package aqueous chemistry than do any possible variations from the incoming J-13 water composition (CRWMS M&O 1998b). For example, for those waste forms involving codisposal with HLW glass, the rapid glass degradation will often drive the ionic strength to ~1 molal. Steel degradation somewhat faster than normal can drive pH below 5. Under these conditions, the aqueous phase deviates from the nominal J-13 composition by much more than the variety of suggested modifications for the composition of the indripping water.

DOE plans to support any licensing applications of geochemistry codes by a thorough sensitivity analysis with respect to composition of the indripping water. The following is typical of the sensitivity analyses performed thus far. DOE varied the equilibrated  $\log_{10}(f\text{CO}_2)$  values from -2.5 to -3.5, and the  $\text{Ca}^{++}$  concentration constraints were also varied. The calculated uranium loss from the package varied by a factor of <3 (principally due to  $f\text{CO}_2$  variations), but the calculated gadolinium loss varied by less than 20%.

With respect to the last two sentences (accelerated corrosion rates) of this RAI, DOE plans to revise the Topical Report to indicate that if a geochemistry evaluation shows very low pH, or other corrosion-enhancing condition, that geochemistry will be re-evaluated with appropriately enhanced corrosion rates reflecting the affected waste package components.

CRWMS M&O 1998a. *EQ6 Calculations for Chemical Degradation of PWR and MOX Spent Fuel Waste Packages*. BBA000000-01717-0210-00009 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980701.0483.

CRWMS M&O 1998b. *EQ6 Calculations for Chemical Degradation of Fast Flux Test Facility (FFTF) Waste Packages*. BBA000000-01717-0210-00028 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981229.0081.

### **Section 4.2.3 External Geochemistry Models**

**RAI 4-31** Describe how colloidal deposition will be incorporated into modeled chemical deposition.

*Indicate whether the approach will be the same as those adopted under TSPA. Evaluation of models of fissile material accumulation requires full understanding of colloid modeling. A previous analysis of external criticality (CRWMS M&O, 1998p) concluded that colloidal transport and accumulation of fissile materials would be insignificant. It should be clear how new analyses will differ and to what extent they are supportable and conservative.*

Response:

DOE plans to use the same model for colloids (formation, transport, and adsorption) in criticality evaluations as it will use in TSPA. DOE plans to revise the Topical Report to state this. This model is currently under development.

### **Section 4.2.4.1 Validation of Degraded Methodology**

**RAI 4-32** Provide more information on validation methods for the "pseudo flow-through" internal and "open system" external EQ6 models.

*With regard to the "pseudo flow through" model, topical report section 4.2.4.1 refers only to hand calculations supporting the solute concentration adjustments (CRWMS M&O, 1998q). This exercise only partially addresses the question of the validity of the model results.*

*In discussing the "open system model," it is stated that the results are conservative, but the pertinent reference (CRWMS M&O, 1997f) is missing from the chapter 6 reference list. The report acknowledges that validation has not yet been done, but does not describe how it will be done. This information is vital to assessing the methodology (see also discussion of topical report section 4.2.4.2 below). Validation approaches should provide confidence that models will not underestimate the effects of processes that could lead to criticality.*

Response:

The pseudo flow-through mode of EQ3/6 mentioned in the Topical Report has been replaced by a modification to the EQ6 portion of the code, called the solid-centered-flow-through code, which automatically incorporates the adjustment of water volume at each timestep. This enables the modeling of water inflow and outflow to track the timestep adjustment process exactly. Use of this code will ensure that the chemical changes are accurately resolved in time and that they also accurately reflect the volume of water in the waste package at any given time. This new version of EQ6 had been qualified (CRWMS M&O 1998, CRWMS M&O 1999a, CRWMS M&O 1999b). The Software

Qualification Report for this new version of EQ6 (CRWMS M&O 1998) includes tests of the solid-centered flow-through method. The tests include comparisons against analytical solutions, and also comparisons against results obtained by chaining several thousand individual EQ6 runs (with adjustment of the water mass between each run). The agreement among the different methods was quite good.

With respect to the open system model for external accumulation of fissionable material discussed in the Topical Report, it should be mentioned that DOE has added the geochemical transport code, PHREEQC, to our tools library. The open system external model discussed in the Topical Report was a temporary expedient and has been replaced by the industry standard geochemical transport code, PHREEQC, which is expected to be supplemented with a new version of EQ3/6 incorporating a Lagrangian transport model. The validation of these codes is discussed in the response to RAI 4-33, below.

DOE plans to revise the Topical Report by modifying the first two paragraphs and adding a third paragraph at the beginning of Section 4.2.2, to read as follows:

“Version 1 of 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 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<sup>3</sup> 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. For version 1 of the model, 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 kilogram).

Version 2 of the model has replaced the pseudo flow-through mode of EQ3/6 by a modification to the EQ6 portion of the code, called the solid-centered-flow-through code, which automatically incorporates the adjustment of water volume at each timestep. This enables the modeling of water inflow and outflow to track the timestep adjustment process exactly, thereby ensuring not only that the chemical changes are accurately resolved in time, but that they also accurately reflect the volume of water in the waste package at any given time. This new version of EQ6 has been qualified (CRWMS M&O 1998, CRWMS M&O 1999a, CRWMS M&O 1999b). The Software Qualification Report for this new version of EQ6 (CRWMS M&O 1998) includes tests of the solid-centered flow-through method. The tests include comparisons against analytical solutions, and also comparisons against results obtained by chaining several thousand individual EQ6 runs (with adjustment of the water mass between each run)."

Note that the reference citations in the third paragraph of the proposed modification to Section 4.2.2 of the Topical Report are to this response. DOE plans to incorporate these references into the Topical Report with appropriate citations.

CRWMS M&O 1998. *Software Qualification Report (SQR) for Addendum to Existing LLNL Document UCRL-MA-110662 PT IV: Implementation of a Solid-Centered Flow-Through Mode for EQ6 Version 7.2b*. CSCI: UCRL-MA-110662 V 7.2b, SCR: LSCR198, MI: 30084-M04-001. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990312.0336.

CRWMS M&O 1999a. *Software Qualification Report (SQR) for Addendum to Existing LLNL Document UCRL-MA-110662 PT IV: Implementation of a Solid-Centered Flow-Through Mode for EQ6 Version 7.2b*. CSCI: UCRL-MA-110662 V 7.2b, SCR: LSCR198, MI: 30084-M04-001. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990920.0169.

CRWMS M&O 1999b. *Software Change Request (SCR) LSCR198; Addendum To EQ6 Computer Program for Theoretical Manual, Users Guide, and Related Documentation UCRL-MA-110662 PT IV (C)*. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990305.0112.

#### Section 4.2.4.2      *Validation of the EQ3/6 Geochemistry Code*

RAI 4-33      *Provide additional information on the validation of EQ3/6 for the specific applications. The validation examples provided in topical report section 4.2.4.2 (Bourcier 1994<sup>9</sup>, Bruton and Shaw 1988<sup>10</sup>, Bruton, 1996<sup>11</sup>, Wolery and Daveler, 1992<sup>12</sup>) do not adequately cover the conditions and processes to be included in the models. For example, the validated spent fuel and HLW models (Table 4-3) did not include the other waste package components (e.g., metal plates) to be included in the internal models. In addition, no examples are given that are comparable to the external models of low-temperature interaction between drift effluent waters and fracture walls. The DOE should state whether or not any new analyses will be performed that would support validation under the conditions to be modeled and, if not, how model confidence will be improved.*

Response:

As the RAI notes, the validation discussions in the Topical Report were examples and not intended to fully validate EQ3/6. DOE believes that full validation is an application issue and not a methodology issue and, therefore, is not appropriate for inclusion in the Topical Report. Additional validation of the EQ3/6 code will include two activities not used previously, (1) comparison with alternative analyses that implement conservative approximations for processes lacking experimental verification, and (2) comparison with the geochemistry/transport code PHREEQC. This latter code is particularly important because it brings some needed modes for transport and adsorption in the invert and rock. In addition, new versions of EQ6, under validation, include radioactive decay (particularly conversion of Pu-239 to U-235) and a legitimated Lagrangian transport capability. DOE plans to fully validate EQ3/6 in the validation reports and in the supporting documents for the License Application.

Transport calculations, similar to those in the Topical Report, may be repeated by two codes (e.g., PHREEQC and linked EQ6 runs, or PHREEQC and the Lagrangian version of EQ6), if there is reason to believe that it will enhance the credibility of the results. The qualification of these codes involves comparison against each other, against more complex analytical solutions for reactive transport, and against experimental data (both laboratory and natural analogs). With regard to the latter, the following are typical examples.

Soler, J.M. and Lasaga, A.C. 1998. "An Advection-Dispersion-Reaction Model of Bauxite Formation." *Journal of Hydrology*, 209, 311-330.

Steeffel, C.I. and Lichner, P.C. 1998. "Multicomponent Reactive Transport in Discrete Fractures: I. Controls on Reaction Front Geometry." *Journal of Hydrology*, 209, 186-199.

Steeffel, C.I. and Lichner, P.C. 1998. "Multicomponent Reactive Transport in Discrete Fractures: II. Infiltration of Hyperalkaline Groundwater at Maqarin, Jordan, a Natural Analogue Site." *Journal of Hydrology*, 209, 200-224.

The three examples above are relevant for several reasons. First, the time scales of reaction approach those expected for degradation of the waste packages ( $10^2$  to  $10^6$  years). Second, the examples involve slow flow rates and Peclet (Pe) and Damköhler (Da) numbers similar to those expected for transport through the fractured tuff. Third, many of the waste package scenarios that yield highest potential for actinide deposition involve penetration of fractures with hyperalkaline fluids (the subject of one of the Steefel and Lichner test cases). Fourth, the solution method developed by Steefel and Lichner is closely tied to the LaGrangian method currently under development, so it should be straightforward to translate the Maqarin example into a validation case.

It should be noted that natural analogs are not necessarily the strongest tests, because the timing and rates of fluid infiltration are poorly constrained. In fact, for natural analogs, the hydrological parameters are often treated as free parameters. As validation examples, they are principally useful in showing that reasonable mineral assemblages can be achieved and for benchmarking codes based on different algorithms.

Despite the difference in time scales, laboratory tests involving reaction and deposition in flow columns often provide more conclusive tests for benchmark purposes, because flow rates and surface areas are well known. As long as the Da number and Pe number are reasonably close to those projected for near-field reactive transport, and the tests involve similar reactive mechanisms (e.g., pH and  $\text{CO}_2$  controls by reaction with tuff silicates), short-term experiments can serve as adequate tests. Several experiments underway at Lawrence Livermore National Laboratory show promise as code benchmarks. These experiments involve reaction between J-13-like fluids, crushed geomaterials, and actinides or radionuclide simulants. The progress of these experiments will be tracked, and the results will be considered for DOE's benchmark suite in the validation reports.

DOE plans to discuss the additional geochemical codes in a revision to the Topical Report.

*RAI 4-34 Provide additional information on the validity or conservatism of geochemical parameters to be used in EQ3/6 models.*

*As acknowledged in this report, there are large uncertainties in thermodynamic and kinetic data used by EQ3/6. The report states that a range of reaction rate values will be used so that conservative cases may be identified. This analysis should take account of any synergistic effects of varying rates for the numerous solid phases involved in this complex system. Such analysis should also be applied to thermodynamic data, particularly with regard to actinide phases. (Note, for example, that much uncertainty exists regarding appropriate thermodynamic data for U and Pu phases.) Only in this way can the model results be interpreted with confidence.*

Response:

The risk-informed approach to uncertainties in parameters influencing the occurrence of a criticality is to perform sensitivity analyses covering the range of possibilities for these parameters and map the results into probability distributions. The resulting probability distributions can then be used, with *conservative* estimates of consequences, to develop a conservative estimate of risk. Sensitivity of EQ3/6 calculations to uncertainties in kinetic models, and to uncertainties in the composition of incoming water, has been discussed in the responses to RAIs 4-29 and 4-30, respectively. The response to this RAI discusses recent studies of the sensitivity to variations in thermodynamic data to be used in EQ6. The sensitivity studies have all been with respect to one parameter, or one parameter set, at a time. For those variations that have the possibility of synergistic effects, DOE plans additional sensitivity comparisons with multiple parameter variations.

