



TRW Environmental
Safety Systems Inc.

Criticality Abstraction/Testing Workshop Results

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June 13, 1997

Civilian Radioactive Waste Management System

Management & Operating Contractor

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

**Criticality Abstraction/Testing
Workshop Results**

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

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Workshop Results**

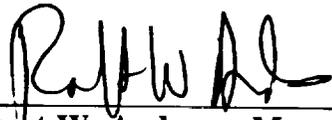
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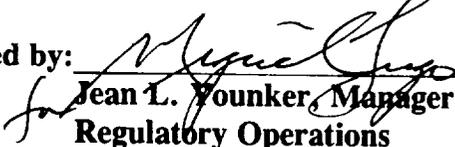
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1. INTRODUCTION

The Criticality Workshop for development of plans and evaluation of criticality in Total System Performance Assessment - Viability Assessment (TSPA-VA) was held on March 18-20, 1997, in Las Vegas, Nevada. This workshop is one of a series of ten workshops intended to provide support to the TSPA-VA (M&O, 1996a). This document serves as a description of the workshop process as well as the analysis plans which were a product of the workshop.

The remainder of this section provides a description of the workshop objectives and process. Also, the approach to abstraction/testing is presented. The additional sections in the report provide the following information:

- Section 2. This section briefly discusses the pre-workshop preparation. A significant effort was expended prior to the workshop to encourage the participants to begin thinking and actually responding to key issues in the area of criticality prior to the workshop. The workshop was meant to be a working meeting, and participants were asked to come appropriately prepared. The correspondence toward this goal is described in this section and provided in the attachments.
- Section 3. The workshop proceedings and results are provided in this section. Each of the three major sessions at the workshop are described. Included in this section are the discussions and development of issues for each major session, ranking and prioritization of the issues, development of major topics from the selected issues, and the initial development of abstraction/testing plans for the major topics.
- Section 4. The finalized abstraction/testing plans for the major topics are presented in this section. The plans required additional work after the workshop in order to be fully realized with appropriate activities, responsibilities, and schedules. The final plans were developed in coordination with the workshop participants.
- Section 5. References are presented in this section.

There are nine attachments to the report, which provide the correspondence for the workshop as well as copy of the viewgraphs presented at the workshop. The attachments also include a series of tables for issues developed in each of the major sessions, ranking of the issues, and summary of the issue prioritization.

1.1 WORKSHOP OBJECTIVES

Nuclear criticality must be considered as part of TSPA analyses because of the potential for increases in the doses and/or releases from the repository system if a criticality event occurs. Furthermore, the NRC design criteria given in 10 CRF 60 specify the k_{eff} (a measure of the ability of a nuclear chain reaction to be self-sustaining) must be less than 0.95. Although waste-packages are designed to no permit formation of potentially critical configurations if the container criticality-control features are

intact, degradation of the waste-package and transport of actinides can result in creation of potentially fissile configurations. Because of the long period of regulatory concern, normal geologic processes can mobilize fissile materials. Therefore, nuclear criticality is included in the TSPA analyses.

The Criticality Workshop attempted to bring together the key project personnel working on criticality including neutronics modelers, process level modelers, and TSPA modelers. These personnel must be integrated in providing the analyses/models of criticality for the TSPA-VA.

This workshop was intended to provide useful integration among these three groups. During the workshop, various key issues regarding criticality were discussed. The TSPA modelers had an opportunity to present the issues which they expect will be important in the repository and how these issues can be incorporated into total system performance assessment models. The process level modelers presented their current level of knowledge. The neutronics modelers presented their current understanding of the various phenomenon as well as their capabilities of gaining additional information.

The primary goals of the workshop as defined in the workshop invitation (see Attachment I) are:

- 1) Identification of Issues. Identify and group the important issues (e.g., processes and parameters) of criticality with respect to long-term performance of the total system. The suggested grouping is based on in-package, near field, and far field criticality evaluations.
- 2) Prioritization of Issues. Prioritize the issues based on the criteria that affect criticality.
- 3) Presentation of Previous TSPAs. Present how the important issues and associated uncertainties have been incorporated in previous TSPAs. Discuss appropriateness of these methods and possible alternatives.
- 4) Treatment of Uncertainty. Decide upon a method for addressing and quantifying uncertainty in the process models and parameters for the topics for which abstraction and testing of the abstraction are being developed.
- 5) Plan for Abstraction/Testing. Develop a plan (or plans) for developing and testing appropriate model abstractions of the most important processes. The plan should consider the following important issues: (a) type of abstraction that is most appropriate, for example, response surface, lower-dimensional process model, analytical model/algorithm, etc., or a combination of these. The abstraction must be sufficiently accurate, and capable of interfacing with the TSPA software in a computationally efficient manner; i.e., the abstraction must be able to be used in a multi-realization probabilistic mode; and (b) representation of spatial and temporal variability in the abstraction.
- 6) Coupling of Criticality Evaluation Modeling with Other TSPA-VA Components. Discuss and, if possible, define how the abstractions for criticality will interface with other abstraction/testing activities in a consistent fashion.
- 7) Post-Workshop Activity Scheduling. Discuss how available resources and scheduling will affect post-workshop activities. These include (a) how do abstraction/testing activities fit into

both overall PA schedule and overall Site, Design and material testing schedules?; (b) can some activities be performed that will satisfy currently planned deliverables?; and (c) develop a tentative schedule for completion and delivery of post-workshop products.

These objectives, although quite ambitious, were essentially met at the workshop. The plans for abstraction/testing were not fully completed at the workshop but are presented in final form in Section 4 of this report.

1.2 SPECIFIC OUTCOMES AND PRODUCTS OF POST-WORKSHOP ABSTRACTION/TESTING ACTIVITIES

The specific post-workshop objectives in the area of disposal criticality are listed below:

- 1) Workshop Report. Write the workshop deliverable, which reports upon the activities and decisions of the workshop and the plans for post-workshop abstraction/testing activities that feed TSPA-VA.
- 2) Abstraction/Testing Activities. Develop and test abstraction methods proposed at the workshop. Compare abstracted models to more detailed models to determine (or test) accuracy (acceptability) of abstractions. Errors in abstractions should be on the conservative side.
 - a) Decide upon the degree of dimensionality reduction.
 - b) Determine how to incorporate spatial and temporal variability.
 - c) Test the interface with TSPA software and see if it is feasible to use the given abstraction in multi-realization fashion.
 - d) Examine predictions of the abstraction compared to the process model. Does the abstraction represent uncertainty appropriately?
 - e) Determine if the abstraction can be coupled with other abstractions such that coupled processes and synergistic effects are still accurately captured by the abstraction(s).
- 3) TSPA-VA Report Sections. Write a section for the TSPA-VA report detailing the models and abstractions to be used for TSPA-VA. All decisions should be documented, along with the sensitivity analyses and abstraction-testing that are performed. The workshop deliverable should serve as a starting point.

1.3 OVERALL WORKSHOP PROCESS

The workshop process essentially followed four major steps. These steps are shown in Figure 1-1 and discussed in the following.

Step 1: Identification of Issues. The Abstraction Core Team (Ralston Barnard, Jerry McNeish, and Peter Gottlieb) produced an initial list of issues which are important to evaluation of disposal criticality. These issues were grouped into three major issues: 1) in-package; 2) near field and; 3) far field. Initial presentations were made on each of the three major categories, and this was followed by small group discussion on the major issues. The small groups developed their own set of sub-issues.

Step 2: Prioritization of Issues. The small groups rated the sub-issues in terms of the criteria which were developed for the criticality evaluation. The sub-issues were rated as to significant, moderate, and negligible effect on the criteria.

Step 3: Consensus on the Key Issues. Overall full group consensus was reached after tallying the small group's results. Discussion was held and, where disagreements arose, a compromise position was arrived at.

Step 4: Development and Prioritization of Analysis Plans. After the important sub-issues for each of the major issues had been selected and full-group consensus had been reached for the selected sub-issues, the participants split into three groups: 1) in-package; 2) near field and; 3) far field. Participants joined a group based on where their expertise would be the most beneficial. Each group discussed what evaluations of criticality are required for TSPA-VA. The groups then discussed what work would be necessary on the part of the data collectors and the process level modelers to facilitate these evaluations. Analysis plans were developed in draft form at the workshop and have been further developed after the workshop.

1.4 APPROACH TO ABSTRACTION/TESTING DEVELOPMENT

The approach to abstraction/testing was described in the TSPA-VA plan (M&O, 1996a) and is briefly presented in this subsection. Figure 1-2 provides an overview of the approach. The key initiators are the identification of issues that are important to evaluation of criticality. These key issues identified are then used to define and develop appropriate analyses to evaluate the issues and uncertainties.

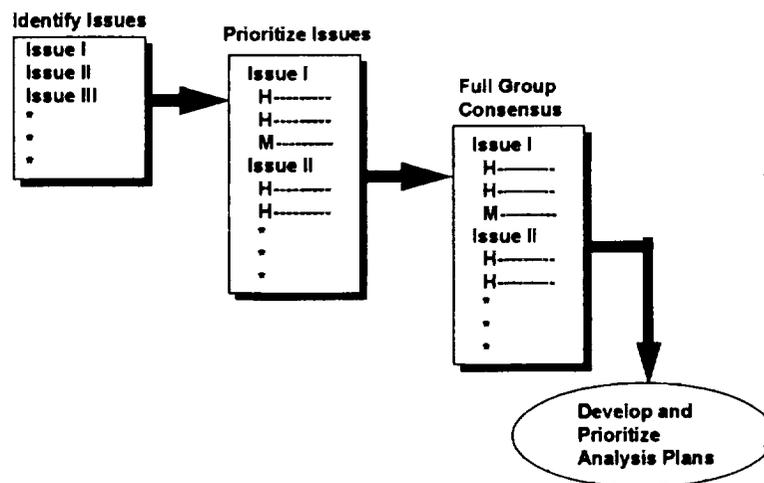


Figure 1-1 Diagram for the overall workshop process. Illustration of the processes for identifying and prioritizing sub-issues and developing analysis plans for the issues most important to evaluation of disposal criticality.

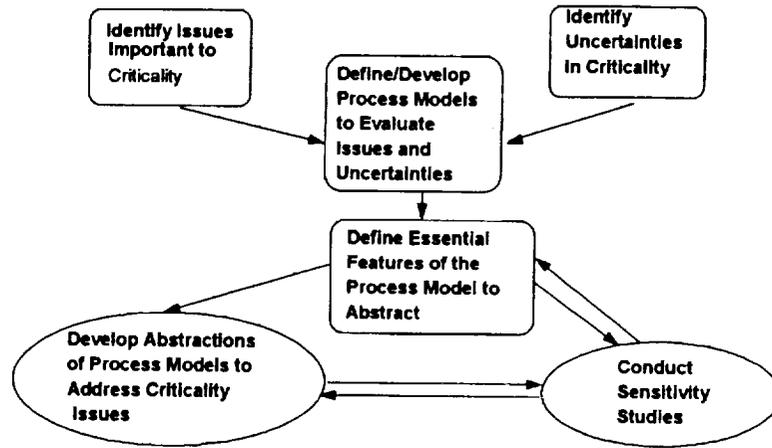


Figure 1-2 Diagram illustrating the overall approach to model abstraction/testing development for criticality evaluation for TSPA-VA.

2. PRE-WORKSHOP PREPARATION

2.1 INTRODUCTION

This section describes the preparation done by the workshop organizers, participants and observers prior to the workshop. There was a significant amount of work prior to the workshop to plan the workshop, to inform participants as the expectations of the workshop in the invitation letter, and to respond to the initial strawman proposals in the invitation letter. These activities and products are described in the following.

2.2 PRE-WORKSHOP PLANNING

The planning of the workshop included efforts to develop a list of issues important to evaluation of criticality, which potentially affect the overall system performance. Meetings were held between PA staff and Waste Package staff involved in criticality evaluation activities. An issue list was developed from these meetings.

A final workshop planning meeting was held on February 21, 1997, with the Performance Assessment Management (Robert Andrews and Holly Dockery), Jerry McNeish, Rally Barnard and Mike Scott (workshop facilitator). This meeting was held to finalize the workshop agenda and review the workshop process and logistics.

2.3 WORKSHOP INVITATION LETTER PACKAGE AND STRAWMAN PROPOSALS

After the list of key issues was developed, a letter for the formal invitation to the workshop was sent to participants, observers, and other interested parties on February 20, 1997. A copy of the letter is provided in Attachment I. The letter included several attachments. These attachments provided the following information:

- 1) Attachment A: Workshop Goals. The overall goals of the workshop were presented in this attachment.
- 2) Attachment B: Introduction to TSPA. Many of the participants were not Performance Assessment personnel. This attachment was developed to provide an introduction to performance assessment and to give the non-PA personnel the perspectives and education on the important aspects of TSPA.
- 3) Attachment C: Discussion of Abstraction. One of the main purposes of the workshop was to develop plans for abstracting and testing the results or information from detailed process models into TSPA evaluations. This attachment provided an overview of the abstraction activity and what it means.
- 4) Attachment D: Important Issues. This attachment provided a concise list of the issues developed by the abstraction core team prior to the workshop. As described above, the issues were developed by incorporating inputs from the workshop participants.
- 5) Attachment E: Coupling of Disposal Criticality to Other Models Developed for TSPA-VA. The criticality evaluation is linked to many other processes in the repository system. This

attachment attempted to describe the important couplings between criticality evaluation and other major components in TSPA-VA.

- 6) Attachment F: Preparation for Workshop. This brief attachment described the specific activities expected of each participant prior to the workshop. The objective was to motivate each participant to begin thinking about the issues important to criticality evaluation.
- 7) Attachment G: Strawman Proposals for Addressing Important Criticality Issues for TSPA-VA. This attachment was one of the key pieces of information passed on to the participants. A discussion of the issues identified by the abstraction core team and proposed method for dealing with the issues was presented.
- 8) Attachment H: Draft Agenda for Disposal Criticality Workshop. The draft agenda was based on the agenda developed for the other PA Workshops held this year.
- 9) Attachment I: Panel Members for Criticality Issues. A listing of the participants expected to make presentations at the meeting was provided.
- 10) Attachment J: References. References for the detailed information included in the letter were provided in this section.

2.4 RESPONSES TO DRAFT PROPOSALS

The participants were asked to provide written responses to the strawman proposals which were included in the invitation letter package. Participants were urged to provide comments on the issues. These responses were compiled and provided to all participants and observers in a letter dated March 14, 1997. A copy of the responses is provided in Attachment II. The participants and observers were asked to study the responses prior to the meeting.

3. WORKSHOP PROCEEDINGS AND RESULTS

3.1 INTRODUCTION

3.1.1 Format of Workshop

The general format of the workshop was to provide introductory material for the participants, followed by issue identification, consensus on the key issues affecting criticality and development of abstraction/testing analysis plans. The introductory presentations included an overview of TSPA-VA, the workshop objectives, TSPA introduction, the status of criticality and guidelines for prioritizing and screening issues.

After the general introductory presentations, each of the three major issues was discussed. For each issue, a TSPA modeler gave a presentation on how the issue had been incorporated into previous TSPAs. This was followed by presentations from data collectors and process level modelers on their current understanding of the issue.

For each of the three major issues, following the formal presentations and brief discussion, the participants split into four groups to discuss and prioritize the key subissues for each major issue. The four groups then combined their respective lists of subissues to form one large list of subissues. Each of the four groups then prioritized the subissues as to their importance to criticality. These prioritizations were tallied for the whole group, and a full-group consensus was reached as to the top priority subissues for each of the major issues.

The participants were then re-grouped into three groups, based on their expertise and experience in developing the abstraction and testing analysis plans for the three topics. The activity for the development of abstraction/testing analysis plans involved each group developing the fundamentals of a plan to address some of the key subissues for one of the three major topics.

3.1.2 Workshop Agenda and List of Attendees.

The workshop agenda is given in Attachment III. This agenda was based on the format for the agenda of previous PA workshops. A list of attendees is given also in Attachment III. The participants included key project personnel who are involved in evaluating criticality.

3.2 INTRODUCTORY PRESENTATIONS

Introductory presentations were given to provide an overview of TSPA-VA, to discuss the workshop objectives, and to introduce TSPA, and to provide the status of repository and waste package design. These presentations were intended to lay the groundwork for the remainder of the workshop. A copy of the viewgraphs for the introductory presentations are given in Attachment IV.

Following an overall introduction by Mike Scott, the facilitator for the workshop, Holly Dockery made the first of the series of introductory presentations. She provided an overview of the abstraction

workshop process to support TSPA-VA, including discussion of: 1) approach and schedule for TSPA-VA, 2) appropriate integration of models into TSPA, 3) documentation of assumptions, 4) the roles and responsibilities of the different workshop participants, 5) the importance of collaboration between the various participants, and 6) technical and programmatic constraints in the abstraction process.

A more specific introduction to the criticality workshop followed (R. Barnard) discussing 1) the workshop goals, 2) scope of the criticality workshop and, 3) structure of the workshop.

An introduction to the TSPA and relevant abstraction activities was presented (J. McNeish). The hierarchy of conceptual models, process models, subsystem models, and the total system model, including the connections between the various process models within the system model were described. It was explained in the presentation why abstractions, instead of detailed process models, are used in TSPAs.

An update on the repository design was presented (D. McKenzie) followed by an update on the waste package design (T. Doering). These presentations provided background information on the details of the current designs being developed by the project.

The status of post-closure process level criticality modeling was presented (P. Gottlieb), including scenarios currently under consideration which could potentially lead to criticality.

The planned and ongoing activities supporting disposal criticality in WBS 1.2.2 were presented (D. Thomas). A significant portion of the work can be incorporated in some manner to the PA disposal criticality evaluations.

3.3 PRIORITIZATION AND SCREENING OF ISSUES

To begin the issue definition and prioritization section of the workshop, a presentation was made by R. Barnard. He detailed the 1) impetus for considering post-closure criticality, 2) development of the major issues for in-package, near-field, and far-field criticality, 3) the issues prioritization process for the workshop, and 4) the three performance related criteria on which prioritization was to be based.

As described previously (Sections 1.3 and 3.1), the workshop participants added/revised the initial list of subissues for each of the three major issues. Since only a limited amount of time and resources are available for TSPA-VA, it would not be possible to address all of the subissues identified by the participants. Thus it was necessary to prioritize the subissues to select only the key issues that are most important to criticality evaluation. For TSPA-VA, efforts will focus on analysis plans to address only the key issues.

3.3.1 Criteria for Prioritization and Screening

The criteria for screening and prioritization of issues were developed based on repository performance related to criticality. The prioritization criteria were as follows: 1) source term inventory, 2) radionuclide release rate, and 3) dose at the accessible environment. Thus, each issue was to be prioritized according to its effect on the criteria with an extreme (5), moderate (3), or slight (1) effect.

3.3.2 Prioritization and Screening Processes

The small groups were instructed to assign each subissue a numerical ranking for each of the three criteria: 5 denotes a extreme effect, 3 denotes a moderate effect, and 1 denotes a slight effect of the subissues on the criteria. Thus, each group assigned three numerical scores to each subissue. Adding these three scores gives each subissue a score between 3 and 15 from each group. Adding the total scores from the four groups gives each subissue a score between 12 and 60. Viewgraphs in Attachment V describe this prioritization method. The list of participants in each group is given in Table 3-1.

3.4 SESSION I: IN-PACKAGE CRITICALITY

3.4.1 Panel Presentations

One TSPA modeler, two data-collectors and one process-level modeler gave presentations on various issues on in-package criticality. A copy of the viewgraphs of the presentations is given in Attachment VI.