When there is uncertainty in the solubility of a fundamental phase, such as  $\text{PuO}_2 \cdot 2\text{H}_2\text{O}$  ( $\equiv \text{Pu}(\text{OH})_4$ ), the  $\log_{10}K$  of the phase is varied in the EQ6 (or other geochemistry code) reference files, to determine the total system sensitivity. Figure 4.34-1 shows a comparison of gadolinium (Gd) solubility for two alternative thermodynamic datasets, SKB and Weger (Spahiu and Bruno 1995, Weger et al. 1998). Also shown in this figure is a comparison of the concentration of the controlling Gd mineral phase, gadolinium carbonate, for the two alternative datasets. There is a significant difference in concentration (between the two alternative datasets) over most of the time. However, during times of peak Gd concentration and minimum gadolinium carbonate concentration, the two datasets give identical results.

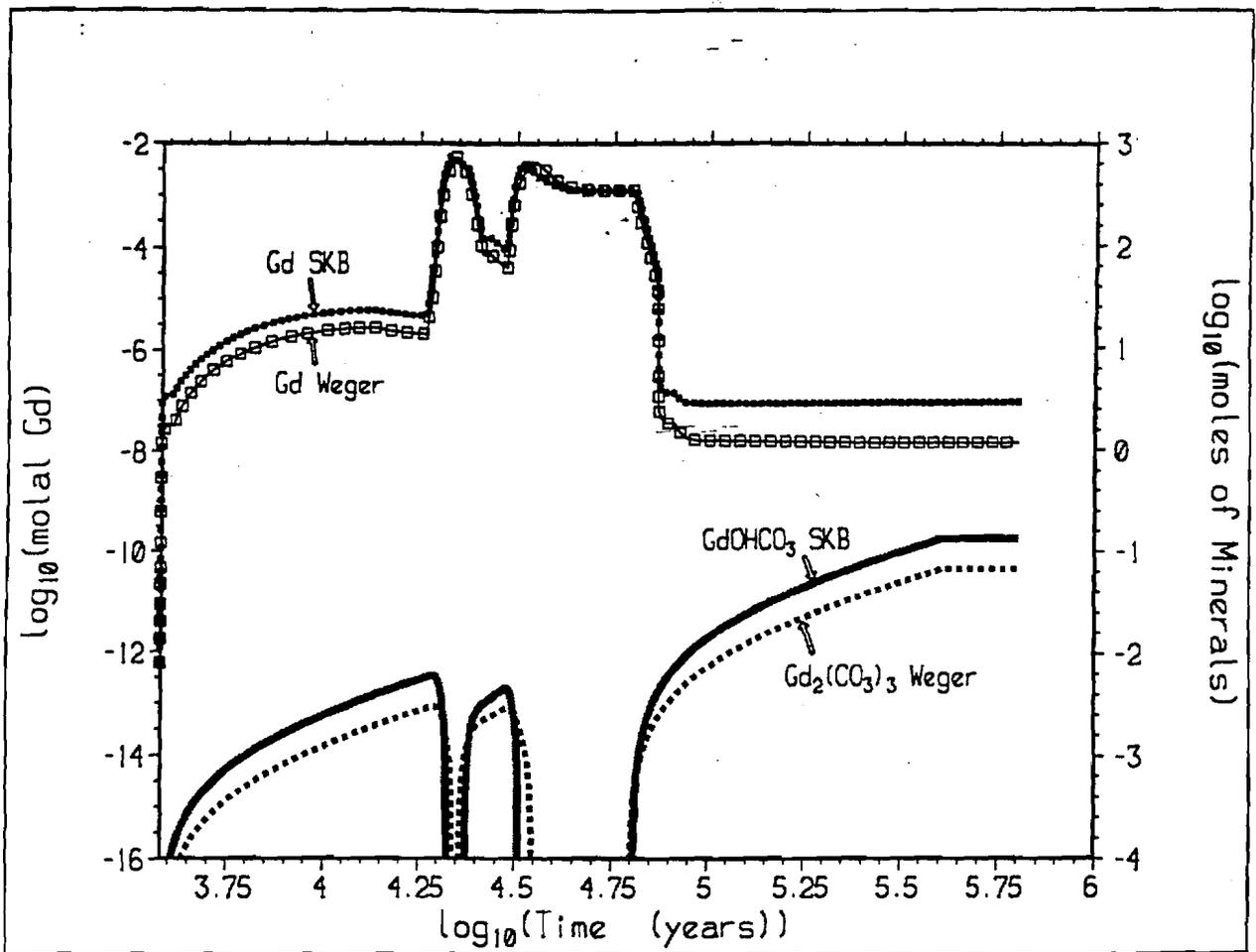


Figure 4.34-1. Comparison of Aqueous Gd Molalities and Moles Gd Minerals Formed, Using Two Different Sets of Thermodynamic Constants. (CRWMS M&O 1999, Figure 5-5)

DOE believes that the parameter of greatest interest to criticality is the loss of Gd from the waste package. This value is equal to the integral over time of the product of the Gd concentration in solution multiplied by the volumetric flow rate out of the waste package. In all the cases analyzed that show significant Gd loss, most of the loss is found to occur during the peak aqueous Gd concentration (CRWMS M&O 1999, Section 5). Therefore, since the SKB and Weger thermodynamic datasets give nearly identical peak aqueous Gd concentrations, the difference in Gd lost from the waste package is expected to be small. This comparison is given in Table 4.34-1. In this table a comparison between the two sets of thermodynamic constants is presented for two examples, which are labeled Run 4 and Run 6, and which have representative, but different, conditions. It can be seen from the table that use of the SKB database was slightly conservative, giving a slightly greater loss of Gd from the waste package for both evaluations.

Table 4.34-1. Percent Loss of Gadolinium, For Entire waste package, Thermodynamic Data Sensitivity Study (CRWMS M&O 1999, Table 5-6)

	Run 4	Run 6
<b>SKB database</b>	14.8625	12.9599
<b>Weger database</b>	14.4983	12.9537
<b>Fractional Difference</b>	0.024	0.00048

CRWMS M&O 1999. *EQ6 Calculation for Chemical Degradation of Pu-Ceramic Waste Packages: Effects of Updated Materials, Composition and Rates*. CAL-EDC-MD-000003 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990928.0235.

Spahiu, K. and Bruno, J. 1995. *A Selected Thermodynamic Database for REE to be Used in HLNW Performance Assessment Exercises*. SKB Technical Report 95-35. Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Co. TIC: 225493.

Weger, H.T.; Rai, D.; Hess, N.J. and McGrail, B.P. 1998. *Solubility and Aqueous-Phase Reactions of Gadolinium in the  $K^+ - Na^+ - CO_3^{2-} - OH^- - H_2O$  System*. PNNL-11864. Richland, Washington: Pacific Northwest National Laboratory. TIC: 242377.

### Section 4.3.1 Probability Concepts

*RAI 4-35 Indicate how correlations between sampled parameters will be identified, quantified, and accounted for in the criticality configuration generation codes.*

*Use of the Monte Carlo method requires that correlations between sampled parameters are taken into consideration if they are not truly independent variables. For example, the drip rate onto the package may affect the WP lifetime. Failure to account for these correlations could result in erroneous results.*

Response:

The Monte Carlo process will always represent correlations between parameters by using appropriate conditional probability distributions for parameter sampling. For the Monte Carlo example presented in Appendix C of the Topical Report, the waste package lifetime was sampled from a probability distribution abstracted from another Monte Carlo analysis, which used the waste package degradation code, WAPDEG. The WAPDEG code used a waste package corrosion model that captured the strong negative correlation between drip rate and waste package lifetime (specifically time to first penetration). This dependence was explained in the Topical Report, Section 3.5, item #1. Although the exposition of the configuration generator in Section 4.3 of the Topical Report indicates that the drip rate is sampled (Section 4.3.2, subheading Internal Criticality, item #1), it is only used for determining the rate of removal of dissolved species (item #5 of the same subheading). Because the drip rate is not used as a determinant of the penetration time, its sampling is not directly correlated with the completely independent sampling of the

waste package barrier penetration time. There may, however, be some indirect relation because the effects of fissionable species removal may depend on the time since emplacement (e.g., how much Pu has decayed to U).

### **Section 4.3.2 Monte Carlo Technique**

*RAI 4-36 Justify the assumption that it is acceptable to only consider the potential for one external criticality for a given realization.*

*DOE argued that the small probability of a realization yielding a critical configuration obviates the need to analyze the realization for multiple criticalities. This argument is acceptable only if each criticality is an independent event. Since having a single criticality in a realization requires that several sampled parameters are favorable to produce a criticality, additional criticalities are not independent events and the probability of having multiple criticalities for a single realization may not be small enough to be ignored. Failure to consider the potential for multiple criticalities in a realization may lead to an underestimation of the probability of a criticality event occurring.*

Response:

The example applications of the methodology in Appendices C and D of the Topical Report considered multiple criticalities as independent events. This is not conservative if the occurrence of one criticality increases the probability of additional criticalities. The strongest example of such positive correlation is the common mode failure. DOE plans to evaluate such possibilities in the comprehensive criticality consequence evaluation performed in connection with TSPA, as noted in the response to RAI 1-2.

*RAI 4-37 Justify the exclusion of water chemical parameters other than pH in regards to item A of the External Criticality list on page 4-39.*

*Water chemistry will be greatly altered during Waste package and WF interaction, and concentrations of other components such as carbonate influence the geochemical behavior of U and Pu.*

Response:

The list of sampled parameters in the first sentence of Item A on page 4-39 was only meant to be illustrative, not exhaustive. The next to last sentence of that paragraph alludes to solution characteristics in general, which would include the concentrations of all chemically significant elements (not just the fissile ones listed in the first sentence) and solution parameters (e.g., ionic strength, eH). DOE plans to provide an exhaustive list in the revision to the Topical Report.

*RAI 4-38 Clarify how the path selection process does not constitute an additional, non-conservative reduction in probability for a given configuration.*

*In item B of the External Criticality list, it is stated that random selection of external pathway is weighted according to probability. Subsequent transport modeling utilizes probability sampling of parameters. It should be made clear that this approach does not constitute redundant application of probability screening of external pathway.*

Response:

The essence of the Monte Carlo process is the probability sampling of parameters that are used in the calculation of the result parameter (typically  $k_{eff}$  for our cases). The statistical summary of many Monte Carlo repetitions is used to generate the probability distribution for these result parameters. Any allusion to a probability of a pathway, scenario, or configuration is really to a probability distribution calculated in this manner, so there is generally no redundant or external source of probability calculation. DOE plans to clarify these points in the revised Topical Report. The principal exceptions to this rule are for the waste package time to breach and bathtub duration. The probability distribution for these parameters is abstracted from the official series of WAPDEG runs performed for the performance assessment evaluations. The example criticality probability calculation in Appendix C of the Topical Report showed that this can be accomplished, while preserving independence of the two domains.

### **Section 4.3.3 Configuration Generation Code**

*RAI 4-39 Regarding item II.C of Section 4.3.3 on the invert configuration generation code (CGC) geochemistry modeling, justify the exclusion of water chemical parameters other than pH in computing solubility dependence.*

*In the WP CGC, solubility dependence on other species such as carbonate is included (item I.D.). Such dependence - which, for example, is strong for carbonate content in computing U solubility-should also be included in external cases.*

Response:

As explained in the response to RAI 4-37, there was no intention to exclude any items not listed in the first sentence of Item A on page 4-39. DOE plans to clarify the text in the revised Topical Report.

*RAI 4-40 Clarify how matrix-fracture distribution of water below the WP is calculated (item III.B and III.C). Reconcile the distinction between fracture and matrix travel times discussed in section 4.3.3 with the attribution of all flow to the fractures apparent from the discussion in section 4.2.3.*

*The distinction between matrix and fracture flow has profound implications for modeled travel times and water-rock interaction. For example, it is typically assumed that solutes are not sorbed during fracture flow. The distribution of groundwater flow between the fracture and the matrix will strongly affect U and*

*Pu transport because of contrasting sorption and groundwater travel times. U and Pu transport rates and concentrations are central to models of external criticality.*

Response:

The allocation of transport to the fractures gets the fissionable material to the potential accumulation zone sooner. The earlier potential criticality is generally conservative and, specifically, is conservative in minimizing the decay of plutonium. The methodology actually implemented is expected to include the capability to calculate flow through the matrix and diffusion from fractures into the matrix. DOE expects to use the geochemical transport code, PHREEQC, for this purpose. DOE plans to clarify the text in the revised Topical Report.

#### **Section 4.4.1.1      Steady-State Criticality**

*RAI 4-41      Justify the methodology used for analyzing the steady state criticality condition with no iron oxide.*

*One of the reasons provided in the "Second Waste Package Probabilistic Criticality Analysis: Generation and Evaluation of Internal Criticality Configurations" report for not including no-iron oxide or no-B-10 configurations in the analysis was that the corresponding  $k_{eff}$  values are "below any possible range of linearity." This is a questionable basis for excluding these types of realistic configurations. Knowing that taking credit for boron retention in the iron oxide has been dismissed in a later report, it is very possible that the combination of a high acidic environment would cause most of the iron oxide to be dissolved and flushed out of the waste package.*

Response:

The steady-state criticality with *no* iron oxide was not evaluated because it is an extremely unlikely configuration. DOE plans to evaluate the effect of reduced iron oxide concentrations and expects to provide a basis for any decision to use a minimum iron oxide concentration for evaluation. DOE does not expect that reduced iron oxide concentrations will have any effect on the consequences (increased radionuclide inventory) for the steady-state criticality, but it could effect potential insertion rate mechanisms for the transient criticality.

#### **Section 4.4.1.2      Transient Criticality**

*RAI 4-42      Provide an analysis for the seismic event using the time scales such as 0.3 seconds for reactivity insertion as part of the transient criticality analysis.*

*The cited reference (CRWMS M&O 1997e) does not provide the transient criticality analysis with a duration of 0.3 second as implied in the topical report. The report uses 30 seconds, which is based on the terminal velocity of iron oxide particles, for the duration of reactivity insertion. However, reshuffling of spent fuel in a time duration of one second or less as the result of the seismic event with no iron oxide must be considered.*

Response:

Although the reference cited described a concept that could support a 0.3-second insertion rate, subsequent analysis for intact commercial SNF assemblies showed that event to be incapable of producing a significant increase in  $k_{eff}$ , as was explained in the response to RAI 3-19. As was also explained in the response to RAI 3-19, DOE plans to evaluate the possibility of such a transient criticality for a waste package with a limited number of collapsed criticalities. This evaluation is expected to include the probability of the specific partially collapsed configurations required to support such a transient criticality.

*RAI 4-43 Justify the transient criticality analysis using a computer code which does not have the restrictions that are associated with RELAP5/MOD3.*

*The one-dimensional RELAP computer code has been developed for reactor cores, which have, flows parallel to the fuel bundles. The code is not intended to be used for systems with cross flows of more than 10%. First, the validity of using a one dimensional code for two dimensional analysis is not demonstrated. Secondly, the flow in both dimensions in the waste package model are perpendicular to the fuel assemblies in which the RELAP has not been designed. Thirdly, no benchmarks which would demonstrate the degree of applicability and accuracy of RELAP5/MOD3 for the waste package transient criticality conditions, are offered. Other codes which have the capability to perform three dimensional thermal hydraulics analysis might be the more appropriate computer code to use for analyzing the waste package transient conditions.*

Response:

It is recognized that the primary hydrodynamic flow in RELAP5 is along the fuel axis. DOE has overcome this limitation by developing RELAP models for components that represent the cross-flow, as explained in Section 4.4.3.2 of the Topical Report. Any licensing presentations of this sort of analysis are expected to demonstrate accuracy by comparison of the behavior of the component models with actual test data.

*RAI 4-44 Justify the use if computer codes that do not have temperature feedback capability to determine the reactivity of these waste package systems.*

*The approach proposed in CRWMS M&O 1997e with regard to compensating of the lack of the temperature feedback in MCNP4A, due to unavailability of "an associated cross section library with sufficient temperature data to calculate*

*reactivity changes," does not appear to be very sound. The use of SAS2H, modified by the buckling corrections developed based on MCNP4A is not accurate. Especially, in deriving the effective radial length of fuel stack, the approach appears to be questionable. The use of another code which has cross section libraries with temperature effects seems to be a more straightforward and accurate way of determining the reactivity insertion as a function of moderator and fuel temperatures.*

Response:

The RAI identifies the potential for an inaccuracy in the DOE method for compensating for the lack of sufficient temperature dependence in the MCNP cross section libraries. However, DOE has mitigated this problem because reactivity tables for the kinetics model in RELAP5 were generated using SAS2H with the SCALE libraries that include Doppler-adjusted cross section evaluations for both uranium and plutonium as well as temperature-dependent scattering cross sections for a number of low-mass isotopes. Because SAS2H is a one-dimensional code, buckling corrections are used to represent the three-dimensional effects. The parameters of the buckling corrections are adjusted to better reproduce the  $k_{eff}$  of a set of MCNP benchmark cases. For any given configuration of waste package components (intact or degraded), the buckling approximation can be improved by matching more MCNP benchmarks.

DOE believes that the ultimate accuracy of this adjustment methodology is only limited by the fact that it is primarily at one temperature. However, three additional points should be noted in evaluating the ultimate accuracy potential of this methodology.

- (a) Some use may be made of the temperature dependence in the ENDF cross section libraries since they are continually being improved by the addition of temperature-dependent cross sections for the most neutronicly significant elements. With these it will be possible to reflect some temperature dependence in the buckling adjustment process.
- (b) The primary sensitivity of RELAP applications is with respect to changes in  $k_{eff}$ , not its absolute value. DOE believes that changes in  $k_{eff}$  caused by changes in configuration can be represented with reasonable accuracy by changes in MCNP geometry. DOE also believes that changes in  $k_{eff}$  caused by changes in temperature are best represented by the change in SAS2H geometry.
- (c) The modeling of transient criticality is usually acceptable within 50% (RELAP5/MOD3 Code Manual, NUREG/CR-5535). A typical RELAP modeling question is whether some component has been seriously damaged, so there is little need for high precision.

*RAI 4-45 Clarify whether in the transient criticality analysis method the code biases and uncertainties, in addition to the Monte Carlo uncertainties, are included in all the  $k_{eff}$  values.*

*Examination of CRWMS M&O 1997b and CRWMS M&O 1997e indicates that the change in reactivity might be based on a subcritical initial condition. This is due to subtracting the code bias and uncertainty from  $k_{eff} = 1$  for initial condition. This would result in the majority of reactivity being inserted while configuration is in subcritical condition. Starting with critical condition (i.e.,  $0.95 + 0.05$  for bias and uncertainties) and adding the bias and uncertainties to the other transient conditions (e.g.,  $k_{eff} = 1.0189 + 2\sigma + 0.05$ ) would place the reactivity insertion above the critical condition.*

Response:

Bias and uncertainty are not directly relevant to the transient criticality analysis because the RELAP calculation is only concerned with differences in  $k_{eff}$ . DOE believes that bias would not change much with a small change in  $k_{eff}$ . The change in  $k_{eff}$  for the example reported in Appendix C of the Topical Report was based on changing from a subcritical configuration (uniform oxide distribution) to a critical configuration (settled oxide) with a  $\Delta k_{eff}$  of approximately 0.07. Since that calculation, the design concept has been changed somewhat so that the difference between these configurations is no longer significant, as explained in the response to RAI 3-19. The Topical Report will be revised to clarify this point. Future application of this methodology is expected to continue to follow the principal of computing differences in  $k_{eff}$  between possible physical configurations. The parameters for these configurations are expected to be chosen so that they closely straddle the point  $k_{eff} = 1$ , both before and after the onset of transient criticality.

*RAI 4-46      Discuss the approach for transient criticality analysis for high-enriched spent fuels in view of absence of negative Doppler feedback.*

*The approach in selecting configuration classes for transient criticality presented in the topical report is with respect to low-enriched commercial spent fuel assemblies. The high-enriched spent fuels, such as DOE-owned spent fuels, will have no negative fuel temperature feedback (i.e., not enough U-238 for Doppler feedback). This type of configuration class must be also analyzed.*

Response:

DOE plans to revise the Topical Report to clarify that the methodology of RELAP5 is expected to be applied to high-enriched SNF. The code is expected to handle a broad range of values for all the feedback coefficients. DOE expects to perform transient evaluations for SNF with upwards of 20% enrichment during FY2000. Although highly enriched fuel has a small Doppler temperature coefficient, the moderator density reactivity feedback is large.

*RAI 4-47 Discuss the over-moderation effect within the waste package in view of the large uncertainty associated with the flow rate into the waste package.*

*Another transient criticality configuration which must be addressed is the over-moderation configuration. Configurations with large flow rate into the waste package and a subsequent seismic event can result in a positive-feedback criticality.*

Response:

The example of transient criticality in Appendix C of the Topical Report did not directly address the issue of overmoderation. However, in practice the MCNP calculations cover the range of water volumes, starting with the initial configuration and reducing in steps to a value small enough to accommodate the blown-down configuration. Hence, RELAP would automatically calculate any positive void coefficient associated with an overmoderated condition. DOE plans to revise the Topical Report to state this.

*RAI 4-48 Explain how the point neutron kinetics and flow models in RELAP5/MOD3.2 will be adapted for broad applicability to the analysis of internal criticality transients involving all intact and degraded waste forms and packages.*

*The staff notes that the feedback coefficients in RELAP5/MOD3.2's point neutron kinetics formulation are limited to those feedback mechanisms needed for modeling selected PWR transients. For example, the "void coefficient" formulation assumes that "coolant" and "moderator" are one and the same, which is not valid for certain non-PWR reactor types and likewise not valid for the many intact and degraded waste form/package configurations that involve more than one "moderator/coolant" medium (e.g., see example configurations in Appendix D of the report). The NRC Office of Research, which oversaw the development of RELAP5/MOD32 at INEEL, has noted that significant revisions to the code's neutron kinetics and flow models would be needed for applying the code to other reactor types such as CANDU, RBMK (i.e., Chernobyl), etc. Similar revisions may likewise be needed for applying the code to the full range of criticality transients in the repository. This potential code deficiency is closely related to the previously noted deficiencies in the concept of over/under-moderation which does not address the full range of neutronic phenomena that govern positive and negative feedback effects.*

Response:

DOE recognizes that the application of RELAP to transient criticality is only appropriate when water is the principal moderator. In addition to the PWR waste package, RELAP5 is intended for application to the BWR waste package, although the accuracy will be reduced because the BWR channels will limit the flow across an assembly that dominates the PWR waste package transient criticality. The dominant flow in the BWR SNF transient criticality will be along the waste package axis inside the assembly channel, with a return flow outside the channel volume to the exit area(s). The turnaround at the

ends of the waste package will be modeled conservatively (to produce a component resistance at the high end of the uncertainty range). The resistance of the turnaround and the conservative model of the turnaround are expected to make the peak pressure and temperature considerably higher for a BWR transient criticality than for a PWR SNF transient criticality.

The RELAP applications are expected to be limited to configurations with the fuel pins in their nearly intact configuration so that water can flow between the pins. There may be some potential for increasing  $k_{\text{eff}}$  by precipitation of silica directly on the fuel pins or on basket material. DOE expects to model this by increasing the resistance of the junction component models used to represent the flow through, and around, the assemblies. DOE plans to apply the coupled thermal-hydraulic-neutronic code mentioned in the responses to RAIs 3-21, 4-49, and 4-53, rather than applying RELAP5, to the case in which the waste package becomes primarily silica-moderated.

With respect to the coolant issue, it should be noted that in a waste package criticality there is nothing analogous to a coolant, and none is modeled. Inputs to the RELAP waste package criticality runs specify no feedwater or other coolant source.

#### **Section 4.4.2.1      Steady State Criticality**

*RAI 4-49      Discuss the approach for consequences of external criticality, some of which are presented in Probabilistic External Criticality Evaluation report, in the topical report.*

*The above report presents some qualitative discussion with regard to only an increase in radionuclide inventory. More in-depth quantitative approach is needed to address the steady state external criticality consequence, especially with regard to high enriched spent fuels.*

Response:

The principal consequence of a steady-state criticality (internal or external) is radionuclide increment. Any large pressure or temperature cannot be sustained on a steady-state basis and would be evaluated as a transient criticality. As stated in the response to RAI 3-21, for criticality external to the waste package, the Topical Report states that a code with fully coupled thermal, hydraulic, and neutronic effects is expected to be used to assess consequences of steady-state criticalities (Section 4.4.1.2). This code is expected to be applicable to any time-dependent criticality, even if it appears more steady-state than transient.