The previous PA representation of in-package criticality was presented (J. McNeish). The presentation focused on the approach used in the Disposal Criticality Analysis Method Report (M&O, 1996b). The issues, potential representation, and abstraction of the in-package criticality were also presented.

Presentation by the neutronics modelers described the WP degraded internal configurations and consequences in terms of inventory (W. Davis). WP in-package criticality configurations were also described (C. Stockman). Some information on natural analogues was also presented (E. Siegmann).

Alternative waste forms (i.e., DOE SNF, and naval fuel) were discussed (H. Loo and R. Beyer). The special criticality issues of these wastes were presented.

3.4.2 Development and Prioritization of Issues

After the presentations, each of the four small groups reviewed the list of subissues that were developed before and during the panel presentations and prioritized.

Each of the four groups rated each of these subissues according to the criteria and following the approach described in Section 3.3. The subissues and their ratings by group are provided in Attachment VI, starting on p. 28, including a summary of the total scores by group for each of the subissues sorted by their importance. There was a significant drop in the scores after the top 3 issues. These top 3 issues were:

- 1.1 Failure Model of waste package (bathtub, flow-through)
- 1.3 Removal of absorbers from WP and/or basket (particularly boron)
- 1.14 Waste form characteristics

The analysis plans presented in Section 4.1 will provide plans to develop models and abstractions to address some of these key subissues.

3.5 SESSION II: NEAR-FIELD CRITICALITY

3.5.1 Panel Presentations

In this session, several presentations were given on the subject of near-field criticality. A copy of the viewgraphs of the presentations is given in Attachment VII.

The TSPA perspective on near-field criticality was presented (D. Sassani). Previous TSPA analyses did not evaluate near-field criticality. Potential near-field aspects important for criticality as well as uncertainties in those factors were discussed.

Criticality evaluations conducted by Sandia National Laboratory (SNL) were presented (R. Rechar). In particular, the presentation covered the screening analyses conducted for evaluating criticality.

An example near-field criticality evaluation was presented (P. Gottlieb). The analysis considered the potential scenario of concentrating critical mass in zeolites. Detailed nuclear dynamics consequence analysis was presented (L. Sanchez). This presentation covered work conducted at SNL for analysis of DOE SNF.

A discussion on the behavior of Boron was presented (R. Van Konyenburg). The characteristics and potential for removal of boron were presented.

3.5.2 Development of Issues

After each of the presentations, the facilitator asked whether or not the existing sub issue list captured the important issues in the presentation. The issue list was modified appropriately according to a group consensus.

3.5.3 Prioritization of Issues

Each of the four groups then rated each of these subissues according to their effect on the performance criteria. The subissues and their ratings by group are given in Attachment VII, starting on page 12. A summary of the total score by group for each of the subissues is presented and the issues are sorted by their importance. There was a significant decrease in scores for the sub issues after the top 5 subissues.

- 2.1 Seepage into Drift
- 2.2 Separation of fissile and neutron absorbing materials
- 2.3 WP corrosion products
- 2.4 Design of invert materials (filtering and sorbing properties)
- 2.5 Total time of release of radionuclides

The analysis plans presented in Section 4.2 will provide plans to develop models and abstractions to address some of these key subissues.

3.6 SESSION III: FAR-FIELD CRITICALITY

3.6.1 Panel Presentations

In this session, several presentations were given on the subject of far-field criticality. A copy of the viewgraphs of the presentations is given in Attachment VIII.

The TSPA perspective on far-field criticality was presented (J. McNeish). Previous TSPA analyses did not evaluate far field criticality. A potential approach to such analyses and some of the uncertainties were presented.

An example probabilistic calculation for far-field criticality was presented (P. Gottlieb). The example was concerned with evaluation of an organic reducing zone effect on criticality.

The stratigraphic interfaces which may contribute to far field criticality were also discussed (D. Jolley). Both UZ and SZ interfaces were presented.

3.6.2 Development of Issues

After each of the presentations, the facilitator asked whether or not the existing sub issue list captured the important issues in the presentation. The issue list was modified appropriately according to a group consensus.

3.6.3 Prioritization of Issues

Each of the four groups then rated each of these subissues. The subissues and their ratings by group are provided in Attachment VIII, including a summary of the total score by group for each of the subissues sorted by their importance. There is a significant decrease in total after the top 7 subissues. These top 7 subissues are:

- 3.1 Location of criticality event (UZ or SZ)
- 3.2 Dispersion/dilution/mixing during transport to criticality location
- 3.6 Organic concentrating environments (reducing zone)
- 3.12 Type of fissile material transported (consider enrichment, depleted uranium as necessary)
- 3.7 Other stratigraphic or chemical concentrating mechanisms (sorption, colloids, filtration, etc.)
- 3.3 Fracture focussing of radionuclides
- 3.14 Composition of plume

The analysis plans presented in Section 4.3 will provide plans to develop models and abstractions to address the top 5 of these key subissues.

3.7 SELECTION OF IMPORTANT ISSUES

3.7.1 Selection of Key Issues

As described in Sections 3.4 to 3.6, the key important issues were identified after each sessions, based on their important to the selection criteria (or scores) the sessions, the key important issues were presented to the full group for the full-group consensus. The top 10 issues for each session are listed in Table 3-2. The intention was for the top issues to be addressed in some manner in the abstraction/testing plans.

3.7.2 Issues Not Covered or Resolved

At the workshop, the participants generated a total of 42 subissues for the three major issues, which they felt should considered in criticality modeling. Because of the constraints on the *time* and *resources* that are available for TSPA-VA, it is not possible to address all of the subissues. Thus it was necessary to prioritize the subissues and select only the key issues that are most important to criticality. This is one of the two major goals of this workshop. [The other major goal of the workshop is to develop plans for developing and testing models and/or abstractions to address the selected key subissues in the criticality evaluation.]

The plans presented in Section 4 address the top subissues (as well as some issues of less importance) identified in each of the three major categories in package, near field, and far field criticality.

There are several reasons that many of the subissues identified at the workshop will not be addressed in the abstraction/testing plans. The issues which were given a lower ranking by workshop participants were deemed to be of less significance to disposal criticality and to overall repository performance. As noted previously, time and resources are limited, so we must focus on those subissues ranked the highest by workshop participants. Other subissues were filtered out by the determination that the subissue will be addressed by the National Spent Nuclear Fuel program.

3.8 DEVELOPMENT OF PRELIMINARY ABSTRACTION/TESTING PLANS

The participants formed three new small groups to discuss the three major issues. These new groupings were independent of the four groups which had prioritized the issues earlier.

After developing the three small groups, the participants were asked to develop the abstraction and testing plans to address the major issues. A short presentation (J. McNeish) was given to provide the participants with the required components of the analysis plan. The components or information required were: 1) Title; 2) Objectives; 3) Hypothesis(es); 4) Inputs to criticality evaluation and TSPA, 5) Issues to be covered, 6) Model development plan including approach, source of data, code(s) to be utilized, and others, 7) Potential problems, 8) Model assumption(s) and uncertainty(ies), 9) Potential follow-up work, 10) Potential inputs/feedbacks to other WBS elements, and 11) What is covered in the existing worksopes? A copy of viewgraphs of the presentation is given in Attachment IX.

Additional presentations were made to assist the groups in developing their abstraction/testing plans. Input from other workshops important to criticality was presented (R. Barnard). A brief presentation

Each of the three groups discussed the basis for a plan to develop an abstraction dealing with their major topic. These plans were developed within the framework discussed above. Prior to departure from the workshop, each group developed a draft version of the analysis plan.

Table 3-1 List of participants in each group.

Group #	Participants*
1	Mike Wilson, Peter Gottlieb, George Barr, Cliff Ho, Joel Atkins, Henry Loo, Bob Rundberg
2	Rob Rechard, Chris Stockman, Darren Jolley, Wes Davis, Paul Sentieri, David Sevougian
3	Ralston Barnard, Dan McCright, Jack Gauthier, Rich Von Konynenberg, Eric Siegmann, Dick Beyers, John Massari
4	Jerry McNeish, Michael Brady, Dan Thomas, Larry Sanchez, Sarvajit Sareen, David Sassani

* Affiliation of the participants is given in Attachment III.

Table 3-2 Key Issues

In Package	<ul style="list-style-type: none"> 1.1 Failure model of waste package 1.3 Removal of absorbers from WP and/or basket (particularly boron) 1.14 Waste form characteristics
Near-field	<ul style="list-style-type: none"> 2.1 Seepage into Drift 2.2 Separation of fissile and neutron absorbing materials 2.3 WP corrosion products 2.4 Design of invert materials (filtering and sorbing properties)
Far-field	<ul style="list-style-type: none"> 3.1 Location of criticality event (UZ or SZ) 3.2 Dispersion/dilution/mixing during transport to criticality location 3.6 Organic concentrating environments (reducing zone) 3.12 Type of fissile material transported (consider enrichment, depleted uranium as necessary) 3.7 Other stratigraphic or chemical concentrating mechanisms (sorption, colloids, filtration, etc.) 3.3 Fracture focussing of radionuclides 3.14 Composition of plume

4. FINALIZED ABSTRACTION/TESTING PLANS

Detailed abstraction/testing plans for the three major topics are presented in this section. The plans were developed based on the plans outlined in the workshop.

4.1 ABSTRACTION OF IN PACKAGE CRITICALITY

Dan Thomas, Jerry McNeish, Henry Loo, Christine Stockman, Eric Siegmann, Paul Cloke, S. Sareen

4.1.1 Objectives.

- 1) Evaluate the factors important to initiate an in-package criticality and their likelihood
- 2) Evaluate the consequence of in-package criticality

4.1.2 Hypotheses

- 1) In-package criticality is highly improbable and has very low consequences.
- 2) We can screen in-package criticality scenarios to reduce the number of scenarios which must be included in TSPA-VA.

4.1.3 Products for TSPA-VA

- 1) Based on models of dripping water, boron and other neutron absorbers, fissile materials (uranium, plutonium), and Fe with time, determine criticality event initiation trigger external to TSPA model.
- 2) Develop response surface of consequences of in-pkg criticality (modified source term, modified solubilities, modified temperature) which is implementable in TSPA.

4.1.4 Issues Covered by Products

This activity covers the following key issues that were identified at the workshop (refer to Attachment starting on page 28).

Issue 1.1	Failure model of waste package
Issue 1.3	Removal of absorbers from WP and/or basket (particularly boron)
Issue 1.14	Waste form characteristics
Issue 1.4	Extent of degradation of waste form (physical, chemical, cladding)
Issue 1.8	Chemical composition and other properties (including materials)
Issue 1.2	Extent of degradation of basket materials

4.1.5 Abstraction Testing Plan

a) Approach

Phase I.

- 1) Evaluate the following waste forms:

- a) CSNF,
- b) co-disposal (aluminum fuel/DHLW).
Co-disposal evaluation may require simplification due to resource constraints.
- 2) Obtain aluminum fuel degradation information/models from H. Loo.
- 3) Obtain dripping model results from M. Wilson abstraction group.
- 4) Obtain waste package degradation results from WP group.
- 5) Obtain geochemistry of inflowing water from NF group.
- 6) Obtain absorber loss with time from WP group.
- 7) Obtain fissile material content with time from WF degradation group.
- 8) Obtain definition of criticality environment requirements from WP group.
- 9) Define most probable scenario(s) for in-package criticality

Phase II.

- 1) Based on modeling, determine whether or not criticality occurs
- 2) Determine consequence of criticality
 - modified inventory
 - modified solubilities
 - modified temperature
- 3) Create response surface of criticality consequences as $f(\text{time, location, dripping flux, absorber removal, water chemistry, iron oxide, chromium oxide, WP degradation configuration})$

b) Metrics

Screen scenarios for exclusion from TSPA-VA which produce less than a factor of 5 increase in the total peak dose.

c) Existing Workscopes

- 1) Fuel characteristics - WP Design
- 2) Dripping water model - TSPA abstraction group
- 3) Geochemistry of incoming water - TSPA abstraction group
- 4) WF degradation - TSPA abstraction group
- 5) Modeling of WP (outer/inner barrier, basket materials) materials degradation - WP Materials
- 6) Probabilistic determination of configuration(s) - WP Risk Analysis
- 7) Consequence model development and application - WP Risk Analysis

d) Information Sources

[(see c) above]

e) Programs to be utilized

Multiple codes used in the other parts of the system which are required to conduct these analyses including MCNP, SCALE, WAPDEG, AREST-CT, dripping water model, and EQ3/6.

f) Roles and Responsibilities

Dan Thomas (group leader) - Conduct MCNP analyses

Jerry McNeish (PA integration)-Integrate PA aspects of the evaluation with WP Group.

H. Loo/P. Cloke-scenario development
C. Stockman - expert reviewer

g) Schedule

Formulate scenarios
Develop approach.
Determine likelihood of scenarios
Determine consequences of criticality events.
Abstraction effort concluded: November 1, 1997

h) Model Assumptions and Uncertainties

- 1) Seepage rate into package will be developed by M. Wilson abstraction team.
- 2) WP degradation information will be developed by/ J. Lee/B. Bullard.
- 3) Spatial distribution of waste forms within repository
- 4) Scenarios:
 - a) Intact CSNF, barrier degradation leading to bathtub
 - b) Degraded CSNF in bathtub
 - c) Intact aluminum fuel in codisposal package in bathtub
 - d) degraded aluminum fuel in codisposal package in bathtub with partially degraded canister
 - e) degraded aluminum fuel/DHLW mixtures.

i) Potential Follow-up Work

Develop model which incorporates a more detailed representation of the key parameters affecting the in-package criticality.

j) Inputs/Feedbacks from other WBS elements

- 1) Site: current infiltration rates
- 2) WP: (see above)

k) Potential Problems

- 1) High level of uncertainty in many of the processes
- 2) Lack of resources
- 3) Lack of information on aluminum fuels.

4.2 SENSITIVITY STUDIES FOR NEAR-FIELD CRITICALITY PROCESSES

Ralston Barnard, Dave Sassani, Dick Beyer, Rob Rechard, Larry Sanchez, Wes Davis, David Sevougian, Rich VanKonynenburg

4.2.1 Objectives

- 1) Develop source term from near field criticality for use by far-field flow and transport.
- 2) Bound effects on near-field due to near-field criticality.

4.2.2 Hypotheses

There are several mechanisms for concentrating fissile material in the near-field materials that can potentially lead to criticality. These criticalities will produce changes in the radionuclide inventory that can be tracked to the accessible environment. The degree of change for each criticality mechanism can be evaluated.

4.2.3 Products

- 1) Incremental source term that provides isotopic abundances and spatial and temporal distributions of radionuclides.
- 2) Effects on near-field environment due to thermal and chemical changes from criticality.
- 3) Relative probabilities of occurrence for FEPs (as part of the overall FEP diagram for criticality scenarios).

4.2.4 Issues

Issue 2.1	Seepage into drift
Issue 2.9	Physical/chemical form of fissile materials (particulates, colloids, solutes)
Issue 2.2	Separation of fissile material and absorbers
Issue 2.4	Design of invert materials (filtering and sorption properties)
Issue 2.12	Waste-form characteristics

4.2.5 Abstraction/Test Plan

a) Approach

The mechanisms for concentrating fissile material have been incorporated into FEP diagrams to make scenarios (see attached). The parameters and important factors for each FEP are identified. Calculations are proposed that will test the sensitivity of the various parameters. These sensitivity calculations will be used to indicate which scenario causes the greatest change in radionuclide inventory and/or greatest change in near-field environment. The sensitivity studies will also be used to indicate which parameters can be used to characterize changes in the inventory due to that criticality.

Four potential critical configurations have been identified. They have in common that an effluent from a degraded waste package flows into the tuff and invert beneath the waste package. Depending on the mobilization mechanism for the fissile material (as a solute, colloid, or clay mixture), concentration is postulated to occur by precipitation, sorption, filtration, or mechanical deposition. The important FEPs for these scenarios include a transport mechanism for the waste, some process to separate neutron absorbers from the fissile material, and establishment of a potentially critical configuration by the presence of a neutron moderator and/or a suitable geometry. In order to model the processes leading up to a potentially critical configuration, models and parameters from other components of the TSPA analyses will be used. Thus, the Waste-Package Degradation and Waste-Form Degradation and Mobilization activities will provide information on the time of release of effluents from the waste package, composition of the effluent, rate and amount, location of release, etc. Transport will use information from Waste-Form Mobilization, Near-Field Environment, and Thermohydrology to model

diffusion/advection in the tuff and invert, mixing of other groundwater with the effluent, fracture/matrix flow, water saturation and matrix water capacity.

Criticality calculations consist of evaluating K_{eff} for configurations as a function of numerous variables (such as fissile-material density, matrix composition, water saturation, volume, etc.) using neutronics codes such as RKEFF and MCNP. Values of K_{eff} greater than 0.95 are interpreted as meaning that the configuration is self-sustaining critical. Based on the conditions postulated for generating the critical configuration, the power output and termination can also be calculated. Using these factors, the radionuclide inventory from the criticality can be calculated using a code such as ORIGEN. The inventory from the criticality can be combined with the "nominal" radionuclide inventory in TSPA calculations to determine the impact of the criticality on overall TSPA measures (such as dose at the accessible environment). The criticality calculations require that parameter-value distributions be provided for all the variables of the models (examples listed above). These will be provided by the other TSPA components (listed above).

Estimates of the relative probabilities of occurrence for the FEPs in each scenario are important for completely addressing the criticality problem. It is expected that the NRC will not be satisfied unless we can show that even if there is no TSPA consequence from a criticality we can also provide some estimate of the probability that the criticality event will occur.

b) Metrics

Rationale for excluding or analyses for including FEPS. A scenario diagram complete enough to provide relative probabilities.

c) Existing workscopes

Scenarios development covered in 1.2.5.4.1. Interface between Waste-Package design and PA covered in 1.2.2.2.

d) Information sources

Prior work by 1.2.2 (WP development)

e) Programs

MCNP, RKEFF, NARK, SCALE43, EQ3/6, AREST-CT, ORIGEN-S

f) Roles & Responsibilities

PA will produce a complete scenarios diagram, including both FEPs that describe how a criticality can occur and FEPs for mitigating situations. PA will provide inputs from other workshop activities (e.g., WFD&M, WPD, NFE, T/H).

WP design will perform the criticality calculations, using the parameter variations developed at the workshop.

- g) Schedule**
Abstraction Effort concluded: November 1, 1997
- h) Model Assumptions and Uncertainties**
 - 1) Processes to Separate fissile material and absorbers.
 - 2) Reconcentration mechanisms for fissile materials (chemical, physical)
- i) Potential Follow-up Work**
None identified at this time.
- j) Inputs/Feedback from other WBS elements**
WP: see (f).
- k) Potential Problems**
Lack of resources to complete the analyses, due to constraints on WP personnel.

4.3 SENSITIVITY ANALYSIS OF FAR-FIELD CRITICALITY

Mike Wilson, Cliff Ho, Jack Gauthier, Joel Atkins, George Barr, Peter Gottlieb, Darren Jolley, Bob Rundberg

4.3.1 Objectives

Construction of scenarios (from locations and mechanisms); initial screening for possibility and consequences.

4.3.2 Hypothesis

Many of the possible scenarios for external criticality can be screened out on the basis of available geochemical information and fundamental physical and chemical calculations.

4.3.3 Products for TSPA-VA

Screened scenarios for far field criticality.

4.3.4 Issues

Issue 3.1 Location of criticality event (UZ or SZ)

Issue 3.2 Dispersion/dilution/mixing during transport to criticality location

Issue 3.3 Fracture focussing of radionuclides

Issue 3.6 Organic concentrating environments (reduction or oxidation state)

Issue 3.7 Other stratigraphic or chemical concentrating mechanisms (sorption, colloids, filtration, etc)

Issue 3.12 Type of fissile material transported (consider enrichment, depleted uranium as necessary)

4.3.5 Abstraction Testing Plan

a) Approach (Activities, many of which may be performed in parallel):

- Determine fissile carrying capacity of the flow out of the repository (solutes and colloids)

- As a preliminary screening, evaluate characteristics of 11 representative far-field locations, including geochemistry and maximum U concentrating capability. The principal purpose is to identify locations which can be eliminated from further, detailed evaluation.
 - Near drift fractures which collect colloids.
 - Dead-end fractures near the drift, particularly at the bottom of the excavation stress-relief zone, which can trap solutes and colloids remaining uncollected by the nearer fracture walls.
 - First zone of pH change encountered in the rock, where the pH drops from high to neutral.
 - Zeolites (upper portion of layers)
 - Altered vitrophere (lower portion of layer immediately above): Dead-end fractures, Topographic "bowls"
 - Paleo-soils as a possible organic source.
 - Upwelling of hydrothermal fluids (in the SZ, presently identified by water temperature maxima at the water table along portions of the main faults, which are believed to provide a fast path for this upwelling).
 - "Pinch-out" zone: transition from tuff aquifer to alluvial aquifer (likely to contain organic reducing zones)
 - Possible focusing mechanism from selective hydrothermal precipitation (from WP heating of water) - UZ
 - Possible focusing mechanism from selective hydrothermal precipitation (from WP heating of water) - SZ
 - Outfalls (Franklin Lake Playa, springs): Organics (possible reducing zones), Evaporation
- Evaluate transport/retardation mechanisms appropriate to each location, including how much fissile remains in the flow when the location is reached. Specific attention will be given to the potential time periods for the transport and re-concentration.
 - Colloids & filtration
 - Solutes and their sorption
 - Carrier plume (extent of confinement of contaminant plume)
 - Precipitation
 - Dispersion/diffusion (molecular, hydromechanical mixing)
 - Mixing of plumes from several waste packages: Dilution of U concentration, Dilution of U enrichment (from interspersing HEU and LEU packages).
- Criticality calculations (MCNP), for configurations which are possible from the above analyses, using representative enrichments, including consideration of mixing of outflow from HEU and LEU packages, as appropriate.
- Consequence calculations for configurations determined to be critical from the above calculations (increased radionuclide inventory).

b) Metrics/Acceptance criteria

Suitability for inclusion in TSPA-VA as explanation of alternatives screened out.

c) Existing workscopes

1.2.2 activities:

- (1) Criticality calculations
- (2) Chemistry of the fissile bearing solution

- d) Information sources**
 - 1) Reports on geology and geochemistry of the repository, Yucca Mountain, and nearby outfalls of the saturated zone
 - 2) Reports on natural analogs
 - 3) Reports on naturally occurring uranium orebodies
 - 4) Other abstraction teams: UZ flow, UZ transport, UZ thermal-hydrology, SZ flow
 - 5) Source term produced by PA-WPD (reflecting the variety of waste forms to be covered by TSPA-VA)
 - 6) PA colloid evaluation team already supporting several other abstraction teams.

- e) Programs**

MCNP for criticality, EQ3/6 for chemistry, FEHM for transport

- f) Roles and responsibilities**

Co-leaders D. Jolley (PA), P. Gottlieb (WPD); assignments: G.Barr (saturated zone transport), J.Massari (MCNP), C.Ho (unsaturated zone transport), R.Rundberg (fluid carrying capacity, together with P.Cloke EQ3/6 calculations), D.Jolley (geology), P.Gottlieb (modeling), J.Gauthier & M.Wilson (coordination with other abstraction teams).

- g) Schedule**

Brief letter report with scenarios specified, all information sources identified (6/97); Final report (8/97).

- h) Assumptions and Uncertainties**

Pu decayed to U

- i) Potential Follow-up work**
 - 1) Sensitivity to mitigating measures (e.g. depleted uranium, sorbers in the invert)
 - 2) Calculations of flow from criticality location to the accessible environment
 - 3) Immobilized plutonium waste form

- j) Inputs**

From other WBS elements: Scientific Investigations (formerly Site Characterization)

- k) Potential Problems**
 - 1) Resource limitations,
 - 2) Unavailability of information/data,
 - 3) Timely input from other abstraction teams.

5. REFERENCES (reduce to only those listed in report)

M&O (Civilian Radioactive Waste Management System, Management and Operating Contractor [CRWMS M&O]), 1996. Total System Performance Assessment - Viability Assessment (TSPA-VA) Plan, B00000000-01717-2200-00179, Las Vegas, NV.

M&O 1996b - Disposal Crit Method Report

ATTACHMENT I

Workshop Invitation Letter Package and Strawman Proposals



TRW Environmental
Safety Systems Inc.

1180 Town Center Drive
Las Vegas, NV 89134
702.295.5400

WBS 1.2.5.4.1
QA: N/A

Contract #: DE-AC01-91RW00134
LV.PA.RWB/JAM.01/97-007

February 20, 1997

To: Distribution

From: Ralston Barnard - M&O/SNL, Albuquerque, New Mexico
Jerry McNeish - M&O, Las Vegas, Nevada
Peter Gottlieb - M&O/F-C, Las Vegas, Nevada

Subject: Invitation to the TSPA-VA Disposal Criticality Abstraction/Testing
Workshop

We would like to invite you to a three-day Disposal Criticality Abstraction/Testing Workshop to be held at the **CRWMS Summerlin M&O Facility (Bldg. 11, Room 1111) in Las Vegas, Nevada on March 18-20**. More detailed information on the workshop location and schedule will be sent to the participants and observers at a later date. The workshop is the seventh of a series conducted by the Performance Assessment (PA) group on abstractions and testing of important aspects of the Total System Performance Assessment-Viability Assessment (TSPA-VA).

The workshop is intended to be a working meeting. Therefore, the number of participants is limited to keep the meeting as productive as possible. In addition to the participants, a small number of observers are also invited. Their role is to observe, not to participate in the presentations, discussions and planning that will take place during the workshop. In contrast, all participants will have to do preparation work prior to the workshop. Many will be asked to give short presentations during the workshop, and small working groups will be writing proposals during the workshop for abstraction/testing activities. This letter defines the goals and describes the process of the Criticality workshop.

Introduction

This workshop is the seventh in a series of ten which have the ultimate goal of helping to develop a valid, defensible TSPA-VA using the most complete and

current information available. In order to achieve these goals, we need to incorporate reasonable models that reproduce the essential behavior of key processes important to long-term performance in a computationally efficient manner. In addition, we need to describe alternative conceptualizations and parameter sets that reflect the variability and uncertainty of the system. The TSPA-VA schedule calls for completion of all calculations and documentation by June 1998. During the 1997 fiscal year it is therefore necessary to completely define how TSPA calculations will be made, what input parameters will be used, and the uncertainty associated with these input parameters. The Criticality workshop is intended to bring together geologic-process modelers, neutronics modelers, subsystem modelers, and TSPA modelers in order to address issues seen as important for TSPA-VA. The primary goal of the workshop is to provide technical guidance to Performance Assessment for developing criticality initiation and consequences models, and associated parameter distributions that are to be used in TSPA-VA. A list of activities and products for both the workshop and post-workshop is presented in Attachment A.

All participants in the workshop must stay focused on the goals of the workshop. Another important point is that we are deciding how to handle issues for TSPA-VA calculations. We are not necessarily trying to resolve the issues at the workshop.

To assist those who are not used to thinking with a TSPA perspective, an introduction to TSPA focused on criticality is attached (Attachment B). It is very important for all the workshop participants to read this Attachment B carefully and keep what is said in mind while preparing for the workshop.

Overall Workshop Structure

This workshop is part of a series of workshops for TSPA-VA that address different "parts" of the TSPA model. These parts have been selected, partly along boundaries in the calculation that make the pieces relatively independent, but also to reduce the complexity of any one part so that it could be effectively treated in a workshop format. The subject of this workshop, is linked to the subjects of other workshops. Criticality is expected to be coupled with certain aspects of waste package degradation, waste-form degradation and mobilization, near-field alteration processes, UZ and SZ flow and transport, and biosphere models. The coupling to processes treated in other workshop areas will be part of the workshop discussions.

Abstractions

The physical size, complexity, and time domain of the complete radioactive waste disposal system to be evaluated for TSPA is too computationally demanding to be performed with a set of fully integrated, fundamental, process-level models. Furthermore, the uncertainty in system characteristics, both at present and in the future, lead to the requirement for multiple probabilistic TSPA calculations in order to explore the potential range of system performance. The need for multiple calculations places an even greater emphasis on computational efficiency for TSPA. Therefore, approximations (also called abstractions) to the more commonly used models and parameters for processes that affect system performance are needed for TSPA. A more detailed discussion to help clarify the meaning and use of abstractions is given in Attachment C.

Description of the Disposal Criticality Workshop

The Criticality workshop will concentrate on the abstracting and testing of issues pertinent to the initiation of and the ultimate consequences of nuclear criticality events potentially occurring at three general locations at Yucca Mountain that have a significant influence on long-term performance. Criticality events have been postulated to potentially occur in the waste package (called In-Package criticality), in the rock or engineered materials (e.g., concrete) immediately surrounding the waste package (Near-Field criticality), or in the rock of the unsaturated or saturated zones of Yucca Mountain (Far-Field criticality). In preparation for this workshop, TSPA and subsystem modelers have assembled a list of issues that need to be addressed in order to conduct appropriate abstractions for the Criticality portion of TSPA-VA calculations (Attachment D). This list was developed in collaboration with waste-package design and criticality-analysis personnel in an attempt to provide a complete list for the participants. The goal of the workshop will be to address all of the issues listed in Attachment D. Areas that are not easily resolved, or for which there is some disagreement between participants (herein referred to as problem areas) will be noted and methods of resolving these problem areas proposed and assessed. A brief discussion of the coupling of criticality with other processes such as waste package degradation and waste-transport processes is presented in Attachment E.

Prior to Workshop

In order to make the workshop successful, much work has gone into the planning and it is asked that the participants also conduct some work prior to the workshop. Attachment F contains complete instructions for the workshop participants. As a mechanism to begin the discussion, and to start participants thinking about the issues involved in TSPA modeling of nuclear criticality in Yucca Mountain, we present, in Attachment G, a series of "strawman" proposals for improving TSPA calculations in the criticality area. The proposals represent current ideas in the TSPA and waste package design group for implementing Criticality evaluations into the TSPA model. Examination of the proposals shows that there are many issues that need to be resolved at the workshop or during the remainder of the fiscal year. Strategies to define the appropriate modeling methods for TSPA-VA during this fiscal year need to be resolved at the workshop. Workshop participants are asked to review the strawman proposals and provide written comments as appropriate. At a minimum, panel members should send in responses on their panel issues. A short written summary on what each person can contribute to answering the questions is requested in advance of the workshop (see Attachment F for instructions). These summaries will be compiled and distributed to all of the participants. If a proposal is not controversial then it will be assumed to be acceptable for TSPA calculations. The pre-workshop preparation will allow the participants at the workshop to concentrate on the more complicated issues and arrive at plans on how to resolve them. It should be noted that if participants do not comment on a proposal it is assumed that they either agree with the method or do not believe they have the background to comment. Also, as pre-workshop work, many participants will be asked to prepare short presentations, described below.

A draft agenda for the workshop is presented in Attachment H. This agenda may change based on the results of the comments we receive on the issues list and strawman proposals. For example, if general agreement is found on a particular issue, less time will be devoted to that issue. At the workshop, panels will be convened to discuss each question listed in Attachment D. The panel format will consist of presentations by panel members followed by discussion by the whole group. Panel members (Attachment I) will consist of people with neutronics modeling, process-level modeling, subsystem modeling, and TSPA modeling experience who are best suited to discuss the questions. At the end of the panel presentations and whole-group discussions, additional problem areas that need to be further discussed during the

workshop will be identified. In addition to identifying the problem areas, another outcome of the workshop will be a proposal (or proposals) on how to address these problem areas in analyses after the workshop.

Note that the agenda is still subject to change, thus the exact time the panel discussions will end has not been determined. The goal of the small-group discussions will be to develop and document a suite of proposals on how to address the problem areas. The benefits and drawbacks for each proposal will also be documented. As it might not be possible to address all proposals during the fiscal year, the problem areas will need to be ranked in the order of importance of resolving before the TSPA-VA calculations begin.

Schedule of Workshop:

Tuesday, March 18, 1997	Day 1 of Workshop (all day)	8:00 a.m.
Wednesday, March 19, 1997	Day 2 of Workshop (all day)	8:00 a.m.
Thursday, March 20, 1997	Day 3 of Workshop	8:00 a.m. - 2:00 p.m.
Thursday, March 20, 1997	Core Team Wrap-up Meeting	2:00 - 5:00 p.m.

List of Participants:

PA Management:

Robert Andrews - M&O/INTERA, Las Vegas, Nevada, M/S 423
Holly Dockery - M&O/SNL, Albuquerque, New Mexico

Abstraction Core Team:

R. W. Barnard - M&O/SNL, Albuquerque, New Mexico
M. C. Brady - M&O/SNL, Albuquerque, New Mexico
Peter Gottlieb - M&O/F-C, Las Vegas, Nevada, M/S 423
Jerry McNeish - M&O/INTERA, Las Vegas, Nevada, M/S 423

Other Participants:

George Barr - M&O/SNL, Albuquerque, New Mexico
Dwayne Chesnut - M&O/LLNL, Livermore, California
Wes Davis - M&O/F-C, Las Vegas, Nevada, M/S 423
Carl Detrick - Bettis Atomic Power Lab, P.O. Box 79, West Mifflin, PA
Jack Gauthier - M&O/SNL, Albuquerque, New Mexico
Bill Glassley - M&O/LLNL, Livermore, California

Cliff Ho - M&O/SNL, Albuquerque, New Mexico
Darren Jolley - M&O/INTERA, Las Vegas, Nevada, M/S 423
Joon Lee - M&O/INTERA, Las Vegas, Nevada, M/S 423
Henry Loo - INEL, Idaho Falls, Idaho
John Massari - M&O, Las Vegas, Nevada, M/S 423
Rob Rechard - M&O/SNL, Albuquerque, New Mexico
Laurence Sanchez - M&O/SNL, Albuquerque, New Mexico
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Paul Sentieri - INEL, Idaho Falls, Idaho
Dave Sevougian - M&O/INTERA, Las Vegas, Nevada, M/S 423
Eric Siegmann - M&O/INTERA, Las Vegas, Nevada, M/S 423
Christine Stockman - M&O/SNL, Albuquerque, New Mexico
Dan Thomas - M&O, Las Vegas, Nevada, M/S 423
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List of Attachments:

Attachment A: Workshop Goals
Attachment B: Introduction to TSPA
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Attachment D: Important Issues
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Attachment I: Panel Members for Criticality Issues
Attachment J: References

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ATTACHMENT A WORKSHOP GOALS

The primary goals of the workshop are:

- 1) **Identification of Issues:** Identify and group the important issues (e.g., processes and parameters) of the criticality abstraction/testing topics with respect to long-term performance. Long-term performance can be measured as the consequences of:

Changes in Releases/Doses at Accessible Environment:

due to modification of Source Term used in TSPA (i.e., the radionuclide inventory)

due to modification of Near-Field Environment (e.g., thermal, chemical alterations)

due to generation of Far-Field Source Terms (i.e., inventory, transport processes at locations nearer the accessible environment)

The three main issues are identifying credible criticality FEPs and scenarios for:

In-package events

Near-Field events

Far-Field events

The suggesting grouping of issues is as follows based on the relative priority: high, medium, low, and "to be determined."

- 2) **Prioritization of Issues:** Prioritize the issues as to which are most important to be evaluated as a post-workshop activity. For criticality, a prioritization of consequences should consider the following (to be rated as high, medium, low or to-be-determined) measures:

Degree of impact on Waste-Package/Waste-Form Degradation & Mobilization

Degree of impact on Near-Field Environment

Degree of impact on UZ and SZ radionuclide transport

Degree of impact on Biosphere model

Develop alternative methods for evaluating "to be determined" issues and document strengths and weaknesses of each alternative.

- 3) **Treatment of Uncertainty:** Decide upon a method for addressing and quantifying uncertainty in alternative process models and parameters used for criticality analyses. (The eventual outcome of this method during post-workshop activities should be probabilities and/or probability distributions.)

- 4) **Plan for Abstraction/Testing:** Create a plan for developing and testing appropriate model abstractions of the most important processes. The plan should resolve (or outline a procedure to resolve) the following important issues:
 - a) Which type of abstraction is most appropriate: response surface, lower-resolution/ dimensional process model, analytical model/algorithm, etc.(or a combination of these)?
 - i) The abstraction must be sufficiently accurate.
 - ii) The abstraction must be capable of interfacing with TSPA software in a computationally efficient manner; i.e., we must be able to use it in a multi-realization probabilistic mode.
 - b) How should neutronic variability be represented in the abstraction?
 - i) How is heterogeneity affected or represented if dimensionality is reduced?
 - ii) What degree of spatial/temporal discretization is acceptable in the abstracted model?

- 5) **Coupling of Disposal Criticality Workshop with Other Workshops:** Discuss and, if possible, define how the above abstractions will interface with other abstraction/testing topics in a consistent fashion: with respect to time, space, processes, and parameters.

- 6) **Post Workshop Activity Scheduling:** Discuss how available resources and scheduling will affect post-workshop activities:
 - a) How much time/personnel/funds is required and available to conduct post-workshop abstraction/testing activities?
 - b) How do abstraction/testing activities fit into both overall PA schedule and overall Site schedule?
 - c) Can some activities be performed that will satisfy currently planned deliverables?
 - d) Develop a tentative schedule for completion and delivery of post-workshop products.

Specific Outcomes and Products of Post-Workshop Abstraction/Testing Activities

- 1) **Workshop Report:** Write workshop deliverable, which reports upon the activities and decisions of the workshop and the plans for post-workshop abstraction/testing activities that feed TSPA-VA.
- 2) **Abstraction/Testing Activities:** Develop and test abstraction methods proposed by the workshop. Compare abstracted models to more detailed models (if available) to determine accuracy (acceptability) of abstractions. Errors in abstractions should be on the conservative side.
 - a) Determine how to incorporate spatial and temporal variability.
 - b) Test the interface with TSPA software and see if it is feasible to use the given abstraction in multi-realization fashion.
 - c) Examine predictions of the abstraction compared to the process model. Does the abstraction represent uncertainty appropriately?
 - d) Determine if the abstraction can be coupled with other abstractions such that coupled processes and synergistic effects are still accurately captured by the abstraction(s).
- 3) **TSPA-VA Report Sections:** Write a section for the TSPA-VA report detailing the models and abstractions to be used for TSPA-VA. All decisions should be documented, along with the sensitivity analyses and abstraction-testing that were performed. The workshop deliverable should serve as a starting point.

ATTACHMENT B. INTRODUCTION TO TOTAL SYSTEM PERFORMANCE ASSESSMENT

Purpose. The purpose of total-system performance assessment (TSPA) is to calculate various measures of repository safety, such as a peak individual radiation dose, and to estimate the uncertainty in the calculations. Essentially, we want to estimate the radiation dose and put error bars around the estimate, just as any experimental result should always be accompanied by an error estimate. (There are other "performance measures" of interest as well, but for the rest of this discussion we'll just speak of peak doses.)

Uncertainty. The uncertainty estimate complicates the problem and increases the difficulty of the task considerably. Suppose for the sake of discussion that we need to consider four design cases (e.g., with and without backfill, high and low thermal load). If we were confident enough of our models and their input parameters, we would just need to make four deterministic model calculations, and it might be feasible to use models so complicated that they take several weeks to run.