#### **Section 4.4.2.2      *Transient Criticality***

*RAI 4-50      Discuss the approach for addressing consequences of transient criticality such as autocatalytic criticality from possible re-concentration of fissile masses in the near-field and far-field.*

*Re-concentration of fissile material in the near or far field combined with subsequent sudden flow of water can result in external transient criticality situations. An approach to address possible consequences of this configuration class is needed.*

Response:

As stated in the responses to RAIs 1-4 and 3-22, DOE expects to evaluate all potentially autocatalytic configurations that can be reached by conceivable scenarios. Preliminary evaluations of external accumulation thus far indicate that such accumulations are not possible for commercial SNF in the near field (CRWMS M&O 1997), and DOE is continuing to explore the possibility of reducing zones in the far field. Other waste forms are also being evaluated in this respect.

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

#### **Section 4.4.3.1      *Validation of the Steady-State Criticality Consequence Methodology***

*RAI 4-51      Provide a discussion of the approach used to identify applicable experiments which would quantify the bias and uncertainty associated with the steady-state criticality analysis.*

*Qualitative discussion with respect to conservatism does not provide the quantitative values for uncertainties and bias which need to be identified. For example, examination of the reference material indicates that there is a large uncertainty associated with predicting the steady state power. The analysis indicated that the power produced can be between 0.5 KW and about 4 KW. The average of these two numbers was used. Other areas of analysis have large uncertainties which need to be quantified and taken into consideration for predicting the consequence of the steady-state criticality.*

Response:

For any critical configuration, the consequences of a steady-state criticality will be calculated according to the methodology outlined in Section 4.4.1.1 and 4.4.3.1 of the topical report. Because the only neutronics calculation is with ORIGEN-S to determine the radionuclide generation over the duration of the criticality, there is no need for a separate bias-uncertainty determination once the criticality has been identified. It should

also be noted that the power level used to determine the burnup/depletion will be based on a specified probability distribution. The averaging between high and low power levels in the Appendix C example was a temporary expedient in the absence of a probability distribution; it will not be used again. This process is specified by the addition to Section 4.4.1.1 of the Topical Report given in the response to RAI 3-23.

Because the steady-state criticality consequence analysis is a mixture of classical physics and neutronics calculations, it is worthwhile to provide the following outline here. This information is already contained, implicitly or explicitly, in Sections 4.4.1.1 and 4.4.3.1 of the Topical Report.

**Inputs:** Inputs are the drip rate distribution with time. Such distribution will be derived primarily from the climate and mountain-scale hydrology model. The latter may also give a distribution with time for the drip location. If the drip location distribution shifts significantly with time, the reaction will be shut down accordingly. Other parameters of importance are the "bathtub" duration, the thermal conductivity of the material in contact with the waste package barriers (primarily the invert and backfill), the assembly condition, and the water level in the waste package. All are specified probabilistically, with the latter two having distribution determined by the degradation processes leading to the critical configuration.

**Calculation:** The calculation begins with the determination of the waste package temperature so that the evaporation rate over the waste package pond surface equals the volumetric drip rate into the waste package. The criticality power is equal to the heat loss rate at this temperature (the sum of conduction and radiation heat losses, although radiation heat loss will be very small if there is significant backfill). This gives a probability distribution for power, which varies as a function of drip rate, which, in turn, varies as a function of time. The radionuclide increment is determined from ORIGEN-S as a function of power, integrated over the duration of the criticality. This duration is at least the duration of the climate period, but should also include the possibility of a return of the moister climate so that the reaction can start again. Ultimately the time is limited by the duration of the "bathtub" (time that the waste package can be filled with water). It should be noted that, in this consequence methodology, ORIGEN-S is the only neutronics calculation. All the other calculations are very well understood classical physics. There is uncertainty associated with these calculations, primarily due to the uncertainty of the degraded waste package configuration parameters. DOE plans to capture these uncertainties in probability distributions, and the effects of these degradation parameter uncertainties are expected to be reflected in the final risk calculations, based on these figures.

**Result:** The result is the expectation of the radionuclide increment integrated over time and averaged over the probability distribution of drip rates (over the evaporation threshold) at each time-step, with the ultimate criticality duration limited by distribution of bathtub durations.

#### **Section 4.4.3.2 Validation of the Transient Criticality Consequence Methodology**

*RAI 4-52 Justify the applicability of RELAP5 to the waste package in light of differences in orientation and presence of iron oxide.*

*As indicated in the above questions, the RELAP5 has been developed for reactor cores with moderator and coolant flow in the direction parallel to fuel assemblies with minimal cross flow across the fuel assemblies. The situation in the waste package is the reverse of that in the core. Applicable experiments need to be identified in order to provide confidence in predicting transient criticality consequences.*

**Response:**

As explained in the response to RAI 4-43, DOE expects that any licensing presentations of this sort of analysis will demonstrate accuracy by comparison of the behavior of the component models (that are used to represent cross-flow) with actual test data.

*RAI 4-53 Provide a discussion of the approach used to identify the super critical experiments which will be used to validate the appropriate transient criticality model.*

*This section needs to discuss the benchmark experiments which will be used in validating the transient criticality computer code. The discussion should be in terms of area and range of applicability.*

**Response:**

The approach used to identify the super-critical experiments, which will be used to validate the appropriate transient criticality model, is based on the benchmarks that the NRC has accepted (Carlson et al. 1990). As suggested by previous licensing evaluations using RELAP, if the geometry of the fissile configuration remains in a quasi-static form during the transient, the spatial and spectral integrals of the neutron kinetics equations are appropriate to model the time-dependence of the reactivity transient.

The area and range of applicability of the RELAP5 model include all reactivity transients. The super-critical experimental condition representing the most severe transient in terms of power is prompt criticality with more than a dollar of reactivity inserted. The benchmarks that have validated the neutron kinetics for prompt criticality are associated with the control rod ejection accident in a reactor. The experimental condition representing the least severe power transient is power escalation in a reactor. By using a very slow escalation, DOE could use some of the sophisticated modeling features (such

as the vaporization model) of RELAP to model the steady-state criticality more accurately than was done in Appendix C, Section 5.1 of the Topical Report.

Validation of RELAP will proceed by showing that it exhibits proper behavior over a set of complex examples. DOE is presently using four standard RELAP benchmarks: Marviken III Test 24 (EPRI 1992), Loft Test L3-1 Accumulator Blowdown (Bayless et al. 1980), SemiScale Natural Circulation Experiment (Dimenna 1983), and MIT Pressurizer Experiment (Saedi 1982), to secure quality assurance validation for the use of RELAP for transient criticality. Although none of the cases duplicates our conditions, DOE expects to demonstrate that the essential features of the code reproduce experimental results. This process will also identify the uncertainty (and/or bias) in using the code as a predictor.

Ultimately, the validation of a consequence code for repository applications is expected to be concerned with two types of criticality impact, (a) maximum pressure and temperature which can cause damage to the fuel and/or the waste package barriers, thereby enhancing the release of radionuclides and (b) the maximum energy (or steady-state criticality) to produce the greatest increment in radionuclide inventory. The Topical Report, Sections 4.4.1.1, 4.4.1.2, and Appendix C, Section 5.1, indicate how RELAP5 would be used to estimate impacts of type (a) and how a simpler analysis methodology could be used for the steady-state criticality [impacts of type (b)]. As mentioned above, certain features of RELAP5 could enhance the accuracy of the evaluation of type (b) impacts as well.

For evaluation of transient external criticality consequences and other configurations not suited to RELAP analysis, DOE plans to use a coupled thermo-hydraulic-neutronic code. Either the code developed by the University of California Berkeley Nuclear Engineering Department, and mentioned in Section 4.4.1.2 of the Topical Report, or a similar code to be identified later, may be used. The validation of such a code would include comparison with the standard criticality accident/transient experiments (e.g., Godiva, Kiwi).

DOE plans to revise the Topical Report to reflect the information provided in this response.

EPRI 1982. *The Marviken Full-Scale Critical Flow Tests. Volume 32: Results from Test 24*. EPRI-NP-2370 vol.32. Palo Alto, California. ACC: MOL.19990929.0079.

Bayless, P.D.; Marlow, J.B.; and Averill, R.H. 1980. *Experiment Data Report for LOFT Nuclear Small Break Experiment L3-1*. NUREG/CR-1145. Idaho Falls, Idaho. TIC: 243817.

Dimenna, R.A. 1983. *RELAP5 Analysis of Semiscale Mod-2A Single-Loop Single-Component Steady-State Natural Circulation Tests*. EGG-SEMI-6315, Idaho Falls, Idaho. ACC: MOL.19990929.0078.

Saedi, Hamid Reza 1982. *Insurge Pressure Response and Heat Transfer for PWR Pressurizer*. M.S. Thesis, Department of Mechanical Engineering, Massachusetts Institute of Technology. TIC: 243870.

**Appendix C Example Application of the Methodology for Commercial Spent Nuclear Fuel**

*RAI C-1 Provide information on plans for geochemical model validation in this example analysis and the Appendix D example analysis (see discussions above on model validation). This information will make clearer the scope and rigor of the validation approach.*

Response:

The main body of the Topical Report contains the validation process for the geochemical models. The response to RAI 4-51 provides more detail on this process. As indicated in the responses to earlier RAIs, DOE plans to provide the detailed validation information in separate validation reports. The reports referenced in the main body of the Topical Report contain the details of the evaluations performed to date, and some plans for future evaluations. The example in this Appendix is intended only to briefly demonstrate various aspects of the methodology.

The best way to validate the code is to show that it exhibits proper behavior for all the relevant output parameters, over a set of complex examples. It is not critical that the test cases match exactly the time and chemical conditions of the waste package models. It is important that the test cases span the Damköhler number ( $Da$ ) and Peclet number ( $Pe$ ) expected in the waste package/near-field models, and the test cases and waste package models involve rate laws and chemical behaviors of similar complexity. In essence, this is a restatement of the principle of similarity. For example, one scenario for precipitation of actinides, in a crushed-tuff invert, involves dissolution of Ca- and Fe(II)-silicates. The Ca may reprecipitate as calcite, indirectly destabilizing actinide carbonate complexes; the Fe(II) may act as a reductant for Pu; and the excess silica may act as a precipitant for U. The dissolution of the silicates is a rate-limiting step, and the density of precipitant is partly controlled by the ratio of the characteristic diffusion, or advection time, to the characteristic dissolution time (the  $Da$ ). In addition, the amount of precipitation is limited by the total availability of Ca and Fe(II) in the system. If there are no relevant data, it may be necessary to develop an additional experiment that flushes J-13 through crushed Topopah Springs Tuff. The experiment may involve much higher flow rates than are proposed for flow through the invert; however, the same  $Da$  can be achieved in the experiment by careful control of the grain size and, thus, the surface area (which acts with the dissolution rate per unit area per unit time to determine the total dissolution rate per unit time).

### **Section C.1.4.3 Waste Form Degradation Characteristics**

*RAI C-2 Expand the discussion of the structural and corrosion characteristics of Zircaloy cladding to include the effects of irradiation, reactor water chemistry, operating history, and pre-disposal storage conditions.*

*Commercial SNF exhibits a wide range of Zircaloy material characteristics, including large variations in the degree of hydriding, oxidation (corrosion), erosion thinning, embrittlement, pallet-cladding interactions, pinhole/crack formation, crud deposition, etc.*

Response:

As noted in the response to RAI 4-26, future licensing documents relying on cladding credit, which will be based on the extensive testing and carefully reviewed modeling programs, is now ongoing.

*RAI C-3 Clarify the intent of the statement that "At sufficiently high temperatures in an oxidizing environment, the fragments will oxidize ..."*

*Oxidation of UO<sub>2</sub> does not, in general, require elevated temperatures.*

Response:

The referenced statement was based upon earlier work, and DOE agrees that it is not valid. It is irrelevant to the topics under discussion in Appendix C. The statement will be deleted from Appendix C.

### **Section C3.3 Criticality Regression Expression**

*RAI C-4 Justify the applicability of  $k_{\infty}$  which was based on all isotopes in spent fuel, to spent fuel with the 29 principal isotopes.*

*The  $k_{\infty}$  regression equation developed by ORNL is based on all the isotopes included in SAS2H. If these results are used for binning the spent fuels with the principal isotope assumption, the  $k_{eff}$  appears to be under-predicted.*

Response:

Use of  $k_{\infty}$  was established as a temporary expedient to distinguish SNF requiring more, or less, criticality control measures. The  $k_{\infty}$  regression was never used for determining probability of criticality. Now that DOE has enough cases of  $k_{eff}$  calculation (over 2000 for the various waste forms and various degradation parameters), DOE can quickly estimate  $k_{eff}$  for a range of waste forms and a number of ranges for individual degradation parameters by table lookup and interpolation. Therefore, DOE will have no further use for  $k_{\infty}$ . The discussion of  $k_{\infty}$  in Appendix C of the Topical Report will be deleted.

*RAI C-5 Assess the impact of not including axial burnup profile and the reactor*

*operating history bounding parameter values in the regression equation.*

*Using single uniform axial burnup profile and nominal values for reactor operating history parameters would result in a regression equation under-predicting the  $k_{eff}$  values.*

Response:

The combined impact of not including axial burnup profiles and bounding depletion parameters in the example evaluation is expected to be, as noted in the RAI, an under-prediction of  $k_{eff}$  values. If the example included axial profiles and bounding parameters, it would be expected that more potential criticalities would be predicted. The effect of axial burnup profiles on regression equations has been calculated in an initial evaluation (CRWMS M&O 1998, page 32, Figure 6.1-1), and the effect was found to be minor. As noted in the response to RAI 3-2, DOE is currently using the multi-node model for commercial SNF criticality calculations for the methodology. The effect of using the bounding depletion parameters has not been assessed yet, since the bound parameters have not been established for any commercial SNF.

DOE plans to update the example evaluations in the revision to the Topical Report to incorporate the available axial burnup profile and bounding depletion parameter information or to note what the expected effect of not including the information would be.

CRWMS M&O 1998. *Supplemental Criticality Evaluation for Degraded Internal Configurations of a 21 PWR Waste Package*. BBA000000-01717-0210-00022 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980918.0086.

#### ***Section C4.1 Probability Estimation***

*RAI C-6 Evaluate the potential for axial displacement of the disposal control rods relative to the active fuel.*

*The topical report takes credit for the control rods as the basis for not considering the most reactive fuel, i.e., fuel with burnup below the loading curve, as part of the population of PWR fuel capable of exceeding the critical limit. Any upset or degradation mechanisms that could produce axial displacement (e.g., tilting of the package or basket) should be identified.*

Response:

If control rods are used, DOE plans to use one or more mechanisms to ensure that they cannot be axially displaced while the fuel is intact. Such mechanisms may include friction fitting of the control rods, pinning at one end, or space limitation inside the waste package. Furthermore, based on current preliminary designs, there is not expected to be enough room in the fuel assembly cavity of a waste package for the rods to slide out. Nor have any credible degraded waste package scenarios, that could result in such a

displacement, been identified. The criticality evaluations used to support the License Application for waste packages containing disposal control rods are expected to fully evaluate this possibility.

DOE plans to update the example evaluations in the revision to the Topical Report to incorporate any available credible degraded waste package scenarios that would result in axial or radial displacement of disposal control rods.

### **Section C5.1 Criticality Consequence Estimation**

*RAI C-7 Justify limiting the reactivity insertion scenario to the relatively slow ones described here.*

*The reasoning for not considering rapid reactivity insertions resulting from sudden movements such as those caused by collapse of the degrading basket structures, rock fails, etc., should be provided.*

Response:

Justifications for the reactivity insertion rates used here are discussed in the responses to RAIs 3-19, 3-20, and 4-42.

*RAI C-8 Justify the apparent conclusion that long-term steady-state criticalities bound the consequences of all criticality events.*

*During a long-term steady-state criticality, many of the radionuclides produced will decay or be burned out. High power transient events resulting from rapid reactivity insertions and/or autocatalytic effects, perhaps in conjunction with steady-state criticalities, have a potential to produce a burst of short-lived fission products and actinides (i.e., short-half life equates to high activity) as well as transient thermal-mechanical effects that may promote their early release from the repository.*

Response:

The additional burnup from the long-term steady-state criticality was approximately 820 MWd/mtU, while the additional burnup from the transient criticality was  $1.8 \times 10^{-3}$  MWd/mtU (CRWMS M&O 1996, CRWMS M&O 1998a). As can be seen in the response to RAI C-9, higher amounts of the short-lived radionuclides are present at the end of the steady-state example than at the end of the transient example. This is also true for the long-lived radionuclides important to performance assessment.

The possibility of the criticality event accelerating the release of the additional radionuclides generated (e.g., by damaging previously intact fuel cladding) has already essentially been addressed in the TSPA evaluation reported in Appendix C. This evaluation (CRWMS M&O 1998b) assumed that the additional radionuclides are

available for removal from the waste package immediately following termination of the criticality.

CRWMS M&O 1996. *Second Waste Package Probabilistic Criticality Analysis: Generation and Evaluation of Internal Criticality Configurations*. BBA000000-01717-2200-00005 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19960924.0193.

CRWMS M&O 1998a. *Criticality Consequence Analysis Involving Intact PWR SNF in a Degraded 21 PWR Assembly Waste Package*. BBA000000-01717-0200-00057 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980106.0331.

CRWMS M&O 1998b. *TSPA-VA Total System Model Base Case Modified to Include Nuclear Criticality Disruption of the Repository*. Las Vegas, Nevada: CRWMS M&O. DTN: SNT05072098001.004. ACC: MOL.19981125.0027.

*RAI C-9* Verify that short-lived isotopes arising in high-power transients are considered in evaluating dose consequences.

*It is not clear that the short-lived isotopes potentially important to the dose consequences of rapid transient events (e.g., Kr-85, I-131, Sr-89, Cs-134) are included in the isotopes evaluated under this methodology. This section limits its evaluation to the 36 TSPA-95 isotopes.*

**Response:**

Radionuclide inventories for the short-lived radionuclides were also calculated as part of the consequence evaluations performed for the steady-state and transient criticality examples. The table below provides information on the inventories of various short-lived radionuclides at the termination of each of the example criticality events shown in Appendix C. As is indicated on page C-57 of Appendix C, gas travel times from the repository block to the surface were estimated to be in the range of 200 to 600 years. This is the same order of magnitude as the 300-year minimum groundwater travel time to the accessible environment given in (DOE 1998, *Viability Assessment of a Repository at Yucca Mountain*, Figure 4-18). Therefore, because both gas and groundwater travel times are at least an order of magnitude greater than the half-life of any of the radionuclides listed below; it is not expected that any significant quantity of these radionuclides could reach the surface via a gaseous pathway.

Radionuclide	Half-Life (GE 1989)	Ci/assembly at end of criticality event	
		Steady-state example (CRWMS M&O 1996, Att. X)	Transient example (CRWMS M&O 1997, long.out)
H-3	12.3 y	$1.1 \times 10^{-2}$	$1.2 \times 10^{-3}$
Kr-85	10.7 y	0.19	$1.1 \times 10^{-5}$
I-131	8.0 d	2.73	-
Sr-89	50.5 d	3.29	$6.7 \times 10^{-2}$

Sr-90	29.1 y	3.97	$1.8 \times 10^{-3}$
Cs-134	2.1 y	1.15	$1.4 \times 10^{-6}$
Cs-137	30.2 y	5.49	$2.0 \times 10^{-3}$
Ru-106	1.0 y	1.42	$1.7 \times 10^{-2}$

Furthermore, even if all of the fuel rods in a 21 PWR waste package were assumed to fail immediately after termination of the criticality, and all of the radionuclides were assumed to be quickly transported to the surface, the dose from the event would still be very low. The total effective dose at a distance of 5 km from such a non-mechanistic scenario would be less than 1 mrem for the steady-state example, and less than  $< 10^{-4}$  mrem for the transient example. The total effective doses were estimated by summing the inhalation and submersion doses for the radionuclides of interest. The inhalation dose from isotope i ( $ID_i$ ) is estimated using:

$$ID_i = S_i * N * IDCF_i * RF_i * BR * [\chi/Q]_{5km}$$

The submersion dose from isotope i ( $SD_i$ ) is estimated using:

$$SD_i = S_i * N * SDCF_i * RF_i * [\chi/Q]_{5km}$$

The parameters in the above two equations are as follows:

- $S_i$  = Inventory of radionuclide i per assembly (Ci)
- $N$  = Number of PWR assemblies in waste package (21)
- $IDCF_i$  = Effective inhalation dose conversion factor for isotope i (From EPA 1988, pp. 122-137; for isotopes with multiple lung clearance classes, the class with the highest effective DCF was used).

Nuclide	Effective IDCF (Sv/Bq)
H-3	1.73E-11
Kr-85	N/a
I-131	8.89E-9
Sr-89	1.12E-8
Sr-90	3.51E-7
Cs-134	1.25E-8
Cs-137	8.63E-9
Ru-106	1.29E-7

Conversion to mrem/ $\mu$ Ci made by multiplying by 3.7E9.

SDCF<sub>y</sub> = Effective submersion dose conversion factor for isotope i  
(From EPA 1993, pp. -65)

Nuclide	Effective SDCF (Sv per Bq*sec*m <sup>-3</sup> )
H-3	3.31E-19
Kr-85	1.19E-16
I-131	1.82E-14
Sr-89	7.73E-17
Sr-90	7.53E-18
Cs-134	7.57E-14
Cs-137	7.74E-18
Ru-106	N/a

Conversion to mrem per μCi\*y\*cm<sup>-3</sup> made by multiplying by 1.168E23

RF<sub>i</sub> = Release fraction for isotope i, defined as the fraction of the inventory of the radionuclide that is present in the waste form that is released to the environment during an event (see Table 7.1, NUREG 1536 or CRWMS M&O 1998, p. 8)

Nuclide	Release Fraction
H-3	0.3
Kr-85	0.3
Iodines	0.1
Cs and Sr	2.3E-5
Ru	1.5E-5

BR = Breathing rate; 3.3E-4 m<sup>3</sup>/sec (CRWMS M&O 1998, p.9)  
 [χ/Q]<sub>5km</sub> = Best-estimate atmospheric dispersion factor at 5 km distance for assumed meteorological conditions and duration of release; 1.44E-5 sec/m<sup>3</sup> (CRWMS M&O 1998, p. 9)

Additional credit for dispersion in the fracture network as the gas is transported from the drift to the surface, and "filtration" by particle filled or dead-end fractures, would further reduce these estimates.

CRWMS M&O 1996. *SAS2H Generated Isotopic Concentrations for B&W 15x15 PWR Assembly*. BBA000000-01717-0200-00012 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19961218.0190.

CRWMS M&O 1997. *Criticality Consequence Analysis Involving Intact PWR SNF in a Degraded 21 PWR Assembly Waste Package*. BBA000000-01717-0200-00057 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980106.0331.

CRWMS M&O 1998. *Preliminary Preclosure Design Basis Event Calculations for the Monitored Geologic Repository*. BC0000000-01717-0210-00001 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981002.0001.

DOE 1998, *Viability Assessment of a Repository at Yucca Mountain, Volume 3, Total System Performance Assessment*, DOE/RW-0508/V3. ACC: MOL.19981007.0030.

EPA 1993. *External Exposure to Radionuclides in Air, Water, and Soil: Federal Guidance Report No. 12*. EPA 402-R-93-081. Washington, DC: EPA. TIC: 225472.

EPA 1988. *Limiting Values of Radionuclide Intake and Air Concentration and Dose Conversion Factors for Inhalation, Submersion, and Ingestion: Federal Guidance Report No. 11*. EPA-520/1-88-020. Washington, DC: EPA. TIC: 203350.

*RAI C-10 Justify why the presence of boron and corrosion products dissolved or suspended in the water and that can affect the moderator void coefficient of reactivity is not addressed in the TR.*

*The presence of absorbers in the "moderator" can produce a positive void reactivity, resulting in autocatalytic feedback effects that are apparently not considered in the proposed methodology.*

Response:

The proposed methodology can consider the potential for a positive void coefficient provided by dissolved neutron absorber. The nominal tool for evaluating the consequences of a transient internal criticality, RELAP 5, is capable of exhibiting behavior reflecting the presence of dissolved neutron absorber (e.g., boron) in moderating water. This capability was not used in the transient criticality example of Appendix C of the Topical Report, because the waste package is only exposed to such a criticality threat for a relatively brief period of its history. For most of the time there is boron in the waste package, the boron will serve to prevent criticality entirely. When the boron has essentially been completely removed from the water, and from the waste package, there may be a criticality, but there can no longer be a positive void coefficient. In the brief period between these conditions there could be such a positive void coefficient, and DOE plans to evaluate this possibility in the documents that will support the License Application.

*RAI C-11 Justify the assumption of one-year decay time in assessing the consequences of a fast transient criticality. In particular, explain how the one-year decay time bounds the travel times of all important radionuclides.*

*Fast transient criticality events resulting from rapid reactivity insertions and/or autocatalytic effects have a potential to produce a burst of short-lived fission products and actinides. However, it is not clear why the one-year decay time assumption is used in assessing the consequences in this case.*

Response:

The assumption of one-year decay time was considered conservative because several of the long-lived radionuclides shown are not at their peak activities at the time the criticality event is terminated but reach their peak at various times during the first year (e.g., Pu-238 peaks between 0 and 60 days as a result of build-in from the decay of Np-238 and Cm-242).