However, because of the uncertainty in models and input parameters, we must conduct a probabilistic assessment with multiple runs for each design case in order to look at the probability distribution of peak doses. Uncertainty in peak dose is usually expressed as a complementary cumulative distribution function (CCDF). Such a distribution is equivalent to the more familiar probability density function, but it shows more explicitly what we really want to know: the probability of calculated doses being exceeding some regulatory limit.

The importance of examining system performance probabilistically is illustrated by the fact that the mean dose is often dominated by low-probability occurrences--that is, by "realizations" with one or more input parameters from the tails of their probability distributions. (Incidentally, the measure of risk that the National Academy of Sciences recommended using [National Research Council, 1995] is calculated from the mean of the peak-dose distribution.)

Computational Requirements. Because the effects of criticality will be modeled in TSPA-VA as alterations to the source term (for in-package events), or as alterations to near-field radionuclide transport models (in near-field events). They can be considered additional cases to be modeled as part of the baseline TSPA-VA. Far-field criticality requires the development of additional source-term models.

Previous TSPA's. Past performance assessments (TSPA-1995: M&O, 1995a; TSPA-1993: Andrews et al., 1994, and Wilson et al., 1994) have not included the effects of criticality. For in-package and near-field criticalities, the waste package, waste form, and near-field environment control criticality. The prior TSPA analyses have found calculated peak doses to be sensitive to (1) the distribution of waste package failure (i.e., the meantime of the waste package failure and "spread" of the failure over time), and (2) the rate of degradation of the waste package, (3) the conceptual model for advective release from the waste packages, and (4) the rate of dissolution of the waste form. All four of these factors may be altered by in-package or near-field criticality events. How many realizations are necessary to properly account for the uncertainties in the system? One must ensure that all conceptual models are given appropriate weight, and that the

distributions for parameter values are sampled often enough to obtain coverage of the complete distribution. Various sampling strategies are available including the Latin Hypercube sampling method, and the number of samples actually needed to resolve the behavior depends on how nonlinear the response is. However, it is expected we will need to run hundreds (at least) of model realizations in order to determine the plausible range of calculated peak dose. (As an aside, we used to expect to have to run thousands of model realizations because the remanded EPA standard, 40 CFR 191, placed restrictions on the calculated releases at the 0.1% probability level.)

Because the applicable regulatory standards are not yet in place, it is not entirely clear what time period should be simulated for those hundreds of realizations for TSPA-VA. We expect that the majority will probably be for 10,000 years, but that some of the calculations will cover a million-year period.

TSPA-VA Requirements. Our needs for TSPA-VA can be summarized as follows:

- 1) We must be able to run thousands of model calculations of the entire disposal system, including waste container corrosion, waste-form degradation and radionuclide release, unsaturated-zone flow and radionuclide transport, saturated-zone flow and transport, and biosphere transport and dose to individuals.
- 2) The calculations must cover at least 10,000 years, and some of them will cover 1,000,000 years.
- 3) The in-package and near-field criticality calculations should include an appropriate representation of:
 - a) evolution of in-drift waste-package degradation conditions such as temperature, relative humidity, and chemistry of water contacting the containers,
 - b) effects of water, basket degradation, and waste form degradation on neutronics processes,
 - c) proper representation of the uncertainty in the conceptual and process models and the variability in the processes and in-drift exposure conditions.
- 4) The far-field criticality calculations should include an appropriate representation of reconcentration processes, potential critical geometries in rock, and rock/water moderators.
- 5) The model(s) we use for TSPA-VA will have to be defensible in terms of how well they fit the available experimental and field data.

Please keep the above criteria in mind when considering which models are appropriate for use in TSPA. The simplest choice would be a time-dependent model of incremental radionuclide inventory at a specific location that can be used to modify the detailed TSPA nominal-case

spatial and temporal source term. Such a model may not capture all the important criticality factors. Given this constraint, we must decide on the best approach for "abstraction," which is to say an appropriate set of approximations or simplifications that will allow the calculations to be completed within the time available and at the same time represent the essential behavior of the system. Abstraction is discussed further in Attachment C.

ATTACHMENT C. DISCUSSION OF ABSTRACTION

Definition of Abstraction. As a first step, let us try to remove the "abstractness" from the terms "abstraction" and "abstraction/testing," as used by Performance Assessment. The term abstraction is often used to mean a "simplified model" or the procedure for developing such a simplified model. Perhaps a clearer definition of abstraction is "model." All physical-chemical models are an abstraction of the one reality to a greater or lesser degree. At the simplest level, the "abstraction/testing" procedure would consider two models of a given physical-chemical process, a complex model and a simple model (there may actually be a spectrum of models going from the most complex, and presumably most accurate, to the most simple), and compare the system response predicted by the two models. If the simple model response reasonably bounds (i.e., predicted peak concentration is equal to or higher than) the complex model over the range of uncertainty of the model parameters and boundary/initial conditions, then the simple TSPA model can be said to be validated viz-a-viz the presumably "calibrated" complex model.

Calibration of Models and the Use of Reasonably Conservative Models. All models need to be calibrated and validated against experimental data. In many cases, the most simplified (or most abstracted) TSPA model might just as well be calibrated against the available data as the most complex (or process-level) 3-D model. However, often as a matter of preference the simple model is calibrated against the complex model rather than against the data itself. (For some very simple models, such as the RIP TSPA model, certain state variables are not explicitly used in the simple model, so the simple model cannot really be calibrated, but must be used in a bounding sense.)

Even the most complex process-level models of Yucca Mountain cannot really be validated, due to the lack of data. Thus, a reasonably conservative simple model seems a valid approach. However, there may be multiple "alternative conceptual models" of the processes that may require analyses to incorporate the uncertainty in the process.

Definition of "Alternative Conceptual Models." This brings us to a clarification of the often used phrase "alternative conceptual model." As used in the previous paragraph, this just refers to a form of uncertainty and/or simplification in the modeling of the system or process behavior. In fact, if there is a single agreed-upon TSPA model that can describe processes (such as formation of a critical configuration), including uncertainty in model parameters and/or boundary/initial conditions, then there is no need for a so-called alternative conceptual model.

The phrase "alternative conceptual model" often seems to imply that two or more "alternative" models are equally good representations of the underlying reality. However, this is rarely the case, because as mentioned in the opening paragraph, all models are abstractions or simplifications of varying degree of the underlying physical-chemical processes. One of the primary reasons for using simplified models are the limitations on computational resources and efficiency when running calculations in a multiple realization format. This in turn brings us to

the question of how to ascertain whether a TSPA model provides "an adequate representation" of the system response over a wide range of uncertainty in boundary/initial conditions and phenomenological coefficients. In this context, one important workshop task is to identify how to validate the simple models against the complex model. Criteria for validation must include metrics for how "well" the various processes are captured or addressed in the simpler model. (See below.)

Model Validation/Calibration as a Function of Process Simplification. It is important to classify issues as to how they relate to both model abstraction and total system performance. Broadly speaking there is really only one issue: model validation. For the purposes of attacking this issue from a performance-assessment (and also "abstraction") perspective, it is convenient to discuss it in two parts: (1) how model validation is a function of (or is affected by) process simplification and (2) how model validation is a function of uncertainty. With regard to the former, the important point is to quantify how accurately the key physical-chemical processes and boundary/initial conditions are represented in the various models. To this end, a large part of the workshop discussions will revolve around the components of the various models themselves (rather than around "issues"): processes included in the models, boundary and initial conditions, coupling to other models, methods for calibration/validation of the models and sub-models (both "process-level" and simplified TSPA models).

Presentations should discuss how both the most complex and simple models include or account for the various processes and boundary/initial conditions. This requires a definite proposal for a simple TSPA model. Furthermore, there should be a presentation/discussion of processes and boundary/initial conditions not adequately addressed in the complex and simple models, and a ranking of if/how/which processes need to be included in complex and TSPA models. This should be done in light of the effect of these things on system performance (and also keeping in mind the limitations on computer resources). First, the absent processes need to be addressed in the process models. Then the absent processes need to be addressed in the TSPA models. For TSPA models, some processes may have been intentionally left out, or represented by a simpler model. The effect of this omission or simplification of an important process needs to be quantified. If the workshop decides that some of these omitted processes need to be included, or simplified processes need to be represented more thoroughly, then a discussion of time/personnel/resources is required to decide the feasibility of this for TSPA-VA.

Model Validation/Calibration as a Function of Uncertainty. Regarding uncertainty, which is caused by lack of data for parameters (phenomenological coefficients) and boundary/initial conditions, and lack of knowledge of the appropriate mathematical representation of the process(es), the workshop must address the major sources of this model uncertainty and how to include the uncertainty in both the complex model and the simple model. Parameter uncertainty seems somewhat more quantifiable than so-called conceptual-model uncertainty, which is really uncertainty regarding the level of detail needed to represent certain processes, such as fracture/matrix interaction, for the purposes of predicting peak dose to humans. Specifically, one must address how parameter uncertainty translates to process uncertainty,

i.e., how input uncertainty translates to uncertainty in the system response, which is a function of the particular process model.

The uncertainty in some model parameters, such as matrix permeability, seems straightforward to quantify, based on the sample space of the lab-measured data for the given parameter(s). On the other hand, the uncertainty in other model parameters is very difficult or impossible to quantify, since these model parameters represent abstractions of reality that are not directly measurable by experiments (or, also that there are too many parameters in the model to assign unique values to the various parameters).

Inherent in validating a simple TSPA model against a complex process-level model is to validate it over the entire uncertain range of the parameters and boundary/initial conditions, or equivalently, over the entire range of likely system response. This would seem to require as many runs of the complex model as the simple model for the purposes of calibration. Since the simple model is the one to be used as the final predictive tool for future doses, it would eventually be run many more times.

Deciding upon the necessary number of runs is a post-workshop activity, and proposing criteria for making this decision is a useful outcome of the workshop itself. As with any physical model of reality, we can only validate the model at a few values of the parameters with a few experiments, and then use the model to predict the system response at other values of the parameters. Ideally, this should be done in an interpolation sense, rather than an extrapolation sense, but that may not always be possible. As mentioned previously, in the case of simple TSPA models, the model validation will generally consist of comparison to the more complex "process-level" models, rather than comparison to the experimental data themselves. In this validation process, it is clear that the simple model response will not be the same as the complex model response. Theoretically, the complex model response should be more accurate, but given the lack of data, that is not necessarily so. In any case, since we believe the more complex models to be more accurate (or at least that they have a higher degree of spatial-temporal resolution), we want the simple model responses to "bound" the more complex model responses, i.e., to always give equal or higher values for the doses. We need to build confidence that significant dose peaks are captured adequately by the simple models.

To summarize, the workshop participants should identify those values of the model parameters at which to compare/validate the simple models against the "calibrated" complex models. In conjunction with this, the workshop should identify/quantify uncertainty ranges for the parameters and boundary/initial conditions of the complex and simple models.

Discussion of Response Surfaces

It may be decided during post-workshop analyses that the proposed simple models are inadequate. Perhaps they have so few measurable parameters, or the dimensionality and discretization have been reduced so much, that they cannot adequately predict system response over the supposed uncertainty range. Or perhaps, they do not allow a high enough degree of coupling to other workshop models, such as thermohydrologic models. In this case, the only

possible abstraction or simplification alternative may be to develop response surfaces based on the complex model. Here we mean that the complex model is run relatively few times to develop a curve fit of the nonlinear system response as a function of time, space, and the key model input parameters. Then, the system response for other values of the input parameters is interpolated from the response function. (Ideally, extrapolation would never be attempted.) This method is in contrast to running the simple model at any and all values of the input parameters.

Variability. Another, possibly separate issue is spatial-temporal variability, which is related to (1) the probabilistic versus deterministic nature of the physical-chemical processes themselves; (2) simplification of the spatial-temporal domain due to lack of knowledge (uncertainty) about the boundary/initial conditions; (3) simplification of the spatial-temporal domain due to constraints on computational resources. When validating the various models, the necessary or desired degree of variability must always be considered in the calibration process.

Relation of Criticality Models to Other PA Models. Models for criticality in spent nuclear fuel include the fissile material, the geometry, and the moderator as components. Calibration of the fissile-material model relies on well-constrained extrapolations from nuclear-reactor core data and neutronics models. Generation of critical configurations (i.e., the geometry and moderator characteristics) by geologic processes relies heavily on the existing PA models. For example, for in-package criticalities the waste-package degradation and waste-form mobilization models provide the basis for supplying the moderator and for removal of the neutron absorbers. In general, criticality models can be layered on top of the existing PA models. A PA model (or models) result in physical and neutronic configurations that can be evaluated for their potential for criticality.

Process models for criticality can be addressed by coupling with the other models being developed for TSPA-VA, and by ensuring that the outputs of those models and the constraints on them permit criticalities to be calculated. These couplings are given in Attachment E.

Uncertainties in Process Models. In addition to the uncertainties associated with the standard PA models, the neutronics calculations introduce additional variability and uncertainty. For example, the amount of silicon in the rock or the water moderator influences the neutron scattering, and thus the value of neutron multiplication factor.

Abstraction of the Criticality Models. To abstract the criticality models, this workshop must identify the important aspects of the supporting process models that affect the criticality process and supplement them with the specifics of criticality. The uncertainties unique to criticality calculations must also be incorporated. Both of these are outlined in Attachment D.

Summary. All of the above abstraction options have potential drawbacks. It might take too many model runs to develop an acceptable response surface (the discussion in Attachment B about the number of runs needed to determine the uncertainty caused by the key parameters applies as well to development of a response surface). And the danger of developing simple

models to explore particular effects is that other important effects may be left out, such as coupling to other physical-chemical processes. Additional discussion of abstraction issues may be found in Chapter 3 of the TSPA-VA Plan (M&O, 1996).

In both the development and the testing of abstractions for TSPA-VA, performance assessment needs the support of site-characterization personnel and process modelers so that we can optimize their models in a realistic fashion for TSPA calculations.

ATTACHMENT D. IMPORTANT ISSUES

Several issues are important for criticality as it affects repository performance. The key issues to be discussed at the workshop are presented below. Attachment G discusses the issues in detail. The italicized lists below may be considered starting points for addressing the issues.

These issues will be addressed in the workshop in the form of panel presentations and discussions as described in the main body of this letter. Workshop participants are also requested to prepare statements on how they feel the issues should be addressed and what they can contribute to resolving the issues. As a starting point, strawman proposals are included in Attachment G for some of the issues.

1. In-Package Criticality

What are models for process that may lead to critical configurations for intact fuel assemblies and intact baskets?

What are models for process that may lead to critical configurations for intact fuel assemblies and degraded basket?

basket degradation, release of absorbers, water chemistry, (pH, ion concentration, dissolved O₂), transport of absorbers from WP

What are models for process that may lead to critical configurations for degraded fuel assemblies?

cladding degradation, basket collapse, release of absorbers, water chemistry, (pH, ion concentration, dissolved O₂), transport of basket absorbers from WP, removal of fission products from the WP, degraded fuel composition (clayey material, slurry, etc.)

What types and amounts of emplaced waste have the greatest chance to lead to criticality?

High initial enrichment, low burnup, ²³⁹Pu more effective than ²³⁵U, short degradation times (Al based fuels)

What are the key uncertainties and variabilities in the parameters and models for in-package criticality?

moderator composition, degraded fuel geometry & composition, moderator concentration & geometry, neutron reflectors/absorber distribution & concentration

2. Near-Field Criticality

What are models for process that may lead to critical configurations in the drift/invert?

waste-form dissolution, colloid/pseudo-colloid formation, fissile mobilization processes, fissile material transport, reconcentration (sorption, filtration) of absorber and fissile species, critical-configuration geometry, reconcentration

What environmental conditions are necessary to establish a critical configuration outside the waste package?

solid and liquid moderators, reflectors, flow rates, concentration/ filtration processes, colloids/pseudo-colloids, fracture network spacing, sorption, concrete degradation to form zeolites, oxidized WP materials for adsorption

What types and amounts of emplaced waste have the greatest chance to lead to near-field criticality?

High enriched, soluble matrix (concentration of release over short time means short reconcentration period which can be handled by one mechanism)

What are the uncertainties and sensitivities in the parameters and models for near-field criticality?

moderator composition, moderator geometry, moderator fraction in material containing fissile species, neutron reflectors/absorbers, enrichment, composition of material containing fissile species, fissile species density

3. **Far-Field Criticality**

What are models for process that may lead to critical configurations in YM tuff (in both UZ and SZ)?

transport processes, reconcentration/diversion/ponding, sorption, sources for reducing environment, criticality event leading to additional (or more severe) criticality events

What are models for process that may lead to critical configurations elsewhere (e.g., Franklin Lakes Playa)?

transport processes, reconcentration/diversion/ponding, sorption sources for reducing environment

What environmental conditions are necessary to establish a critical configuration in undisturbed (country) rock?

reducing environment, accumulation of fissile material (lateral diversion/ponding in geological structures), reconcentration mechanisms (mineralization processes), liquid and solid moderators, flow rates

What environmental conditions are necessary to establish a localized (i.e., in fracture network) reactor?

solid and liquid moderators, flow rates, fracture spacing, sorption/reconcentration processes

What are the uncertainties and variabilities in the parameters and models for far-field criticality?

moderator composition, moderator geometry, neutron absorbers, fissile-material concentration, moderator concentration

The following is an attempt at providing a global view and strategy for addressing criticality for transportation, TSPA, and waste-package design.

FACTORS CONTRIBUTING TO THE LIKELIHOOD OF NUCLEAR CRITICALITY EVENT

	Fuel Composition	Geometry	Environmental Conditions (Moderator/Reflector/Temperature)
Waste Acceptance	wide range of burnup and initial enrichment	intact fuel assemblies	n/a
Transportation (possible misload)	actinide-only Burn-Up Credit (BUC) minimum burnup max initial enrich.	intact fuel assemblies accident Conditions: loss of basket poison	most reactive conditions: fully flooded, pure H ₂ O room temperature (20° C)
Storage: Wet (possible misload) Dry (possible misload)	actinide-only BUC minimum burnup max initial enrich as above	intact fuel assemblies basket poisoned intact fuel assemblies	water chemistry boron concentration limits/water moderator exclusion
Preclosure: Waste Package (possible misload)	BUC - actinides plus Fission Products (FP) minimum burnup max initial enrich	intact waste package intact fuel assemblies emplacement accidents ?	temperature effects (induced stress), radiolysis, cathodic effects moderator exclusion ? presence of inert gas

<p>Postclosure: Waste Package <i>-Intact WP</i> <i>-Degraded WP (breach pkg)</i> <i>-Degraded WF (Waste Form)</i> Near Field <i>(Full WP degradation)</i> Far Field</p>	<p>same as above determined from chemistry (act, FP) determined from chemistry (act, FP) determined from NF chemistry (act, FP, dose, transport nuclides) determined from geochemistry (act, FP, dose, transport nuclides) ▸U-238, U-235 ▸Pu solubility ▸zeolitic adsorption impact of previous criticality</p>	<p>same as above seismic events radiolysis, cathodic, seismic impacts seismic impacts loss of basket, cladding, pellet form rubble pile backfill sandfilter(particle accumulation) solution (fissile concentration) ▸matrix dispersion ▸perched water ▸deposits in fractures ▸lithophysal cavities ▸fast path to CHn ▸adsorption CHn ▸fast path to water table ▸dilution at water table</p>	<p>same as above and humidity external corrosion, pitting loss of inert gas, presence of water/water vapor accumulation of water in WP water chemistry ponding in alcove water chemistry tuff as reflector? Dryout/rewetting water chemistry tuff as reflector? saturated tuff as reflector? fracture flow facilitating transport fissile/moderator concentrations as a function of volume (minimum critical mass curves)</p>
<p>Consequence</p>	<p>source term</p>	<p>particle, colloid, gas</p>	<p>dose to accessible environment</p>

**ATTACHMENT E.
COUPLING OF CRITICALITY
TO OTHER MODELS DEVELOPED FOR TSPA-VA**

In-package criticality modeling is directly influenced by the waste package degradation and the near field environment. Such parameters as the time and rate of waste package degradation, the thermal conditions (temperature), the hydrologic conditions (percolation flux rates), and geochemistry of near field waters affects the critical-assembly process. Coupling to each of these parameters or models is vital to produce acceptable defensible criticality models. Near-field and far-field criticality modeling is influenced by the models for UZ and SZ flow and transport.

Waste Package Degradation. Waste package failure time (or failure history or distribution) provides the time for the potential introduction of water (or water vapor) into the waste package. WP Failure distributions depend on the in-drift environment (i.e., temperature, chemistry of water contacting the waste, and in-drift flux rate). Subsequent pitting and other localized corrosion degradation of the failed waste package provide the area on the waste package surface from which the radionuclides can migrate out of the waste package. Thus, close coupling with the waste package degradation activities is required for consistent TSPA calculations. Corrosion of the internal structural materials (e.g., basket tubes and guides made of carbon steel) is very important in modeling the various stages of in-package criticality.

Waste Form Degradation. The nature of in-package criticality changes as the neutron-absorbing basket degrades. Criticality further changes when the cladding degrades. Near-field and far-field criticalities can only occur when the waste has been transported out of the waste package from the degraded waste form. The release rate and amount of fissile nuclides affect external criticalities. Corrosion of the internal structural materials (e.g., basket tubes and guides made of carbon steel) is very important in modeling the various stages of in-package criticality.

Thermo-hydrology. Criticality events may generate sufficient heat to change the in-drift thermal and hydrological conditions (i.e., temperature, relative humidity, fracture flow onto waste packages, etc.). Additionally, there are some temperature-dependent effects on the neutronics. Thermal loading scenarios and the modeling assumptions in the T-H modeling activity should be compatible with those in the criticality modeling.

NFE Geochemistry. The in-drift geochemistry has a significant impact on the degradation and mobilization of the waste form and the waste package degradation. In addition, criticality events can modify the near-field geochemistry. As part of the consequence analysis for criticality, near-field alterations will be evaluated. Ionic species and concentrations in moderator water can affect neutronics.

UZ Flow. Criticality is indirectly affected by the repository percolation flux, and the areal distribution of that flux. Flux influences waste-package degradation and the rate and availability of water than can act as a neutron moderator.

UZ Transport. Reconcentration of fissile nuclides outside the waste package is dependent on transport mechanisms, including absorption and colloid filtering.

SZ Flow and Transport. Dilution and dispersion of fissile nuclides in the saturated zone will reduce potential far-field criticality. Reconcentration mechanisms in the SZ may enhance potential far-field criticality. The potential for the SZ flow system to cause accumulation of fissile nuclides in the groundwater (such as at locations like Franklin Lakes Playa) must be considered.

**ATTACHMENT F
PREPARATION FOR WORKSHOP**

- 1) Please read this memo carefully. It is important that all participants be well prepared for this workshop.
- 2) Check to see where you are listed as a panel member (Attachment I).
- 3) Prepare write-up for issues for which you are a panel member and any other issue of significance to you.

We strongly request that all panel members send us a short write-up (approximately 1 page) on the issues that they will discuss. These write-ups will be collected and compiled before the workshop and redistributed to all the workshop participants, also before the workshop. This will allow the workshop organizers to ascertain where the most discussion will be necessary and plan accordingly. It will also allow all of the workshop participants to come to the workshop thinking about the important issues and aware of the other participants' opinions. As said in the main part of this memo if a participant does not comment on a proposal it is assumed that the participant either agrees with the method or does not have the background to comment. The write-ups might discuss what data are available, what the participant's modeling experience or field observations have taught, what information can be extracted from certain models, etc. The write-ups should also comment on the appropriate strawman proposal. We welcome comments from all of the workshop participants (and observers) on any issue of their interest.

- 4) Send write-ups by **March 3, 1997**. Write-ups can be faxed to (702) 295-4730 (attention: Jerry McNeish) or e-mailed to Jerry_McNeish@notes.ymp.gov, preferably in ASCII format.
- 5) Prepare for panel presentations. Presentations should be short. We have a lot to cover in a short time. **As a guideline, keep your presentation to five (5) minutes and no more than two (2) viewgraphs (plus a title slide). If you feel it is not possible to cover what is necessary in that amount of time call Rally Barnard at (505) 848-0738 by March 10, 1997.** As with the write-ups, presentations might discuss your opinion of the strawman, what data are available, what your modeling experience or field observations have taught you, what information can be extracted from certain models, etc.
- 6) Come to the workshop prepared to contribute and have a stimulating time.

**ATTACHMENT G.
ELABORATION OF IMPORTANT ISSUES FOR
CRITICALITY MODELING FOR TSPA-VA**

As a mechanism to begin the discussion, and to get all participants started thinking about the issues for TSPA modeling of criticality, we present strawman proposals for some of the questions listed in Attachment D. The proposals represent current ideas in the TSPA and Waste-Package Development groups and how we would abstract and model criticality at this time. Not all of the issues have strawman proposals, because they have not yet been developed.

The strawman consists primarily of a set of credible configurations (not necessarily likely, but having some small probability of occurring), grouped according to the location of the criticality. The question of whether the configurations are actually critical is resolved by use of a neutronics code such as MCNP applied to specific configuration parameters, principally the concentrations of fissile species and neutron absorbers, and the geometry. These parameters are estimated from scenarios which are developed by combining, or abstracting, the results of individual processes analyses. The principal questions, or issues, connected with this methodology involve improvements on the individual process models. The limited scenario analyses performed thus far indicate the process model improvements which will most strongly affect criticality evaluations. However, the question of whether an individual process has a strong enough effect to ultimately lead to a critical configuration cannot be determined from the process, but must await additional scenario analyses, which will be performed in a timely manner as the improved process models become available. There is also a strawman configuration proposed for modeling the power and duration of a criticality. These configurations have all received some analysis as part of M&O Waste Package Development studies of criticality many of which are summarized in the *Disposal Criticality Analysis Methodology Technical Report*, Prepared by the CRWMS M&O for USDOE, August 15, 1996. The most relevant of these results will be presented as an introductory/background presentation at the workshop.

I. Internal Criticality

The configurations that may become critical within the waste package generally require standing water to cover at least half of the SNF. The water acts as a moderator for the neutrons emitted by the fissile nuclides. The presence of water in the waste package has been determined to be a possibility given the models for failure of the waste-packages. Corrosion must occur only at the top of the waste package, in order for the package to hold water. In addition to standing water, if there is the formation of hygroscopic material (such as clay) from the degradation products or from precipitate from the infiltrating water, the moderator for internal criticality can be provided. In addition to pure water, the only dissolved species with significant moderating capability is silica, but it is much less efficient in this respect than is the water that it would be replacing, so water containing silica would lead to a lower k_{eff} than the same volume of pure water.

In general, internal criticality cannot occur until a major fraction of the borated stainless steel component of the waste has been dissolved (by oxidation or otherwise) so that a major fraction of the boron can be removed from the waste package. This requires at least

10,000 years. On the other hand, after the waste package barrier has completely degraded, there can no longer be any significant amount of standing water to provide sufficient moderator to support criticality. This requirement would generally set an upper limit of 100,000 years for the occurrence of internal criticality. [The exception to this upper time limit would occur if sufficient hygroscopic material could deposit in the waste package and retain sufficient water for moderation without any standing water.]

What are the models for processes that may lead to critical configurations for intact fuel assemblies and intact baskets?

Given waste-package failure, there eventually may be water inside the waste package. Because intact fuel assemblies are in the configuration for maximum neutron economy and reactivity (they are designed that way), the presence of enough moderator could result in a critical configuration – if it were not for the neutron absorbers incorporated into the basket structure in the waste package. The basket is constructed of stainless steel loaded with natural boron. The boron is uniformly distributed throughout the mass of the stainless steel. Metal borides appear to be very corrosion resistant so there is no known mechanism for their release at a rate any faster than the general corrosion of the stainless steel basket material. The worst case configuration assumes the waste package voidspace is filled with pure water to serve as moderator. This is conservative because any impurity would have less moderating power than the water it displaced. The basket is designed to provide more than enough neutron-absorbing capacity to prevent criticality in the worst-case situation with the entire package filled with water. Avoidance of criticality under this worst-case configuration is required for licensing for transportation. Nevertheless, there may be more configurations more directly related to geologic emplacement of waste that have not yet been analyzed. The following are some questions that have been suggested:

- Is there a mechanism to leach a sufficient amount of the boron from the basket assembly to permit criticality while maintaining the physical structure of the basket?
- Does water chemistry (e.g., pH, presence of ionic species, presence of dissolved oxygen, etc.) influence the leaching process significantly?
- Under what circumstances can reduction in water density or increase in impurities increase keff? [This can occur in the overmoderated condition which has not been found to occur for commercial SNF, but which may occur for HEU or Pu waste forms.]

What are the models for processes that may lead to critical configurations for intact fuel assemblies and degraded basket?

The waste package basket materials are stainless steel and carbon steel. Most of the commercial SNF assemblies have cladding and spacer grids made of Zircaloy, which is much more corrosion resistant than the basket materials. Hence, it is expected that the basket will degrade before the assemblies. [Those assemblies made of other materials,

may behave otherwise, and are treated in the alternative for intact basket with degraded fuel, below.] The principal effects of basket degradation with intact assemblies are: (1) Relocation or removal of the neutron absorber contained in the stainless steel basket material; (2) Movement of the assemblies into closer proximity, which is generally a more critical (more neutron efficient) configuration. These possibilities raise the following modeling questions:

- What are the models that show the influence of water chemistry on the rate of basket degradation (particularly on the stainless steel and carbon steel)? How does the degradation vary with time?
- What are models for the rates of oxidation of the metal borides and the solubilities of the oxidation products (only poorly known at present)?
- What processes remove the neutron absorbers from the proximity of the SNF, particularly moving the absorbers to the bottom of the waste package, or out of the waste package altogether?
- What are the models for determining configurations resulting from the corrosion of the basket materials which permits the assemblies to settle into closer proximity (driven by the force of gravity)? A structural analysis presently ongoing in Waste Package Development to determine the minimum basket thickness required to support assembly weight will answer part of this question.
- Can materials with hygroscopic properties be formed from the degradation products plus any precipitate out of infiltrating water (e.g., clay)?

What are the models for processes that may lead to critical configurations for degraded fuel assemblies and intact basket?

Certain types of fuel have matrix and cladding which are less resistant to corrosion than the basket materials. The aluminum matrix research reactor fuel is an example. There are two criticality enhancements possible from this behavior: (1) There may be a faster outflow of fissile material from the waste package, thereby enhancing external criticality (this possibility is treated in external criticality, below); (2) The fissile debris from the degraded fuel may collect at the bottom of the waste package where it is not subject to criticality control from the neutron-absorbing material in the basket. The following questions are raised by this second possibility:

- What are the transport processes that can move the degraded waste form through open spaces in the basket or over the ends of the basket to collect at the bottom of the waste package (possibly confined to one end in the case of a tilted package)?

- What are the environmental conditions (particularly infiltration rate) which will determine whether the released fissile material collects at the bottom of the package or flows out of the package?
- Can slurries containing fissile material form and be sustained for long times? What densities of such slurry would be feasible?
- Can materials with hygroscopic properties be formed from the degradation products plus any precipitate out of infiltrating water (e.g., clay)

What are the models for processes that may lead to critical configurations for degraded fuel assemblies and degraded basket?

If, and when, both the basket and the SNF have significantly degraded, criticality can occur internally to the waste package if the fissile material is separated from the neutron absorbers (which are initially in the basket and in the SNF). It should be noted, however, that if the fuel rods or pellets remain intact the assembly degradation will bring them so close together that moderators are excluded, and the criticality of the configuration is lowered by comparison with the intact assembly configuration. It should also be noted that with the increasing overall degradation and increasing time implicit in this case, there is increasing potential for the formation of hygroscopic material, so the requirement for standing water in the waste package (noted as a very necessary overall requirement for internal criticality) may become less important. Other than this exception, criticality can occur internally to the waste package if the fissile material collects in some part of the package while the neutron absorbers collect in some other part of the package or are removed from the package. The following issues relate to the mechanisms for achieving such configurations (and their models). Some of the issues relate to removal rates, which are also important for the external criticality alternatives discussed later.

- How does the oxidation of uranium affect the dissolution rate of the SNF and how does it affect the solubility of the released uranium?
- How does the water chemistry affect the degradation rates of the basket materials and the SNF (both cladding and fuel matrix)? Are there chemistry regimes which favor the degradation of one over the other?
- How are very fine particulates (from degraded, but not dissolved, materials) moved by slowly flowing water?
- What colloids can be formed from the various chemical species (Fe, B, U, Pu, various fission products and actinides, etc.)? What persistence will they have?
- Can materials with hygroscopic properties be formed from the degradation products plus any precipitate out of infiltrating water (e.g., clay)

II. Near-Field Criticality

The environment outside the waste package is divided into near-field and far-field. The former is the invert beneath the waste package and the drift liner; together with the waste package itself they make up the engineered barrier system. The far-field is the native rock which has not been disturbed by the repository excavation. External criticality in the near-field cannot occur until a significant fraction of the waste form has degraded and released the fissile material and until a significant amount of that fissile material has been mobilized and transported out of the waste package. Because of the low solubility of the fissile material, this process is expected to take at least 30,000 years.

What are models for processes that may lead to potentially critical accumulations of fissile material in the invert and/or drift liner?

Evaluation of the potential for such processes begins with a fissile-bearing flow from the degraded waste form. The concentration and rate of this flow are determined from the waste-form degradation process considered for internal criticality. The fissile material is generally assumed to be ^{235}U , because significant SNF degradation is expected to take at least 40,000 years, by which time most of the Pu has decayed to U. [It should be noted, however, that all analyses to support the licensing process will use time-dependent models which do bookkeeping of both Pu and U. As noted above, the research reactor fuel may have degradation times much shorter than 40,000 years, however, this fuel has relatively little Pu to begin with.] It has been assumed that the flow contains no neutron absorbers, except for ^{238}U which is mobilized and transported at the same rate as the fissile ^{235}U . This assumption has been made for conservatism, and because the other chemical species will have significantly different solubilities, so that they are removed either earlier or later than the uranium. The different transport routes and differing solubilities of the other species compared with the fissile material severely reduce their participation at those locations where the fissile might concentrate, but the much greater amounts of waste-package material could still leave this a significant consideration. Comprehensive models of the transport and reconcentration processes may permit fewer conservative evaluations so that some credit can be taken for neutron-absorbing waste package degradation products, particularly the iron oxide from steel corrosion. Reconcentration of mobilized fissile material can occur by any of the following processes (which would need to be modeled if found to have significant effect):

- Ions removed from flow by zeolites in concrete or tuff (invert or liner)
- Particulates removed from flow by filtering through pores and fractures
- Particulates trapped in shallow impermeable depressions (rendered impermeable by filling of cracks with cement from drift liner)
- Colloids being reduced at surfaces

- Precipitation from temperature reduction or change in solution chemistry

In addition, models must be developed to address the following general questions:

- What geometries of fissile materials will be created by the possible transport processes?
- What will be the extent of co-location of the waste package degradation products, particularly the iron oxide, which can be a significant neutron absorber (accumulation by the same mechanism as the fissile material)?

What are the models for environmental processes that will determine the amount of moderator available at the potentially critical accumulations?

For certain configurations silica can be an effective moderator, but generally water is more efficient. The principal issues are therefore concerned with one or the other of the following questions: (1) Will there be sufficient water in the configuration? (2) Is the configuration appropriate for silica moderation? The following are examples of the issues:

- Are there models for transport of the fissile material into configurations which can become critical by the moderation of silica (alone or together with water), typically sphere-like geometry of a radius between 1.0 and 2.5 meters)?
- Retention of water in clay or other hygroscopic material
- Ponding in shallow impermeable depression (rendered impermeable by filling of cracks with cement from drift liner, similar to the trapping of particulates suggested above)
- Saturation of porous rock immediately above a porosity change

III. Far-Field Criticality

The earliest time to occurrence of external criticality in the far-field would be similar to that in the near-field, the only difference being the extra travel time to some zone of potential re-concentration. Since this travel time could be less than 10,000 years, it would not add significantly to the time already estimated for the occurrence of near-field criticality.

What are processes that may lead to critical configurations in Yucca Mountain Tuff?

The conditions that can lead to far-field external criticality are similar to those which can lead to near-field external criticality, with the following principal differences: (1) The fissile material in the flow will be less concentrated, particularly if the flow has

encountered the saturated zone; (2) There is a possibility of focusing of the flow from several waste packages; (3) Particulates and colloids will have been removed from the flow before it reaches the far-field; (4) Zeolites are naturally occurring instead of from concrete. The following are some of the additional issues raised by far-field criticality:

- What hydrothermal or other conditions can result in lateral diversion and ponding of fissile-bearing waters?
- Can a critical configuration form due to subsurface ponding without further reconcentration?

What are processes that may lead to critical configurations beyond the Yucca Mountain Tuff?

To cause criticality in zones beyond Yucca Mountain Tuff, the flow must: (1) pass through the saturated zone; (2) be focused to reverse the large dispersion and dilution that take place in the saturated zone; (3) encounter a strongly concentrating mechanism. These conditions may exist in connection with the Franklin Lakes Playa near Yucca Mountain, which is believed to be the principal outflow area from the Yucca Mountain groundwater. Other nearby areas may receive significant amounts of outflow if the climate becomes considerably wetter. The following are the major issues for this strawman:

- Are there available concentrations of organic or other materials that can form reducing zones?
- What is the appropriate model(s) for the water concentration in the various regions of the Playa?
- Can the flow carry the fissile material to configurations which can be effectively moderated by silica?

IV. Criticality Consequences

What are the processes that determine the power level and duration of a criticality?

The principal consequence of a criticality is the increased radionuclide inventory. The strongest determinants of such increases are the power and duration of the criticality.

A simple model has been constructed for internal criticality with the following features:

(1) A steady state is assumed with constant temperature such that the evaporation from the surface of the water in the waste package just matches the rate of water dripping into the waste package from the external environment; (2) The power level is determined to be that required to maintain the steady state temperature considering the principal energy dissipation mechanisms (radiation exchange with the drift wall, conduction through the rock/rubble in contact with the waste package, evaporation from the water surface; (3)

Duration may be limited by the loss of water confinement due to increased corrosion rates for the waste package bottom due to the increase in temperature caused by the criticality itself. Models of the following processes are presently poorly understood and will strongly affect these estimates:

- Infiltration rate and focusing of fracture flow onto a single waste package.
- Retention of water in the waste package (confinement by concave surfaces that have not been completely penetrated, or retention in hygroscopic material)

A simple model has also been constructed for far-field external criticality with the following features: (1) Maximum sustained power determined by boiling point of water or the maximum inflow of the worst-case high concentration of fissile-bearing water; (2) duration is nominally limited by introduction of fissile material from up to one additional waste package. Models of the following processes are presently poorly understood or implemented, and will strongly affect these estimates:

- Infiltration rate and effect of criticality on this rate
- Flow in porous rock and how it is affected by the criticality
- Heat transfer during criticality
- Cyclic or transient effects (overshoot or criticality spike)
- Combination of fissile material from multiple waste packages

**ATTACHMENT I
PANEL MEMBERS FOR CRITICALITY ISSUES**

Session:

Panelists:

1. In-Package Criticality

- Models
- Waste Forms
- Uncertainties
- FEPs

Peter Gottlieb
W. Davis/J. Massuri
C. Detrick
C. Stockman
E. Siegmann
D. Thomas
M. Brady (?)
J. McNeish - TSPA (?)