*RAI C-12 Explain the design modification needed in light of the change in the radionuclide inventory indicated by Table C-16.*

*The criticality consequence design criterion listed in Section 1.2 states that "the expected radionuclide increase from any criticality event will be less than 10 percent..." Table C-16 indicates a net increase of more than 18% for the five isotopes which are important to the repository performance. Given the results, verify that a design change is needed.*

Response:

The criticality consequence criterion discussed in Sections 1.2 and 3.6.3 requires that the increase in radionuclide inventory be compared with the total inventory for that waste form that is available for release in the entire repository, not in a single package. Furthermore, as is shown in Figure 1-1, failure to meet this criterion requires that the increment in radionuclide inventory be considered in the TSPA. The purpose of this criterion is to avoid performing unnecessary TSPA analyses if the radionuclide increment resulting from the criticality is extremely small.

### **Section C6.1 Total System Performance Assessment Dose Estimation**

*RAI C-13 Evaluate travel times for gases to the surface for the cases of worst-case disruption of the EBS and repository environment from energetic criticality transients.*

*As stated in the discussion, "gaseous fission products such as 85Kr are ignored because only a small amount are produced..." However, there are others that will be produced in significant amounts. Therefore, an evaluation of the travel times for these gaseous fission products to the surface becomes important.*

Response:

Please see the response to RAI C-9.

*RAI C-14 Verify that Figures C-34 and C-35 indicate the incremental dose from just increasing the radionuclide inventory by the numbers in Table C-16 in one waste package which is the result of a single criticality. In addition, discuss the risk from multiple waste packages becoming critical because of juvenile failures.*

**Response:**

The assumption in the RAI that Figures C-34 and C-35 indicate the effect of one criticality is correct. However, the two curves in each figure are based on different assumptions, so the figures are potentially misleading. In the figures, the overall TSPA dose is based on only partial loss of cladding, while the dose increment due to a single PWR waste package criticality is based on all the cladding being lost. This is the reason that the increment Tc-99 peak just after 25,000 years is nearly 15% of the total dose, although the actual Tc-99 increment is only 4% of the total for that isotope. The assumption of complete cladding loss following the criticality was used because it is conservative. DOE plans to make a comparison calculation with increment and base TSPA on the same assumption of cladding loss, to show that the dose from this single isotope is linearly proportional to the inventory of the isotope. DOE plans to revise Appendix C to incorporate the results of these updated calculations and comparisons.

This RAI also suggests that the radionuclide increment would be larger if there were multiple criticalities from a common-mode early failure. This is extremely unlikely for two reasons. First, the fabrication process will be carefully engineered to minimize residual stress on welds, the most frequent source of common-mode failures in pressure vessels. Secondly, even if there are cracks from failed welds, DOE expects to show that there is very low probability of water contacting the penetration (depending on length of crack/fracture, as well as the aperture). DOE expects to show that even if water does contact the penetration, there will be little probability of water being able to transport in and out in sufficient quantity to corrode the borated stainless steel and remove the boron from the waste package. Because of these factors, it is necessary to include the very low probability of multiple criticalities when comparing the incremental dose from criticalities to the TSPA expected (base) case.

A complete list of the radionuclides considered for the example in Appendix C, and the curie inventory for each, is given in the table below. However, the first four radionuclides shown in Table C-16 were the dominant contributors to additional dose from the criticality. The Pu-242 difference was included in Table C-16 to demonstrate that the criticality event actually produced a reduction in some of the radionuclides that were considered important to TSPA.

Isotope	Curie Inventory at 25,000 years			
	Single Assembly* After 10,000 Year Criticality	Single Assembly* Decay Only	Single Assembly* Increase From Criticality	21 PWR WP Increase From Criticality
Pa-231	1.40E-02	6.30E-03	7.70E-03	1.62E-01
C-14	2.40E-06	1.60E-06	8.00E-07	1.68E-05
U-234	7.20E-01	6.50E-01	7.00E-02	1.47E+00
Pu-239	8.70E+01	8.00E+01	7.00E+00	1.47E+02
Se-79	1.20E-01	1.10E-01	1.00E-02	2.10E-01
Tc-99	3.80E+00	3.60E+00	2.00E-01	4.20E+00
I-129	9.20E-03	8.80E-03	4.00E-04	8.40E-03
Np-237	3.90E-01	3.80E-01	1.00E-02	2.10E-01

\* 3 wt% U-235 enrichment, 20 GWd/mtU initial burnup

Juvenile/early waste package failures were not considered in the example evaluation included in Appendix C because a final rate had not yet been developed at the time the criticality probability estimate was performed. However, since the methodology requires that the waste package failure distribution used in the criticality probability calculations be consistent with that used in the TSPA, this issue is expected to be addressed in the references to the License Application. Furthermore, with the change in the waste package barrier materials, it is expected that early waste package failure will be the dominant contributor to the criticality probability during the first 10,000 years. However, this probability is still expected to be very small for the following reasons:

- a) Only a small fraction of packages (on the order of  $10^{-4}$  per waste package) would be expected to have a manufacturing or handling induced defect that could lead to early failure.
- b) The defective package must be located under a dripping fracture to be of concern for criticality.
- c) The defect must result in a failure that is capable of passing a significant fraction of the water dripping on the waste package into the interior and must be located such that ponding of water within the waste package is possible.
- d) The borated stainless steel must become sufficiently degraded and the boron removed from the waste package.
- e) The waste package must remain flooded long enough for the borated stainless steel to degrade to the point where criticality is possible.
- f) The defective waste package must contain fuel that is capable of exceeding the critical limit if the package is flooded, the borated stainless steel is sufficiently degraded, and the boron has been removed from the waste package.

A rough estimate can be made using the probabilities given in Table 4-4 of the Topical Report and substituting the one juvenile failure at 1,000 years assumed in the TSPA for  $P_{\text{breach}}$ . Using this crude approximation, the contribution to cumulative probability of criticality at 10,000 years from juvenile failure for the no-loading-curve case would be  $\sim 2 \times 10^{-7}$  per PWR waste package.

### **Section C7.0 Conclusion**

*RAI C-15 The example and the topical report does not address the classes of criticality events with potentially high consequences.*

*In particular, the report does not give adequate attention to sudden reactivity insertions and the full range of mechanisms for positive reactivity feedback (i.e., autocatalytic criticality).*

Response:

The technique used to identify and evaluate all rapid insertion-rate mechanisms is discussed in the responses to RAIs 3-19, 3-20, and 4-42.

### **Appendix D Example Application of the Methodology for DOE Spent Nuclear Fuel** **Section D2.2 External Configurations**

*RAI D-1 Correct the reference to the discussion in Appendix C of external configurations. Neither Appendices C or D evaluate external criticality.*

Response:

In Section 2.2, it is stated that eventual discussions of external criticality *will include configurations similar to those discussed in Appendix C*. Sections 2.2.2 and 2.2.3 of Appendix C discuss external configurations with the potential for criticality. There is also reference to the documents in which the criticality evaluations associated with these configurations are described.

### **Section D3.1 Evaluation of Critical Configurations**

*RAI D-2 Clarify the application of the methodology in this example, with respect to the flow chart presented in Figure 1.1 in the main body of the report, page 1-10.*

*It appears, in this example, that design changes were made in the choice of poison material ( $GdPO_4$ ) and its concentration, without having evaluated configurations with respect to the probability criterion. This suggests a departure from the methodology described in the flow chart. The staff notes that the flow chart may*

*need to be revised to reflect the fact that the need for design changes may become apparent much earlier in the process.*

Response:

The example application did not follow the full path of the disposal criticality methodology as presented in Figure 1-1. The evaluation included a conservative assumption, based on an engineering judgement that the probability criterion would not be satisfied, and implemented a design option for the DOE SNF Canister. Therefore, the evaluation was not really a departure from the methodology, only a conservative simplification. It is likely that the same results would have been reached if the probability evaluation had been performed.

## Attachment A - -

### Commercial SNF Internal Configuration Validation Planned Workscope

#### I. Isotopic Validation

##### A. Code-to-Code Comparison

Prior to validating the isotopic depletion model with radiochemical assay data and commercial reactor critical integral experiments, the SAS2H one-dimensional depletion code is expected to be compared to a more detailed two-dimensional isotopic depletion code. The objective of this comparison will be to evaluate the analytical assumptions and approximations when applying a one-dimensional depletion code to model heterogeneous fuel types with burnable thermal neutron absorbers. In particular, DOE expects to review the impact of: lattice smearing, gadolinia fuel depletion, moderator density, control blade insertion during depletion, and history effects. Code-to-code comparisons of isotopic concentrations are expected to be performed to demonstrate and quantify depletion endpoint agreement. Isotopic concentration values are expected to be used as input to a waste package criticality model to compare integral  $k_{\text{eff}}$  values resulting from the various modeling assumptions and approximations.

Information from this section is expected to result in an improved understanding of the effects of the analytical assumptions and approximations used in setting up input decks for analyzing the diverse radiochemical assays on a consistent basis.

##### B. Radiochemical Assays

Establishment of isotopic depletion model bias is expected to rely on analyses using radiochemical data and commercial reactor critical integral experiments. Use of assays is discussed in this section.

Fifty-four chemical assay samples were obtained from irradiated fuel assemblies discharged from seven different Pressurized Water Reactors (PWRs) (DOE 1997). Thirty chemical assay samples were obtained from irradiated fuel assemblies discharged from three different Boiling Water Reactors (BWRs) (ORNL 1998). Additional chemical assay samples are expected to be analyzed. These additional assays include 13 PWR samples with enrichments of 4.00 wt% U-235 and 4.65 wt% U-235 and rod average burnups ranging from 27.0 GWd/mtU to 48.5 GWd/mtU. The additional assays also include 13 BWR samples with uranium enrichments of 3.00 wt% U-235 and 3.80 wt% U-235, rod average burnups of about 62 GWd/mtU and about 70 GWd/mtU, and one sample of 2.00 wt% gadolinia. The relevant characteristics and burnup histories of these samples are expected to be modeled in SAS2H and a two-dimensional depletion code.

Historically, radiochemical assay data have significant uncertainties associated with measured values. Also, fuel assembly exposure history and core operation data for assemblies used in the radiochemical assay analyses are not always complete and in sufficient detail to accurately model the isotopic depletion. In addition, most of the radiochemical assay samples are for small segments of a single fuel rod. DOE plans to use a two-dimensional lattice code to transition fuel assembly core operations data to fuel rod data for the radiochemical assay analysis.

The isotopic depletion model bias is expected to be established, in part, as a  $\Delta k_{\text{eff}}$  bias based on radiochemical assay analyses, which include using the measured and calculated isotopic concentrations in representative criticality calculations. DOE plans to appropriately apply this bias in establishing critical limits with the bias obtained from CRC integral experiment analyses (with burnup credit).

#### **C. Commercial Reactor Criticals**

The integral experiments also contain an isotopic bias component. Thus, DOE plans to use CRC integral experiments with radiochemical assay analyses to establish the appropriate  $\Delta k_{\text{eff}}$  bias associated with the isotopic depletion model that is applied in the critical limit. The fuel assembly burnups (exposure) for the CRC analyses are taken from Core Operation Reports and reflect the exposure history of the fuel assembly. The exposure history is reflected with the presence or absence of neutron absorber material (e.g., soluble boron, burnable poison rods, and control rods/blades), moderator density, and fuel temperature. The exposure history is also reflected in the axial distribution of the burnup. The level of detail available with CRC integral experiments will support the development of an integral isotopic depletion model bias component. DOE plans to develop a method during model validation to appropriately account for isotopic bias in the critical limit and avoid repeated application of any portion of the isotopic bias.

#### **D. Statistical Analysis**

DOE expects to perform statistical analyses on the isotopic validation benchmark set. Statistical tests for outliers and normality are also expected to be performed to identify anomalous data points or non-normal data sets.

The measured and calculated isotopic results are expected to be used as input to a consistent waste package criticality model to compare integral  $k_{\text{eff}}$  effects resulting from the various modeling assumptions and approximations and to be used to determine a  $\Delta k$  bias.

#### **E. Isotopic Distribution Effects**

DOE expects to quantify isotopic distribution effects on criticality calculations for various isotopic models. Variations of spectrum, exposure history, and

modeling approaches are expected to be examined for impact on isotopic distribution. Also, variations in isotopic distributions for actinides and fission products are expected to be examined for impact on prediction of  $k_{eff}$ . Together with other isotopic validation activities, these analyses are expected to address the compensating effects issue regarding the integral criticality calculation method.

#### **F. Decay and Branching Fraction Uncertainty**

DOE expects to evaluate the effects of uncertainties in the half-life and branching fractions used in predicting postclosure isotopic concentrations by a statistical method (using Monte Carlo). The approach used is expected to model the entire system of isotopic decay with all of the parent-daughter relationships. Together with the nominal isotopic values, a  $\Delta k$  bias can be determined to account for these uncertainties.

## **II. Criticality Validation**

### **A. Criticality Benchmarks**

DOE expects to define waste form-specific benchmark subsets (from the total Benchmark Database, which consists of laboratory critical experiments (LCE), PWR CRCs, and BWR CRCs) for each applicable scenario/waste class from the master scenario list. The subset development is expected to consider such aspects as material type, geometry, and neutron spectrum.

**Example:** PWR Intact Fuel Lattice: PWR CRCs, low enriched uranium (LEU) rod lattice LCEs, MOX rod lattice LCEs

PWR Fully Degraded Fuel: LEU homogenous LCEs and MOX solutions homogenous LCEs

#### **1. Benchmark Descriptions**

DOE plans to characterize the benchmarks within the given subsets based on various parameters (e.g., flux spectrum, fission spectrum, material type, and geometry).

#### **2. Adequacy of Benchmarks**

DOE plans to compare the benchmarks within the given subsets to the expected configurations. These comparisons are expected to consider a variety of parameters such as isotopic concentrations, actinide ratios (to U-235), and neutron spectrum.

### **B. Statistical Analyses**

DOE plans to evaluate the  $k_{eff}$  values for waste form/waste class-specific benchmark subsets for the purpose of identifying trends in the bias of the criticality code.

1. Equality Analysis

The benchmarks within the given subsets may be analyzed to evaluate the possibility of combining subsets. Potential combinations include, but may not be limited to, combining like geometry MOX and LEU LCE subsets.

2. Trending Analyses

DOE plans to analyze the subsets for trends that may exist within the subsets. Parameters to be considered include spectral parameters (e.g., absorption, leakage and fission spectrums, and neutron spectrum ratios), material type parameters (e.g., enrichment, burnup, actinide ratios, plutonium concentrations, and boron concentrations), and geometry parameters (e.g., fuel pellet diameter, fuel rod pitch, and fuel rod pitch to fuel pellet diameter ratios).

**C. Development of Critical Limits**

DOE plans to develop critical limits using the results of the trending analyses discussed in Section II.B.2 of this attachment. If necessary, other identified sources of uncertainty (e.g., half-life/branching fraction decay uncertainties and temperature uncertainties) may be applied to the critical limit. These adjustments will produce a final critical limit, based on the set of benchmark critical experiments representing a waste form.

**D. Range of Applicability**

DOE plans to use a systematic approach to identify the Range of Applicability for every waste form/waste class pairing. This is expected to involve considering trended and non-trended parameters. For trended parameters, both the benchmarked range and the trended range are expected to be considered.

The subset characterizations and the statistical analyses are expected to define the Range of Applicability for the calculated critical limits. DOE expects the Range of Applicability to include both trended and non-trended parameters. The parameters may include, but are not limited to: isotopic composition, burnup, initial enrichment (wt% <sup>235</sup>U), cooling time, fuel temperature, fuel type, cladding type, fuel density, geometry type (e.g., square lattice, triangular lattice, homogeneous solution), assembly and/or fuel rod pitch, fuel pellet diameter, fuel rod pitch to fuel pellet diameter ratio, absorber types, and absorber concentrations.

DOE plans to develop a procedure for extending the range of applicability. The extension process may include a code-to-code comparison in addition to physical explanations for the trend and statistical analyses of the trend. The procedure is expected to also include a method for determining the penalty ( $\Delta k_{\text{penalty}}$ ) to be included in the extended range.

### III. Application Model

DOE expects that the final step in the criticality validation will be to define an application model and demonstrate that the application model is bounding. This is expected to involve analyzing the CRCs and a number of scenarios in the waste package from the initial enrichment, through the burnup and decay calculations, and demonstrating the reactivity of the CRCs and the waste package is not underestimated for any of the analyzed scenarios.

### IV. Validation Reports

DOE plans to document the results of the work described in Sections I and II of this attachment in validation reports, one for BWRs and one for PWRs. The reports are expected to include sections or volumes specific to the validation of the isotopic and criticality models.

#### References:

DOE (U. S. Department of Energy) 1997. *Isotopic and Criticality Validation for PWR Actinide-Only Burnup Credit*, DOE/RW-0497. Washington, D.C.: U.S. Department of Energy. MOV.19970625.0081.

ORNL (Oak Ridge National Laboratory) 1998. *Validation of SCALE (SAS2H) Isotopic Predictions for BWR Spent Fuel*, ORNL/TM-13315. Oak Ridge, Tennessee: Oak Ridge National Laboratory. TIC 245042.

**Note:** This outline of planned workscope is for Commercial Spent Nuclear Fuel (SNF) Internal Configuration only. It is offered as an example. DOE recognizes that additional validation reports are expected to be necessary. These may include validation reports for: DOE Research Reactor SNF Internal Configuration, DOE Plutonium High Level Waste (HLW) Internal Configuration, and Degraded SNF/HLW External Configuration. There are no plans to have a validation report for Naval SNF, separate from the *Addendum to the Disposal Criticality Analysis Methodology Topical Report for Naval Spent Nuclear Fuel* to be submitted to the NRC in late 1999.

## Attachment B

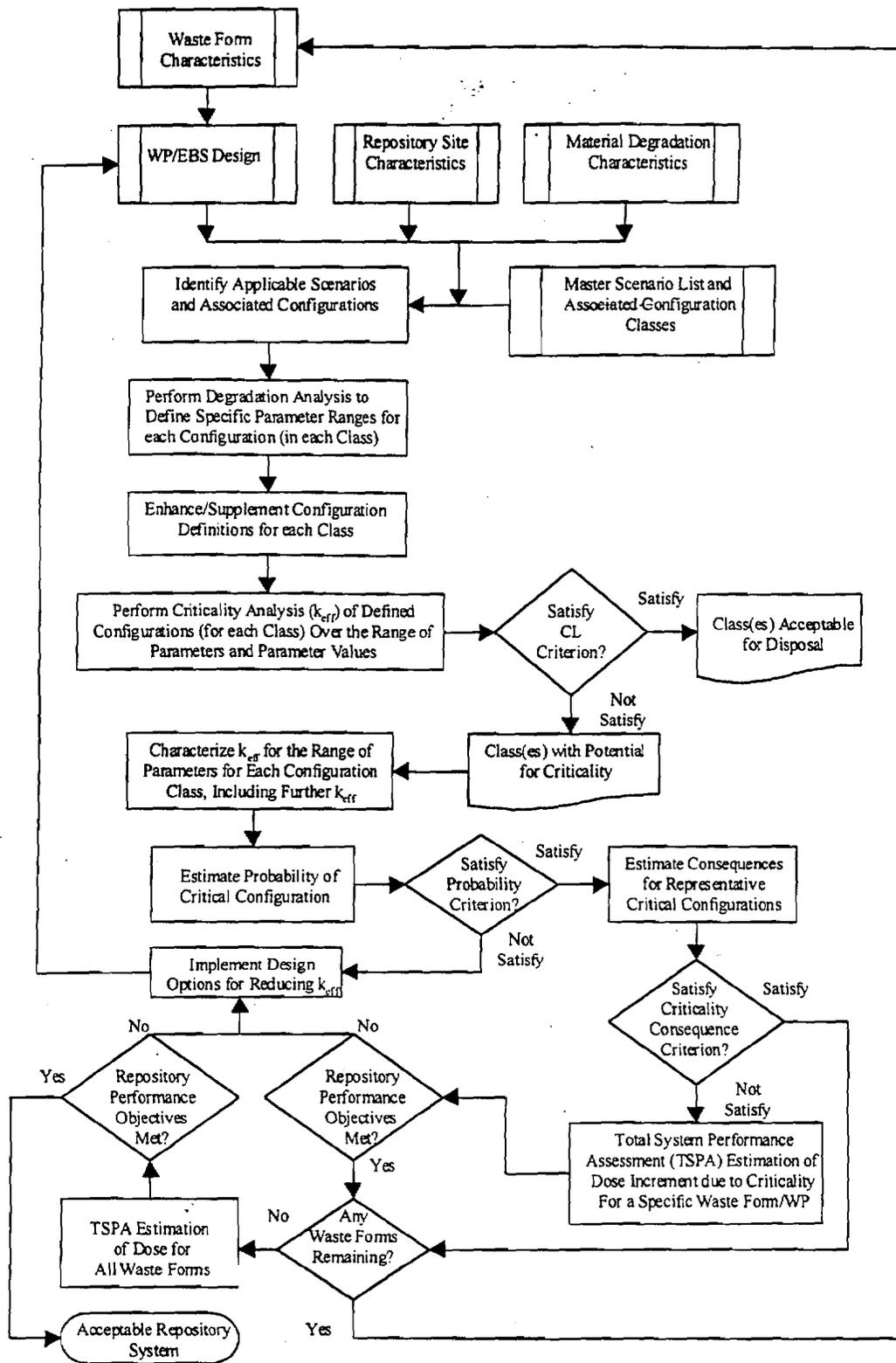


Figure 1-1. Overview of Disposal Criticality Analysis Methodology

# Attachment C

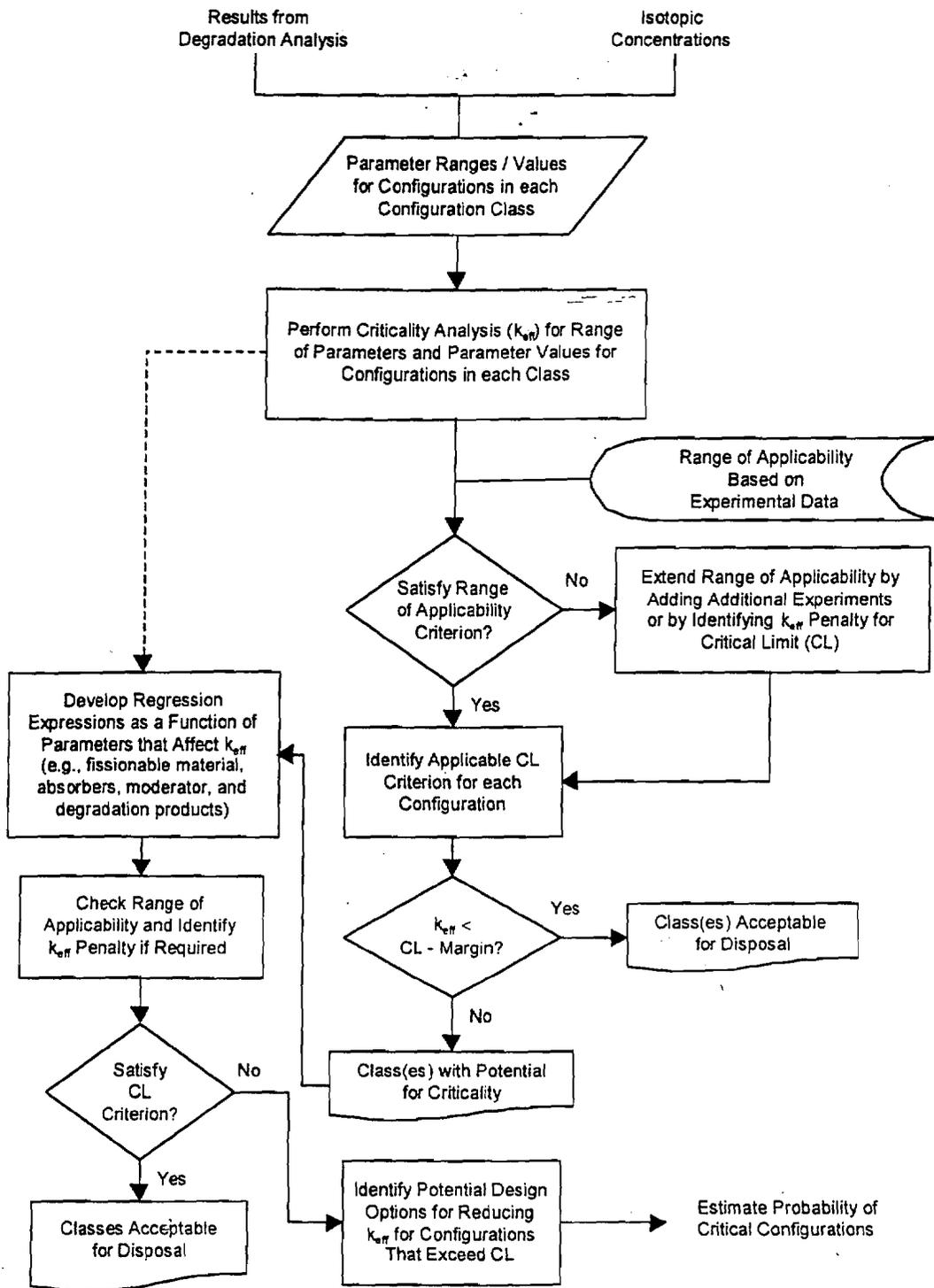


Figure 3-3. Criticality Analysis Methodology

## ENCLOSURE 2

A description is provided below of the aspects of the disposal criticality analysis methodology for which near-term acceptance is sought. Unless otherwise specified, all figures and section numbers refer to the *Disposal Criticality Analysis Methodology Topical Report*, YMP/TR-004Q, Revision 0.