2. Near-Field Criticality

- Models
- Environmental Conditions
- Waste Forms
- Uncertainties
- FEPs

B. Glassley
R. Rechard
L. Sanchez
D. Sassani - TSPA (?)
R. VanKonyenberg
D. Chestnut

3. Far-Field Criticality

- Models
- FEPs
- Uncertainties

G. Barr
R. Rechard
J. Wilson
J. McNeish - TSPA(?)

ATTACHMENT II
Responses to Strawman Proposals

WBS 1.2.5.4.1
QA: N/A

Contract #: DE-AC01-91RW00134
LV.PA.JAM.03/97-XXX

March 14, 1997

To: Workshop Participants and Observers

From: Jerry McNeish - M&O/INTERA (DE&S)

Subject: Responses to Disposal Criticality Strawman for Disposal Criticality
Abstraction/Testing Workshop

The limited comments received from participants regarding the Disposal Criticality Strawman presented in the invitation letter for the workshop are compiled and presented herein. The responses are arranged according to the initial issues presented where appropriate.

Response from Henry Loo, INEEL
DOE EM Fuel Issues: TSPA-VA Disposal Criticality Abstraction/Testing Workshop

The following are presented as issues relating to criticality for DOE spent nuclear fuels.

1. DOE Fuel Characteristics

Some DOE fuel characteristics are significantly different from the commercial fuels that these characteristics should be considered in the criticality workshop abstraction process. If possible, these characteristics should be included in the abstraction. Examples include that certain DOE spent nuclear fuels are very high in U-235 enrichment (over 90%). Other DOE fuel characteristics include different types of fissile materials such as U-233 and much higher concentration of Pu-239 contents (approximately 24%). How enrichment, other fissile materials, and concentration affect the probability of and the consequences of a repository criticality should be considered in the abstraction.

DOE fuels have variable integrity. Examples include the aluminum clad/UA1x fuels which could corrode much faster than commercial spent fuels to the very high integrity Fort St. Vrain uranium carbide and the Shippingport PWR fuels. Similarly, DOE fuel matrixes vary from small pieces of scrap materials in cans, from testing programs, to well-preserved intact spent fuels. The abstraction should consider effect of fuel integrity (matrix integrity and variations, and cladding) on the probability of and the consequences of a repository criticality.

2. DOE Fuel Packages Variations

DOE fuels will be disposed in various packaging options. One option includes the co-disposal of highly enriched spent fuel with high-level waste borosilicate glass logs. Another package difference is the generally lower thermal output from DOE fuel and co-disposal packages, which will likely be much lower than the 14.2 kW/package estimated for the commercial fuels. Thus, how packaging options, and thermal output per package affect the probability and consequences of a repository criticality should be considered in the abstraction.

3. Internal Criticality

In the evaluation of internal criticality, several additional degradation issues should be considered for the DOE spent fuels. For the co-disposal (highly enriched spent fuel with HLW glass) option, as the internal degradation progresses, the effect of large quantity of Si (from the glass) on fissile material solubility should be considered. In a previous evaluation (based on EQ3/6), Si concentration in the water appears to have an impact on uranium solubility. The effect of Si on the probability and consequences of a repository criticality should be considered.

As the waste package basket, fuel canister, and fuel corrode, large quantities of corrosion products will accumulate in the waste package. These corrosion products will displace moderators such as water. If these corrosion products also trap some neutron absorber materials, it will help reduce the

potential of a criticality. Thus, corrosion product credit should be considered as part of the abstraction process.

Even after the waste package has corroded through the bottom, corrosion products (in oxide form) may retain some water. The effect of water hold up in the corrosion products and oxides should be evaluated.

Other neutron absorber materials, such as Hf or Gd, may also be used for criticality control within DOE-owned spent fuel packages. The effect of other neutron absorber materials on the probability and consequences of a repository criticality should be considered in the abstraction process.

4. *Near-Field Criticality*

Again, with the co-disposal (highly enriched spent fuel with HLW glass) concept, as the waste package corrodes, the effect of large quantity of Si (from the glass) on fissile material solubility and retention in the near-field should also be considered in the near-field criticality evaluation. The effect of Si on the probability and consequences on a near-field repository criticality should be considered.

The Nuclear Waste Technical Review Board (NWTRB) and Oak Ridge National Laboratory have suggested that depleted uranium (DU) may provide some benefit in the reducing the chance of repository criticality. In their 1995 report to congress, the NWTRB encouraged the OCRWM to consider the placement of DU in the repository drift to mitigate the potential of repository criticality [Reference page 34, U.S. Nuclear Waste Technical Review Board, Report to the U.S. congress and the Secretary of Energy, 1995 Findings and Recommendations].

The OCRWM has also indicated that other materials, such as zeolite, are being considered for use in the backfilling of repository drifts to retard the movement of radioactive materials. Since such backfill materials will also very likely retain fissile materials, DOE-EM would like to suggest that potential of accumulating large quantity of fissile materials in the backfill be considered in the evaluation.

5. *Far-Field Criticality*

No additional suggestions.

6. *Probability and Consequences*

In estimating the consequences of a repository criticality, the use of bounding scenarios such as a continuous low power reactor may be too conservative. OCRWM should investigate the use of dynamic models to estimate the total number of fissions if a criticality does occur in the repository. These models would take into consideration the feedback mechanisms such as the neutron kinetics and hydrodynamics that would lead to shutdown of the reactions.

It was briefly mentioned that RELAP may be used by OCRWM to model the dynamics of a critical system. The use of RELAP for applications outside of the reactor core, especially in a repository environment, may not be the right tool. This is in part due to the large uncertainties associated with the various input parameters and the physical configuration of the system.

Response from Cliff Ho, SNL

- 1) How do heterogeneities impact focusing of flow (I realize that this is a UZ Flow issue, but it seems to be a required input for criticality models)?
- 2) Is the perched water zone an important area to consider for criticality? What are the mechanisms that are causing the perched water?
- 3) Is criticality likely to occur along fractures or in the matrix in the far field? (The type of model used for UZ Flow and T-H Flow may significantly affect this issue (e.g., DKM vs. ECM)).

Response from Dave Sassani, M&O/INTERA (DE&S)

In-Package Criticality:

It is not clear why consideration is not given to filling the waste package with a material that would assuage concerns over physical movements of fuel rods causing higher potential for criticality. I would suggest that the same material being used for the basket be used as this would provide more abundant moderator and even after reaction continue to provide a supporting mass of, most likely, Fe-oxide to keep the fuel rods in generally the same place. Given the complexity of the system and concurrent uncertainties with respect to the evolution of fluid composition it seems best to stay with a material which is already in use in the system so as to not further complicate it. This would alleviate the need to model so precisely the physical movement of fuel rods in the waste package and would go a long way to constraining their distribution over long time frames. In addition, for concerns regarding uranium criticality, incorporation of depleted uranium into the package design would serve to dilute the fissile material and would behave identically in terms of chemical concentration processes. For Pu, formation of colloidal Pu may occur from shifts in pH via reaction with steels (lower pH) and subsequently glasses (higher pH) in the waste packages. If colloidal transport occurs within the waste package with concentration at the bottom, then Pu-colloids could be ~ 2 orders of magnitude more efficient at localization of Pu compared to transport and precipitation of dissolved Pu.

Near-Field Criticality:

At the very least, any models of the release of fissile materials out of the waste package and concentrations of dissolved fissile materials that are potentially concentrated within the near-field environment should be tested against the long-term drip tests performed at Argonne National Laboratory for both spent fuel and for glass. Such models should be able to reproduce within a

couple orders of magnitude (for both time and composition) the resulting elemental distributions measured in those tests before any results are used to interpret what may be happening to a given waste packages complement of fissile materials. Because the effective quantitative removal by precipitation of an element from solution requires only a two order-of-magnitude decrease in the solubility of a phase containing that element, all calculations should provide explicit assessment of uncertainties and the origin of those uncertainties in order for their utility to be assessed. For example, for a simple system with only a small number of components, even if data need to be estimated for higher temperature conditions, one standard deviation of 0.5 orders of magnitude is feasible for a comprehensively covered system with well-constrained data at 25° C. However, if there are gaps which introduce conceptual-model uncertainties resulting from not having the appropriate solid phases or dominant aqueous complexes at the appropriate conditions, calculations can have one standard deviation of 3 orders of magnitude in terms of how they represent the actual system. The likelihood of producing process-level calculations with large uncertainties increases with increasing complexity of the system considered, and decreasing comprehensiveness of the analysis. Reproducing results of drip tests using uncalibrated process-level calculations would provide a large measure of confidence that the models are capturing the essential behavior of that system, and would provide a basis for interpreting longer time-frame results.

ATTACHMENT III

Workshop Agenda and List of Attendees

POST-CLOSURE CRITICALITY ABSTRACTION/TESTING

WORKSHOP AGENDA

Tuesday, March 18

- 8:00 Welcome and Introduction **Mike Scott**
- 8:10 Overview of TSPA-VA Objectives **Holly Dockery**
- 8:25 Workshop Introduction **Rally Barnard**
- Workshop Objectives
 - Guidelines and Format of Workshop
- 8:30 TSPA Perspective and Overview **Jerry McNeish**
- 9:00 Update on Repository Design **Dan McKenzie**
- 9:10 Update on Waste Package Design **Tom Doering**
- 9:20 Status of Process-Level Criticality Models **Peter Gottlieb**
- 9:30 Initial Presentation of Issues and Prioritization Criteria **Rally Barnard**
- 9:45 Break (collect lunch money for pizza and order for 2nd day's lunch)
- 10:00 Presentation/Discussion/Ranking of issues for Session I (In-Package Criticality)
- TSPA Perspective of the Major Issues (10 min.)
 - Proposal Presentations by Participants (3-5 min./speaker)
 - Clarification/Questions (1-2 min./speaker)
 - Define Issues Presented (3-5 min./speaker)
 - Finalize List of Issues (15 min.)
 - Small Group Prioritization of Identified Issues (30 min.)
- 12:00 Lunch - brought in (if necessary, keep working on in-package criticality)
- 1:00 Presentation/Discussion/Ranking of Issues for Session II (Near-Field Criticality)
- TSPA Perspective of the Major Issues (10 min.)
 - Proposal Presentations by Participants (3-5 min./speaker)
 - Clarification/Questions (1-2 min./speaker)
 - Define Issues Presented (3-5 min./speaker)
 - Finalize List of Issues (15 min.)
 - Small Group Prioritization of Identified Issues (30 min.)

- 3:00 Break
- 3:15 Presentation/Discussion/Ranking of Issues for Session III (Far-Field Criticality)
- TSPA Perspective of the Major Issues (10 min.)
 - Proposal Presentations by Participants (3-5 min./speaker)
 - Clarification/Questions (1-2 min./speaker)
 - Define Issues Presented (3-5 min/speaker)
 - Finalize List of Issues (15 min.)
 - Small Group Prioritization of Identified Issues (30 min.)
- 5:15 Summary and Discussion of Plans for Next Day
- 5:30 Adjourn for the day
- 6:00 Dinner/Social Gathering

Wednesday, March 19

- 8:00 Summary of Linkage with Previous Workshops **Rally Barnard**
- Waste Package Degradation, Waste Form Degradation and Mobilization, Near Field Environment
- 8:30 Relevant Work in Existing Workscopes (5 min./presenter) **Dan Thomas**
Paul Cloke
- In-Package Criticality (Nucleonics Discussion)
 - Out-of-Package Criticality (Geochemistry)
- 8:50 Review of Criticality Issues in Terms of Other Activities **Rally Barnard**
- 9:10 Identification of Abstraction Groups **Mike Scott**
- Issue Criteria Correlation Exercise (dots placement)
 - Binning of Issues for Abstraction Working Groups
- 9:30 Objectives for Strategy/Analysis Plan Development and Working Group Guidelines **Jerry McNeish**
- 9:45 Break
- 10:00 Working Group Strategy Session I
Prepare Proposals to Analyze/Test High Priority Issues Previously Identified
- Title of Abstraction Plan
 - Identify Products for TSPA-VA
 - Define Approach to Abstraction
- 12:00 Lunch

- 1:00 Presentation of Strategies and Whole-Group Feedback for Issues Analyzed
- Presentation of Each Abstraction Plan (5-10 min./group)
 - TCT Comments, Feedback, and Discussion (10-20 min./group)

- 3:00 Working Group Strategy Session II
- Develop Detailed Abstraction/Testing Plans
 - Identify Roles of Group Participants
 - Develop Metrics (Criteria for Abstraction Completion)

5:30 Adjourn for the day

Thursday, March 20

8:00 Review Feedback on Working Group Strategies **Mike Scott**

- 8:15 Finalize Detailed Abstraction/Testing Plans and Schedules by Working Groups
- Schedule
 - Hardcopy of Plan/Overheads for Presentation to Whole Group

9:45 Break

- 10:00 Present Detailed Plans and Schedules for Working Groups
- Presentation (10 min./group)
 - Discussion (10 min./group)

11:30 Wrap Up, Summary, and Observer Comments **Mike Scott**

12:00 Lunch (Workshop Ends for All But Core Team)

2:00 Abstraction Core Team Only Wrap Up

5:00 Adjourn

**Attendees: Criticality Workshop
Las Vegas, NV - March 18-20, 1997**

Name	Organization	Phone #	E-Mail
Andrews, Bob	Intera	702-295-5549	robert_andrews@notes.ymp.gov
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Jolley, Darren	Intera	702-295-4695	jolley@notes.ymp.gov
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ATTACHMENT IV

Viewgraphs of Introductory Presentations

- H. Dockery: Post-Closure Criticality Model Abstraction/Testing Workshop - Objectives and Constraints
- R. Barnard: Post-Closure Criticality Workshop - Introduction
- J. McNeish: Total System Performance Assessment and Abstraction
- D. McKenzie: Repository Subsurface Design Overview
- T. Doering: Engineered Barrier Segment Design Concepts
- P. Gottlieb: Post-Closure Criticality: System and Process Considerations

Post-Closure Criticality Model Abstraction/Testing Workshop Objectives and Constraints

Holly A. Dochary
Deputy Manager, MAO Performance Assessment
March 18, 1997

All Federal Agencies Waste Management & Performance, Inc. Performance Contractors Environmental Contracting Management & Operating Contractors	All Research Laboratories Lawrence Berkeley Laboratory Lawrence Livermore National Laboratory Los Alamos National Laboratory National Institute of Standards and Technology Sandia National Laboratories	State Research Laboratories West Louisiana State University University of Utah University of Wisconsin Virginia Tech West Virginia University
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Viability Assessment Components

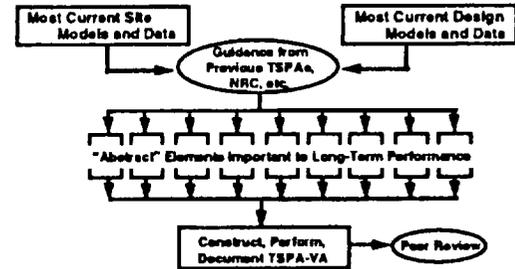
- (1) the preliminary design concept for the critical elements for the repository and waste package;
- (2) a total system performance assessment, based upon the design concept and the scientific data and analysis available by September 30, 1998, describing the probable behavior of the repository in the Yucca Mountain geological setting relative to the overall system performance standards;
- (3) a plan and cost estimate for the remaining work required to complete a license application; and
- (4) an estimate of the costs to construct and operate the repository in accordance with the design concept.

(FY 1997 Energy and Water Appropriations Act)

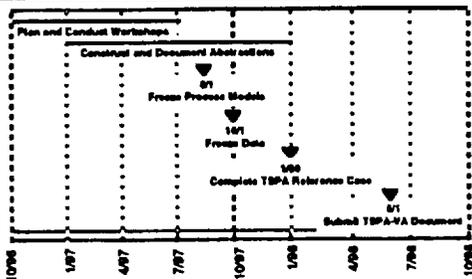
Outline

- Approach and Schedule for TSPA-VA
- Definition of Abstraction
- Goals of Abstraction/Testing Activities
- Goals of Abstraction Workshops
- Constraints

Approach for TSPA-VA



Generalized Schedule for TSPA-VA



What is an "Abstraction"?

- a simplified/idealized model that reproduces or bounds the essential elements of a more detailed process model
 - inputs may be those that form a subset of those required for a process model, or they may be a response function derived from intermediate results.
 - model must capture uncertainty and variability.
 - abstracted model must be tested against process models to assure validity.

Abstraction/Testing: Basis

- TSPA-type analyses are probabilistic/stochastic
 - Goal is to retain key aspects of process model affecting post-closure performance while producing results usable in multiple realization probabilistic models
 - PA assumes that essential elements (e.g., output) of some process models can be represented in a simplified form, thus increasing the computational efficiency of the TSPA

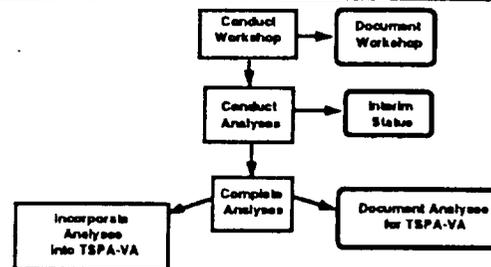
Abstraction Requires Collaboration

- Ensure the most current understanding (observations and models) is incorporated
- Ensure integration across major Project products used as the foundation (=confidence) of TSPA-VA
- Ensure that issues are identified and can be addressed quantitatively/qualitatively in TSPA-VA

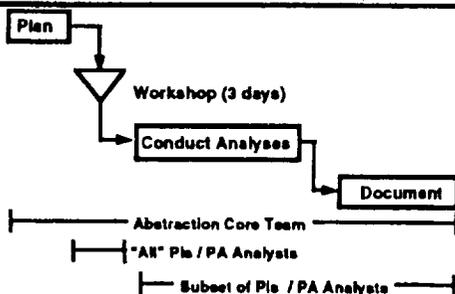
Goal of Abstraction/Testing Activities

- Develop a valid, defensible TSPA-VA:
 - Ensure completeness/representativeness of models used in TSPA analyses with respect to important aspects of process model(s).
 - Ensure appropriate issues (=alternative hypotheses) are identified, quantified and evaluated in TSPA.
 - Ensure model development effort is focussed on most important issues (with respect to performance)
 - Ensure bases for assumptions are well defined, justified and documented.

Format of Abstraction/Testing Activities



Generic Abstraction/Testing Activity Schedule



Schedule for Abstraction/Testing Workshops

Workshop Topic	Workshop Date	Workshop Lead	Workshop Location
Unsat. Zone Flow	1/21-21/97	S. Abram	Albuquerque
Waste Package Degradation	1/8-10/97	J. Lee	Las Vegas
Thermohydrology	1/21-23/97	M. Francis/ C. Ho	Albuquerque
Unsat. Zone Transport	3/5-7/97	J. Houseworth	Albuquerque
Waste Form Alteration and Migration	2/18-21/97	W. Halsey	UNIVERSITY
Near Field Environment	3/5-7/97	D. Seaman	Berkeley
Criticality	3/18-20/97	R. Bernard	Las Vegas
Saturated Zone Flow and Transport	4/1-2/97	B. Arnold	Denver
NEPA	5/8-9/97	A. Smith	Las Vegas
Biosphere	6/3-5/97	A. Smith	Las Vegas

Goals of Abstraction Workshops

- Develop a comprehensive list of issues related to each process that need to be addressed for TSPA
- Prioritize the list of issues according to a consistent set of performance measures or criteria
- Develop analysis plans to address top priority issues (parameter set, numerical analyses, analytical analyses, literature searches, etc.)