### **Overall methodology**

DOE requests acceptance of the risk-informed processes that is the core of the methodology. The risk-informed process is illustrated in Figure 1-1 (discussed in Section 1.5) and revised in Attachment B of Enclosure 1. We do not seek acceptance for a specific application of the methodology, and we understand that we will need to demonstrate acceptability of specific applications to support licensing.

### **Design criteria**

DOE requests acceptance of the four design criteria presented in Section 1.2, Part A of the Topical Report as acceptable for ensuring that design options are properly implemented for minimizing the potential for, and consequences of, criticality. The design criteria are discussed in Sections 3.4, 3.5, 3.6, and 3.7.

### **Master scenario list**

DOE requests acceptance that the list of standard scenarios outlined in Figures 3-1 and 3-2, as supplemented by the new Sections 3.1.3 and 3.1.4 to be added to the Topical Report as discussed in the response to RAI 3-1, comprehensively identifies the generic degradation scenarios incorporating those features, events, and processes associated with the proposed repository at Yucca Mountain that may significantly affect the potential for, and consequences of, criticality.

### **Method for generating internal and external configurations**

DOE requests acceptance of the method for generating a comprehensive set of potential postclosure configurations as discussed in Sections 3.2 and 3.3 of the Topical Report. Acceptance of this item is requested in Section 1.2, Part C of the Topical Report. The principal components of this method are given in the following list. Some of these components consist of codes that will be the subject of validation reports. Acceptance of these codes will not be sought until the corresponding validation reports are submitted. The use of these codes in the Topical Report, the responses to the RAI's and supporting documentation, is intended only to provide background for understanding of the methodology.

- **Degradation methodology:** Ability of the methodology to calculate the loss of fissionable elements and neutron absorbers and calculate the composition of degradation products precipitating in the waste package. For this purpose we are requesting acceptance of the use of a steady-state geochemistry code. Improvements are still being incorporated into this methodology. The example discussed in the Topical Report (EQ3/6 in the pseudo-flow-through mode,

discussed in Section 4.2.2), has been replaced by the solid-centered-flow-through EQ3/6 code discussed in the response to RAI 4-32, which includes proposed modifications to Section 4.2.2. Use of this code is planned to be demonstrated and justified to support licensing.

- Configuration generator: (1) Use of time-dependent first-order differential equations, solved by numerical integration, to track the concentration, or amount, of fissionable or neutron absorber material (Section 4.3.3); (2) Development of coefficients or terms of these equations by abstraction from a steady-state geochemistry code (EQ3/6) calculations (Section 4.3.4); and (3) Random variation of terms or coefficients in these equations as part of a Monte Carlo calculation to reflect the uncertainty in the rates and location of natural processes (Section 4.3.4). In implementing #2, the appropriate balance between the use of EQ3/6 and the Configuration Generator Code will be demonstrated for each major waste form category as part of the License Application process. Examples of the use of #3 are given in Appendix C of the Topical Report, Sections 3.3 and 4.1, in response to RAI 4-38, and in CRWMS M&O, *Probability of Criticality for MOX SNF*, CAL-EBS-NU-000007.
- Accumulation Methodology: Ability of the methodology to calculate the accumulation of fissionable elements external to the waste package. For this purpose we are requesting acceptance of the use of a geochemistry-transport code and/or a geochemistry code used in a mode that simulates transport. The latter has been illustrated by EQ3/6 in the open-system mode described in Section 4.2.3 and Figure 4-7 of the Topical Report. The former is illustrated by the geochemistry-transport code PHREEQC, which is described in the responses to RAIs 3-5, 3-9, and 4-32. Use of the code developed for this application is planned to be demonstrated and justified to support licensing.

#### **Criticality evaluation method**

DOE requests acceptance of the criticality evaluation process discussed in Section 3.4. This process is illustrated in Figure 3-3 and revised in Attachment C of Enclosure 1. Acceptance of this item is requested in Section 1.2, Part D of the Topical Report. Review and acceptance of specific computer codes and isotope sets are not requested. We are not seeking acceptance of any specific application of the process and recognize that we will need to demonstrate the specific applications to support licensing.

#### **Probability estimation method**

DOE requests acceptance of the following aspects of the probability estimation method: (1) Development and use of a table of  $k_{\text{eff}}$  for the range of possible configuration parameters to construct a regression for  $k_{\text{eff}}$  as a function of these parameters or for direct table lookup and interpolation (Section 3.5, page 3-21 and modification of this paragraph given in the response to RAI 3-16); (2) Monte Carlo methodology using random sampling of parameters characterizing configurations and determination of  $k_{\text{eff}}$  by calculation from the regression expression or table lookup and interpolation as a function of these parameters to obtain a sample of up to 1 million values of  $k_{\text{eff}}$  to simulate a

probability distribution (the new paragraph for the Topical Report, given in the response to RAI 3-16); (3) Incorporation of the WAPDEG-generated probability distribution for time of breach and duration of the "bathtub" as two of the parameters (Section 3.5, page 3-22); and (4) Estimate of criticality risk for TSPA (before 10,000 years and to the time of peak dose) (paragraph to be included at the end of Section 3.7, attached to the response to RAI C-14). Acceptance of this item is requested in Section 1.2, Part E of the Topical Report.

#### **Consequence evaluation method for a steady-state criticality**

DOE requests acceptance of the following aspects of the consequence evaluation method for a steady-state criticality: (1) Determination of temperature such that the evaporation rate over the waste package pond surface equals the volumetric drip rate into the waste package (Section 4.4.1.1, page 4-45); (2) Use of the drip rate probability distribution as a function of time (which comes primarily from the climate- and mountain-scale hydrology model) (Section 4.4.1.1 as augmented in the response to RAI 3-23); and (3) Determination of radionuclide increment from depletion code (ORIGEN-S) as a function of power, integrated over the duration of the criticality (Section 4.4.1.1 as augmented in the response to RAI 4-51). Acceptance of this item is requested in Section 1.2, Part F of the Topical Report. It should be noted that acceptance of the ORIGEN-S code will not be sought until the corresponding validation report is complete and referenced in the License Application. The use of this code in the Topical Report, the responses to the RAIs, and supporting documentation, is intended only to provide background for understanding of the methodology.

#### **Validation process for criticality model**

DOE requests acceptance of the criticality model validation process described in Section 4.1.3. Acceptance of this item is requested in Section 1.2, Part G of the Topical Report and discussed further in the response to RAI 1-3. Specifically, DOE requests acceptance that the process presented in Subsection 4.1.3.2 for calculating the criticality limit values and the general approach presented in Subsection 4.1.3.3 for establishing the range of applicability of the critical limit values define the validation process for the criticality model. This validation process will be followed to calculate critical limit values for specific waste forms and waste packages as a function of the degradation conditions. Further clarification is provided in responses to RAIs 4-7 through 4-21. We do not seek acceptance of critical limit values, and we recognize that application to specific postclosure repository conditions will need to be demonstrated prior to licensing.

#### **Requirements for confirmation of bounding isotopic model**

DOE requests acceptance of the three requirements presented in Subsection 4.1.3.1.4 of the Topical Report that describe the acceptance criteria for confirmation of the bounding isotopic model used for burnup credit for commercial SNF. Acceptance of this item is requested in Section 1.2, Part K of the Topical Report. We request acceptance of the method for confirmation of the bounding applications model and not of the method for validation of the isotopic model. Further clarification is provided in responses to RAI 4-1 and RAIs 4-4 through 4-6.

**Validation process for the geochemistry model/codes**

DOE requests acceptance of the validation process for the degradation analysis methodology that uses the solid-centered-flow-through mode (an improvement on the pseudo-flow-through mode described in Section 4.2.2 of the Topical Report, as discussed in the response to RAI 4-32). DOE also requests acceptance for the validation process for accumulation methodology that uses a geochemistry-transport code (e.g., PHREEQC, described in the response to RAI 4-32) or a geochemistry code used in a mode that simulates transport (e.g., EQ3/6 in the open-system mode described in Section 4.2.3). This validation is expected to be provided by comparison between codes (both EQ3/6 and PHREEQC), comparison with experimental data, and comparison with natural analogs. These comparison cases are summarized in Tables 4-2 and 4-3 of the Topical Report. We do not seek acceptance of the bounding cases, which have been identified for the current range of environmental parameters and may be modified for the environmental parameters applicable to the Yucca Mountain repository that will support licensing.

**Validation process for the probability calculation and configuration generator models**

DOE requests acceptance of the validation process for the probability calculation and configuration generator models presented in Sections 3.5 and 4.3 of the Topical Report as modified by responses to RAIs 3-16, 3-19, 4-25, 4-36, and 4-37 that will be implemented by the Monte Carlo probability calculation methodology. DOE plans to validate this methodology by comparison with hand calculations of combinations of probabilities of individual events taken from distributions similar to those used for the Monte Carlo selection process. We also request acceptance that the configuration generator models described in Sections 4.3.3 and 4.3.4 can be validated by appropriate hand calculations.

**Validation process for the steady-state consequence model**

DOE seeks acceptance of the validation process for the steady-state criticality consequence model, specifically that a computer code can be written to perform the numerical integration of power over time and distribution of drip rates, as well as calculating the heat loss according to well-known physics formulae. This process is described in Section 4.4.1.4 of the Topical Report, as modified by the responses to RAIs 3-23 and 4-51. The resulting program will be checked by hand calculation. It is assumed that no validation is required for the use of well-known physics formulae. DOE plans to validate the use of ORIGEN-S to compute the radionuclide increment from steady-state criticality with available data.

**Table 1. Summary of Items for Acceptance**

Item	Requested in Topical Report	Description Provided In
Overall methodology	Section 1.2, Item A	Figure 1-1, Section 1.5
Design criteria	Section 1.2, Item A	Sections 3.4, 3.5, 3.6, and 3.7
Master scenario list	Section 1.2, Item B	Figures 3.1 and 3.2, Section 3.1, RAI response 3-1 (new Sections 3.1.3 and 3.1.4)
Method for generating internal and external configurations (degradation, transport, and accumulation of fissionable materials)	Section 1.2, Item C	Sections 3.2 and 3.3; RAI responses 3-5, 3-9, 4-32, and 4-38
Criticality evaluation method	Section 1.2, Item D	Figure 3-3, Section 3.4
Probability estimation method	Section 1.2, Item E	Section 3.5, RAI responses 3-16 and C-14
Consequence evaluation method for a steady-state criticality	Section 1.2, Item F	Section 4.4.1.1, RAI responses 3-23 and 4-51
Validation process for criticality model	Section 1.2, Item G	Section 4.1.3, RAI responses 1-3 and 4-7 through 4-21
Requirements for confirmation of bounding isotopic model	Section 1.2, Item K	Section 4.1.3.1.4, RAI responses 4-1 and 4-4 through 4-6
Validation process for the geochemistry model/codes	Section 1.2, Item H	Section 4.2.2, Tables 4-2 and 4-3, RAI response 4-32
Validation process for the probability calculation and configuration generator models	Section 1.2, Item I	Section 4.3; RAI responses 3-16 (modified section 3.5), 3-19, 4-25, 4-36, and 4-37
Validation process for the steady-state consequence model	Section 1.2, Item J	Section 4.4.1.1, RAI responses 3-23 and 4-51