Goal is not to resolve key issues/uncertainties

Ch-10 on the Ground for Waste
Management System
Management & Operating
Criteria

Roles and Responsibilities

- **ISPA Core Team (TCT):** ensure approach is implementable in TSPA and process models are consistent
- **Abstraction Core Team (ACT):** coordinate abstraction activities and ensure integration with process model development
- **Abstraction analysts** - conduct sensitivity/uncertainty analyses
- **Process model analysts** - provide most current process model understanding
- **Observation interpreters/synthesizers** - ensure most current interpretations are included in process model

Ch-10 on the Ground for Waste
Management System
Management & Operating
Criteria

Responsible Staff

TCT:

Mike Wilson
David Sevougian
Jack Gauthier
Jerry McNeish

Post-closure Criticality Model ACT:

Ralston Bernard
Peter Gottlieb
Michael Brady
Jerry McNeish

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Management System
Management & Operating
Criteria

Technical Constraints

- Easy to focus on conceptual uncertainties, more difficult to define appropriate methods to address these uncertainties.
- Weighting of alternative hypotheses.
- Alternative data interpretations.
- Some conceptual complexities may be difficult to accommodate.
- Reasonably limiting the degree of conservatism.

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Management System
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Criteria

Programmatic Constraints

- 9 months of abstraction sensitivity analyses by about 1 FTE plus appropriate levels of M&I (plus about 1 FTE support provided by 1.2.2).
- Parallels ESF testing and synthesis.
- Deliverable documenting abstraction/testing results by 5/98 (mid-point status in 7/97).
- TSPA-VA documented 6/98 (analyses completed 2/98).
 - TSPA-VA process will be peer reviewed.

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Criteria

Summary

- TSPA-VA is owned by all.
- Confidence/completeness/consistency in models is our collective responsibility.
- Collaboration is required to ensure success.
- Workshop is just the beginning of the process towards generating a reasonable TSPA-VA.
- At the workshop, we need to focus on approaches to evaluate issues not just identification of uncertainties.

Ch-10 on the Ground for Waste
Management System
Management & Operating
Criteria

Post-Closure Criticality Workshop

Introduction

Ralston W. Barnard
Sandia National Laboratories
March 18, 1997

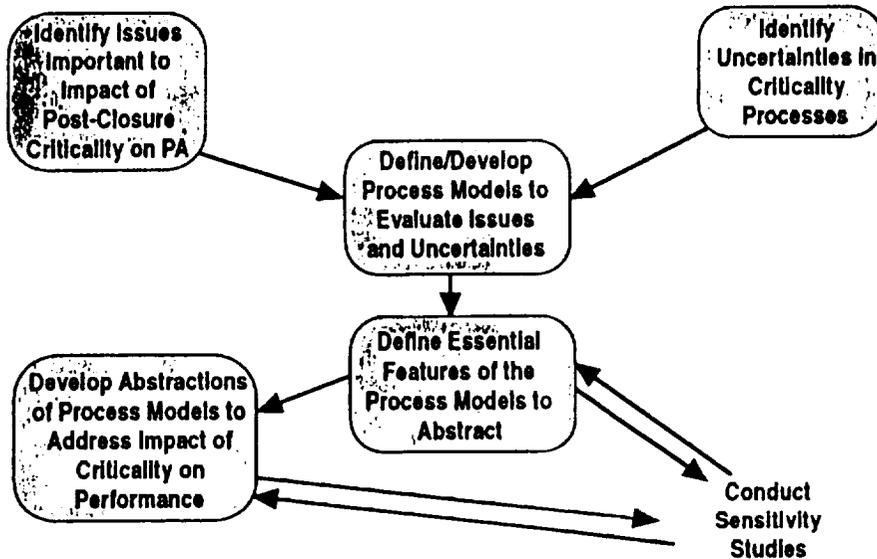


Workshop Goals

- Develop plans/strategies for bounding the impact of nuclear criticality on the total-system performance of the potential Yucca Mountain repository
 - Identify process-level issues
 - detailed discussion of issues
 - Prioritize issues against performance-related criteria
 - select highest ranked issues that can be addressed by further analyses
 - Develop specific plans to test issues
 - structure analyses to identify sensitive/important parameters



Approach to Criticality Abstraction/Testing



3

Scope of the Criticality Workshop

- Criticality in terms of impact on total-system PA
 - in-package criticality
 - near-field criticality
 - far-field criticality



4

Structure of Workshop

- Review factors influencing criticality analyses
 - waste-package and repository design
 - criticality models
 - TSPA requirements
- Discuss and prioritize issues
 - in-package criticality
 - near-field criticality
 - far-field criticality
- Develop abstraction/testing plans
 - problem definition
 - strategies



Total System Performance Assessment and Abstraction

**Jerry McNeish
Performance Assessment
CRWMS M&O/INTERA (DE&S)**

**Post-Closure Criticality Workshop
March 18, 1997
Las Vegas, NV**

CRWMS M&O Workshop JAM 3/18/97 p. 1

Overview

- **Total System Performance Assessment**
- **Evaluation of Uncertainty**
- **What is an Abstraction?**
- **Abstraction and Testing of Abstractions for Post-closure Criticality**

CRWMS M&O Workshop JAM 3/18/97 p. 1

Total System Performance Assessment

- **General**

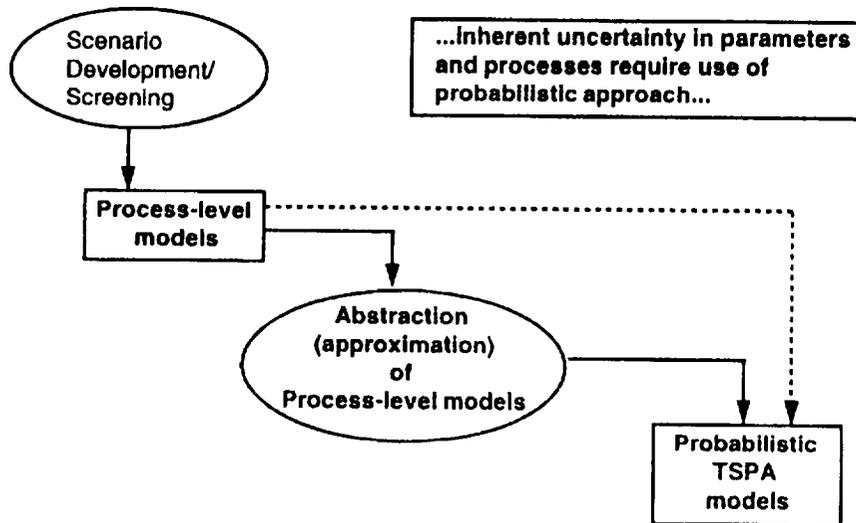
- In a probabilistic framework, evaluate the significance of features, events, and processes (FEPs) at the potential repository using available data, models, abstractions, expert judgement
- Incorporate uncertainty
- Determine potential consequence/risk of the significant FEPs

- **Criticality - specific**

- One of the potentially important FEPs at the repository is the occurrence of a criticality event
- TSPA-VA will include the evaluation of possible criticality events in terms of risk
- For each possible criticality event, the effect on post closure performance will be evaluated

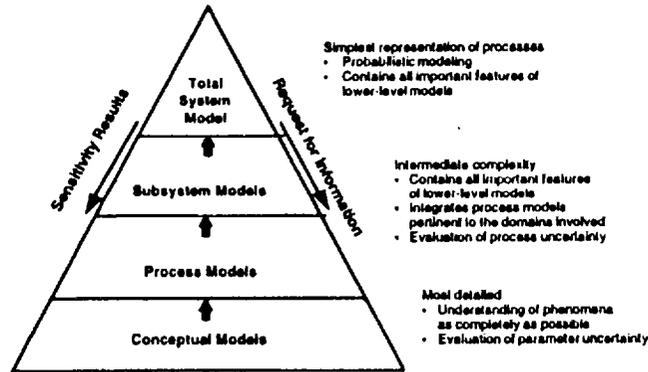
Criticality Workshop JAM 9/16/97 p. 3

TSPA Modeling Philosophy



Criticality Workshop JAM 9/16/97 p. 4

Total System Performance Assessment Model Hierarchy



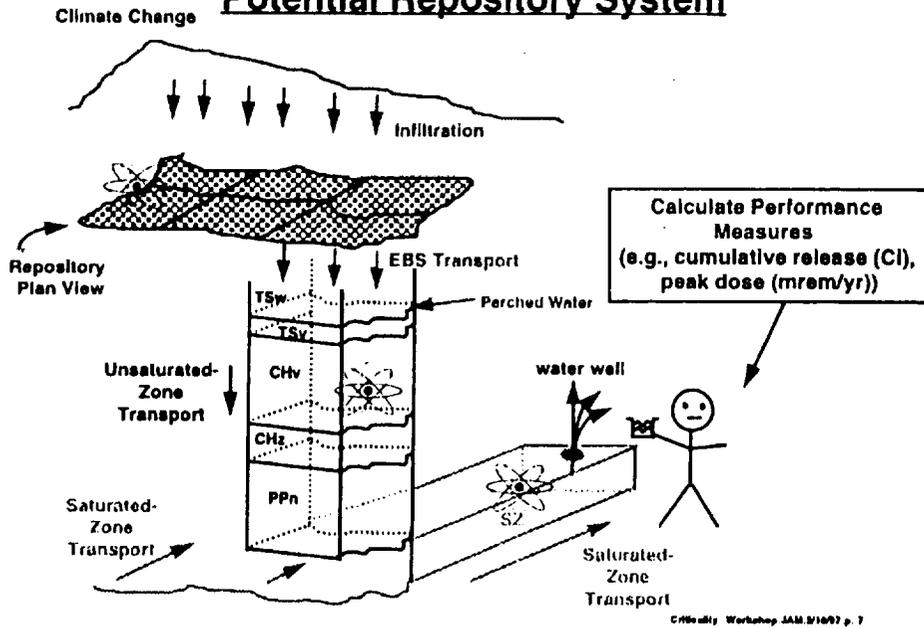
CRS/Health Workshop JAN 2/1997 p. 8

Summary of Key Features of TSPA

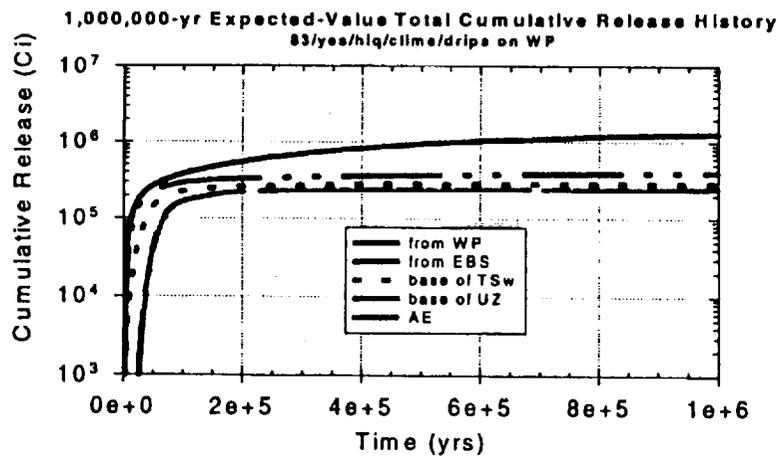
- Identify and quantify uncertainty range for parameters: boundary/initial conditions, phenomenological coefficients.
- Simple model behavior must bound complex model behavior using a peak dose metric.
- Simple models must be computationally efficient.

CRS/Health Workshop JAN 2/1997 p. 8

Schematic of Yucca Mountain Potential Repository System

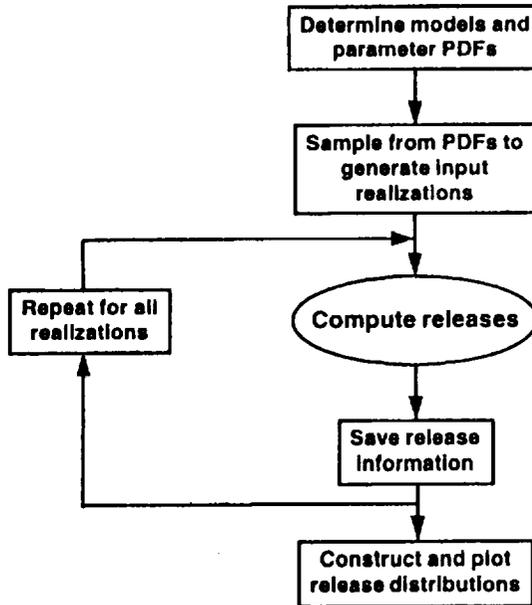


Example Performance Measure: Cumulative Total Release History



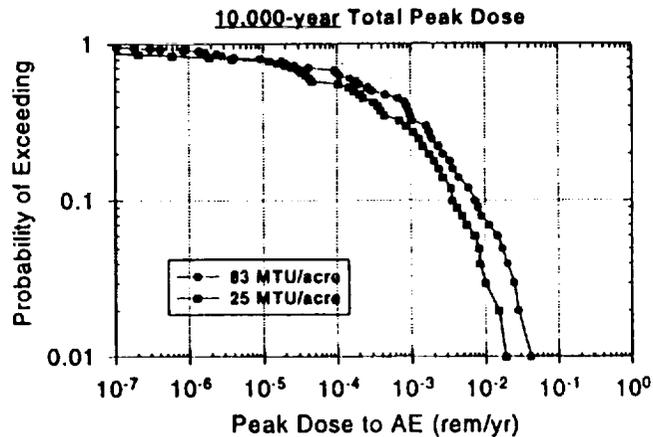
CRW/MS/ Workshop JAM 8/1997 p. 8

Schematic of TSPA Monte Carlo Simulations



Columbia Workshop JAM 3/16/97 p. 8

Example Performance Measure: Peak Dose CCDF's



000 4/16/97 10 2 10

Columbia Workshop JAM 3/16/97 p. 10

What does PA need?

- **Multiple conceptual models of system's components**
- **Defensible process-model abstractions**
- **Integrated model of total repository system**
- **Approach to characterize uncertainty**
- **Multiple realizations of total system (1000's)**
- **Time period of analysis: 10,000 to 1,000,000 yrs**

C/Health Workshop JAM 2/10/97 p. 11

Evaluation/Presentation of Uncertainty

- **Forms of uncertainty**
 - Data
 - Conceptual models
 - Representation of conceptual model
- **Evaluation of Uncertainty**
 - Multiple realizations
 - Focus on key input parameters
 - Expert elicitation
- **Presentation of Uncertainty**
 - PDF/CCDF
 - Multiple conceptual models

C/Health Workshop JAM 2/10/97 p. 12

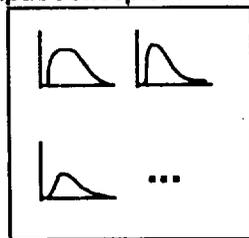
Examples of Uncertainty

- **Uncertainty in boundary conditions:**
 - Current infiltration
 - Future climate change
- **Uncertainty in initial conditions:**
 - Natural system parameters, e.g., fracture/matrix flow parameters
 - Repository design
- **Uncertainty in system processes:**
 - Resolution in physical-chemical process models and spatial discretization required to capture system behavior on scale of human lifespan and behavior
 - Degree of T-H-C-M coupling
- **Regulatory uncertainty in performance measures**
 - Peak dose to maximal individual or average individual
 - 5 km, 20 km, 30 km?

CDM/Elby Workshop JAM 3/10/97 p. 13

Investigation of Uncertainty

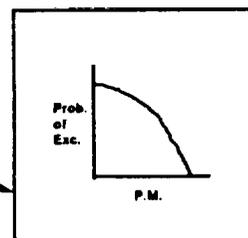
Input/Conceptual Models



Calculation of Performance Measure

-multiple realizations using sampled input values and alternative conceptual models

CCDF of Performance Measure



CDM/Elby Workshop JAM 3/10/97 p. 14

What is an Abstraction?

- **Definition: A simplification of a physical process that captures essential features of the process important to total system performance**

CRMcCarthy Workshop JAM 3/16/97, p. 18

What is an Abstraction? (continued)

- **Examples of Abstractions**
 - Response surface representation
 - Dimensionality reduction in process model
 - Heterogeneity reduction
- **Drawbacks to Abstraction of Process-level models**
 - Simplification, not necessarily representation
 - Coupling with other processes may not be properly addressed
- **Benefits of Abstraction**
 - Include only important processes
 - Requires less time, computing resources

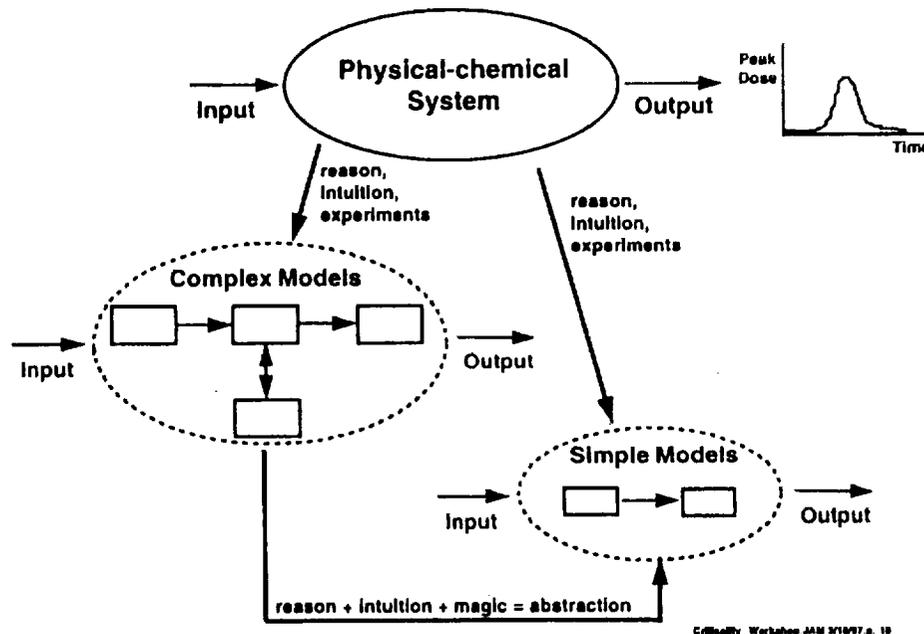
CRMcCarthy Workshop JAM 3/16/97, p. 18

Why do we need TSPA abstractions?

- To help us think about the problem---divide it up into "bite-size" pieces.
- To save time---both human and computer time:
 - Since the overall repository behavior is strongly nonlinear with respect to a number of key parameters and processes, the numerous input uncertainties mean that 100s or 1000s of model realizations are required to adequately characterize the predicted output uncertainties.
 - Predictive time frame for model simulations is at least 10,000 years, with some simulations carried out to 1,000,000 years.
 - Certain multi-process, multi-dimensional, highly discretized "process-level" models require large of amounts of CPU time.
 - Our "ignorance" (lack of data) about the system does not justify using the most complex models in many instances.
- Because some processes have not been adequately represented at the process-level.

C/Health Workshop JAM 3/1997 p. 17

An Abstract View of Abstraction and Modeling



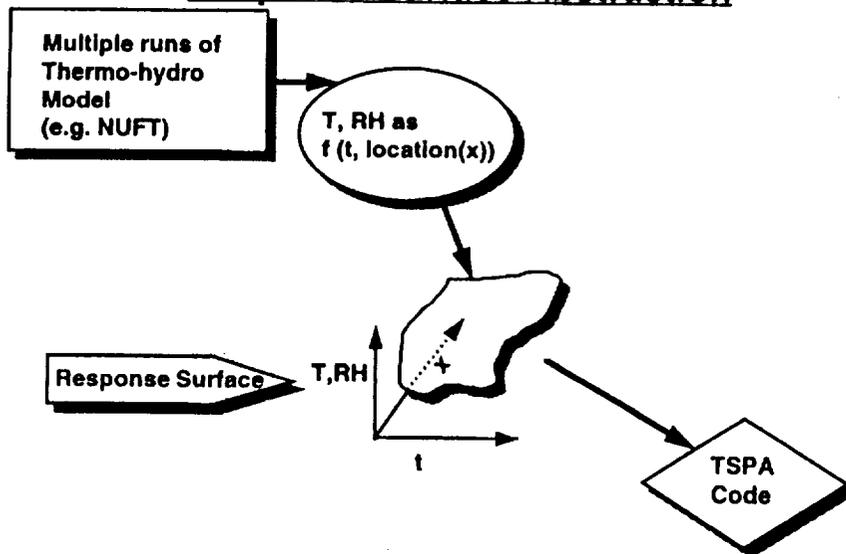
C/Health Workshop JAM 3/1997 p. 18

Response Surfaces

- Use multiple simulations from detailed process models
- Determine model parameters as functions of independent parameters.
- Use those functions, instead of the process model, in the Monte Carlo simulations.
- Define functions as an equation (e.g., from a linear regression) or by a table or library of output.
- Independent parameters should be the key indicators of repository performance

C/Health Workshop JAM 3/1997 p. 19

Example of Thermo-hydrologic Response Surface Abstraction



C/Health Workshop JAM 3/1997 p. 20

Dimensionality Reduction

- Use process models directly in the Monte Carlo simulations, but in 2-D or 1-D rather than 3-D.
- Compare simplified process model with full process model in terms of performance (e.g., calculated peak dose)
- Abstraction should appropriately represent the higher dimension model
- Example: TSPA-1993 used TOSPAC, a 1-D isothermal single-phase process model for UZ flow in the Monte Carlo simulations.

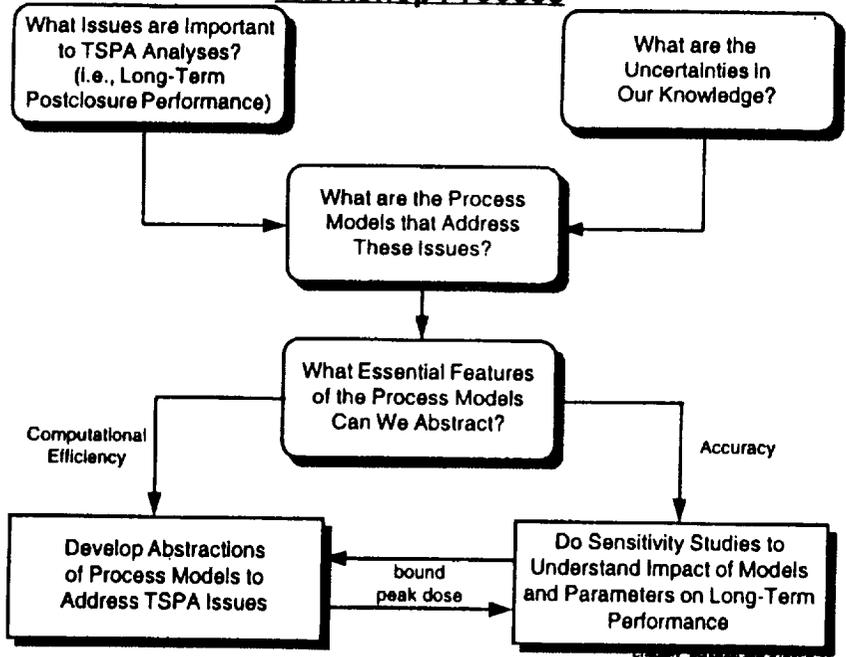
Criticality Workshop JAM 3/16/97 p. 11

Testing/Development of Abstractions

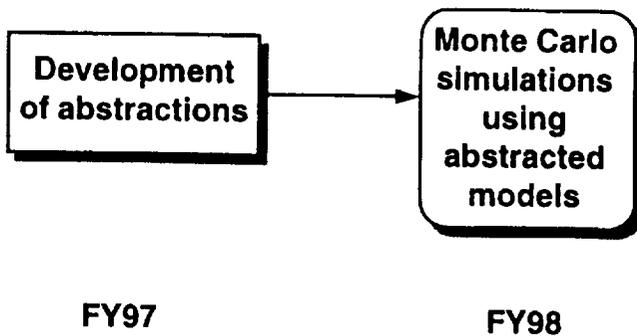
- Sensitivity analyses
 - Multiple conceptual models
 - How much discretization is required?
 - Does the abstraction represent the process model?
- What will be the result?
 - Response surfaces
 - Simplified process models
- What type of abstraction is acceptable for TSPA?
 - lookup tables or libraries of results
 - functional form of results
 - other realizations (e.g., dimensionality reduction, limited coupling, etc.)

Criticality Workshop JAM 3/16/97 p. 12

Workshop Process



Two Stages of TSPA-VA Modeling



CRS Quality Workshop JAM 5/16/97, p. 24

Goals of Abstraction/Testing Workshop

- **Identification of Issues**: Identify and group the important issues with respect to *long-term performance*.
- **Prioritization of Issues**: Prioritize the issues as to which are most important to address in the abstraction proposals.
- **Develop Abstraction Plan**:
 - abstraction should produce reasonably accurate “bounding” behavior.
 - abstraction should be computationally efficient
 - heterogeneity and variability properly incorporated
 - spatial-temporal discretization adequately represented

Criticality Workshop JAM.5/1997, p. 28

Goals of Abstraction/Testing Workshop

- **Treatment of Uncertainty**: Ensure that appropriate parameter and behavioral uncertainty is included in abstractions; discuss how to quantify.
- **Develop Testing Methodology**: How to validate abstraction, e.g., against complex model.
- **Coupling of Abstraction**: How to couple to abstractions from other workshops.
- **Scheduling/resources**: How to mesh with existing workscopes.

Criticality Workshop JAM.5/1997, p. 28

REPOSITORY SUBSURFACE DESIGN OVERVIEW

March 18, 1997

Dan McKenzie
Repository Subsurface Design Supervisor

REPOSITORY SUBSURFACE DESIGN OVERVIEW

- o The design Areal Mass Loading for VA is anticipated to be 85 MTU/acre
- o Only commercial SNF is counted in the AML determination, though all waste heat is accounted for
- o The layout provides for gravity drainage of water out of emplacement drifts
- o WPs will be emplaced in sequence from the exhaust end (far end) of the drift out to the entrance. If removed, they would be taken, again in sequence, last in - first out. [Carry-over not anticipated, nor is it precluded.]

REPOSITORY SUBSURFACE DESIGN OVERVIEW

(Continued)

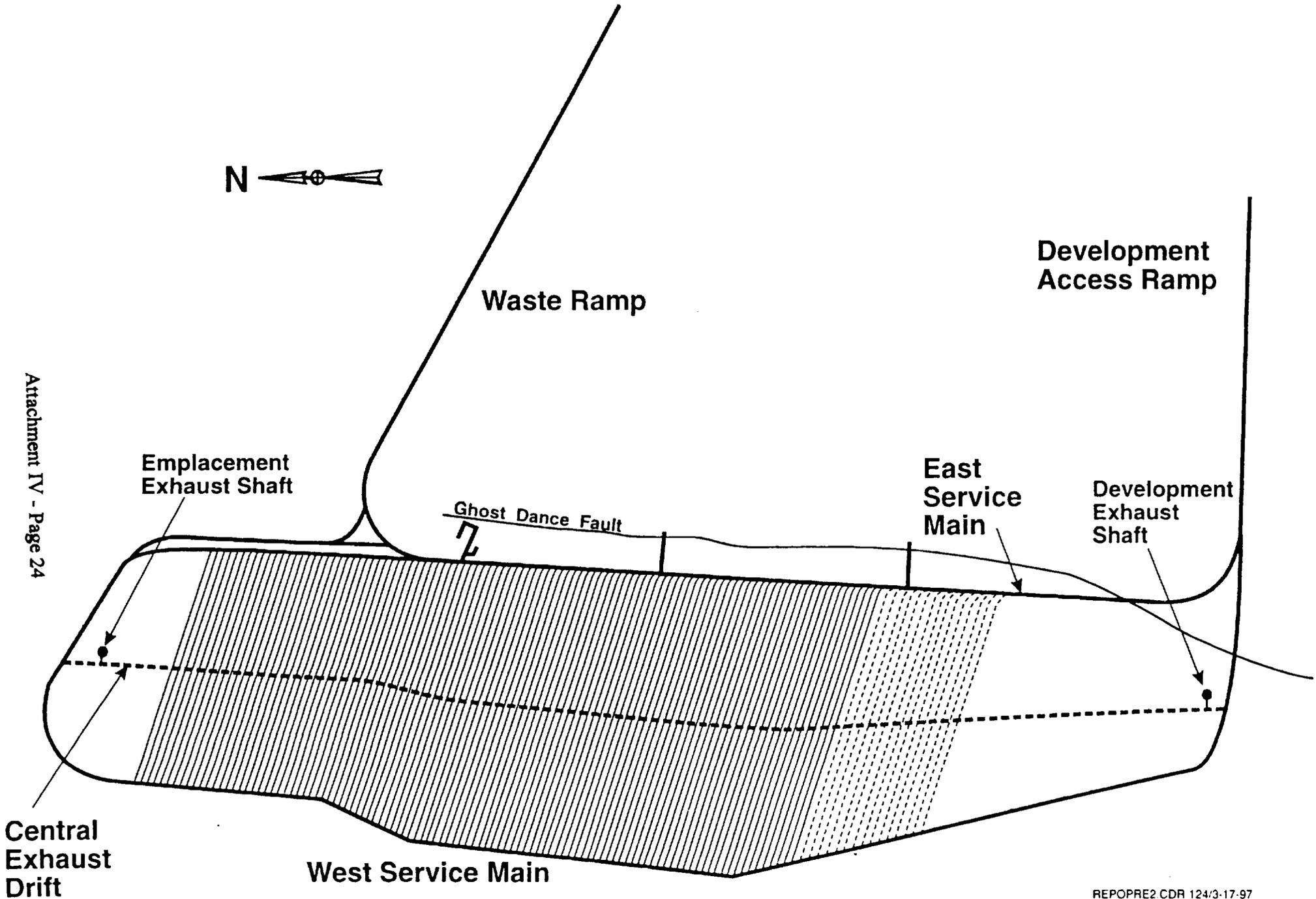
- o It is assumed in the subsurface design is that there are no emplacement limitations regarding criticality. That is, any package can be placed adjacent to any other package with no criticality concerns
- o Emplacement drift spacing for VA is anticipated to be 28 meters (on centers)
- o Waste Packages will be emplaced center in-drift on pedestals
- o The closest WP spacing is assumed to be 1 meter (end-to-end) to allow space for handling

REPOSITORY SUBSURFACE DESIGN OVERVIEW

(Continued)

- o Nominal WP spacing between large CSNF packages should range from 13 to 16 meters (center-to-center)
- o Emplacement drift diameter (OD) currently estimated at 5.5 meters
- o A pre-cast concrete liner is tentatively planned. The liner would be a nominal 200 mm thick, leaving an inside drift diameter of approximately 5.1 meters. Options are also being maintained for cast-in-place concrete, and steel liners.

Preliminary Repository Layout



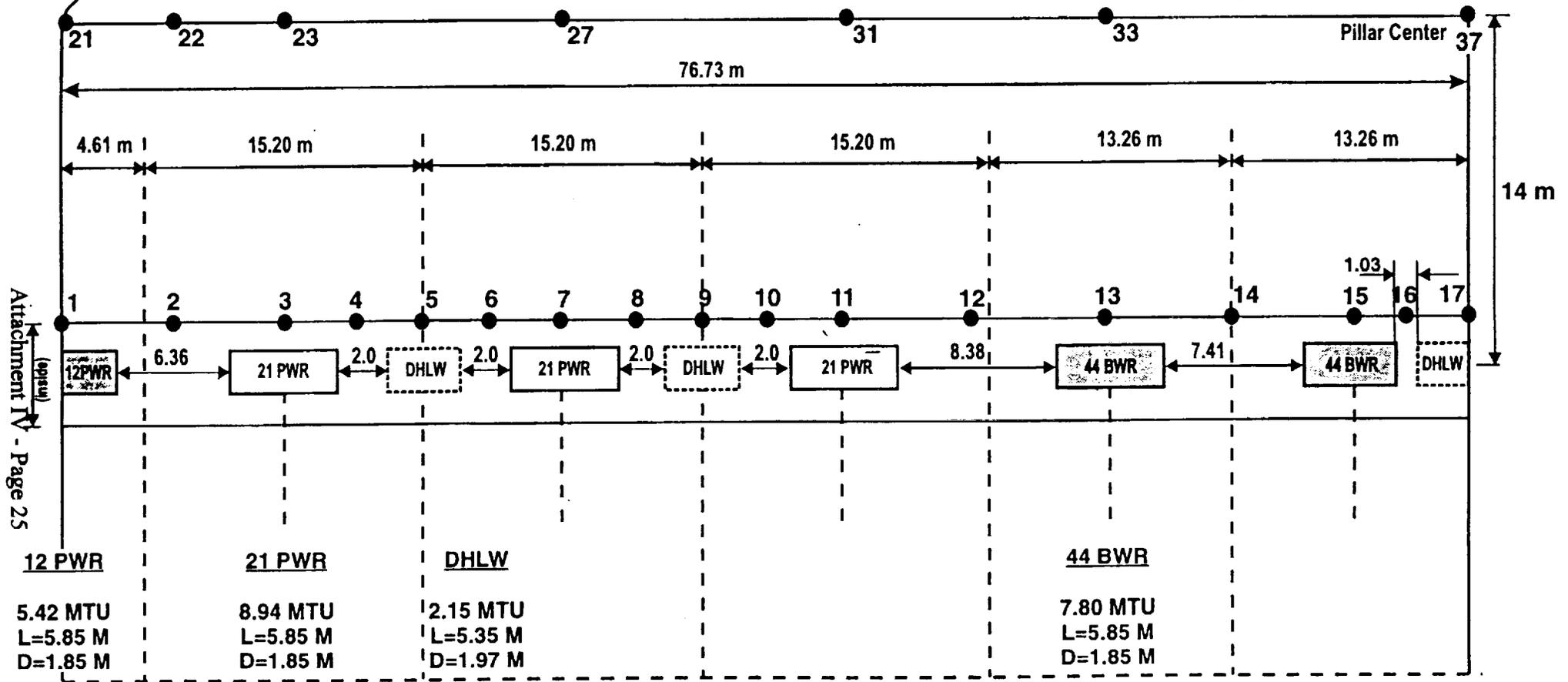
Attachment IV - Page 24

A Typical Emplacement Drift Segment

85 MTU/acre (CSNF)

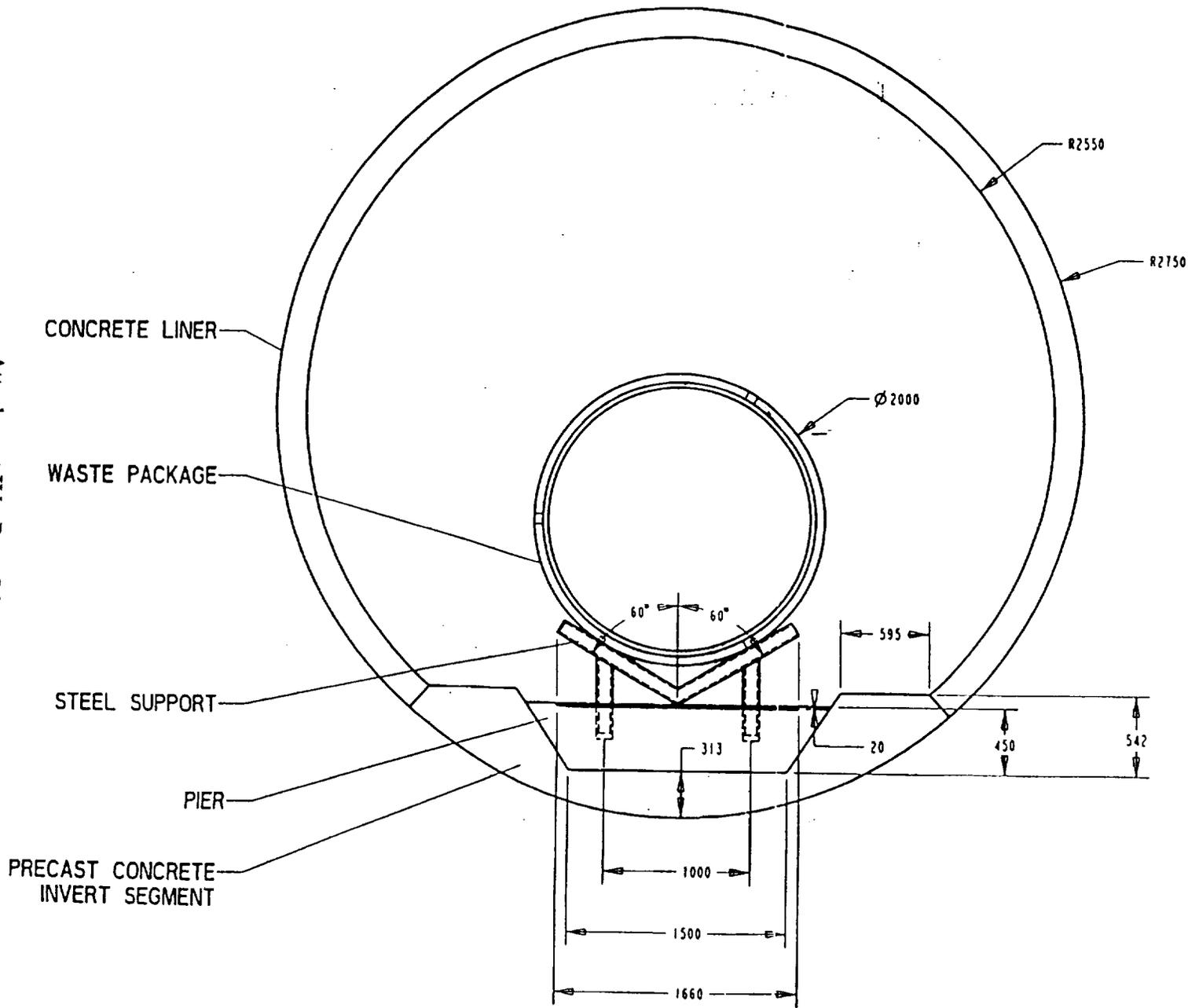
Drift Spacing: 28 m

3 21 PWRs
2 44 PWRs
0.5 12 PWRs
2.5 DHLW
Total 8 WPs
(see note Below)



Note:	44 BWR	21 PWR	12 PWR	DHLW	Total
Actual # of WP	2859	4137	683	3259	10938
(% of Total)	(26.14%)	(37.82%)	(6.24%)	(29.89%)	(100.00%)
Representing WP	2	3	0.5	2.5	8
(% of Total)	(25.00%)	(37.50%)	(6.25%)	(31.25%)	(100.00%)

Attachment IV - Page 25



**Civilian Radioactive Waste
Management System**

Management & Operating
Contractor

TRW

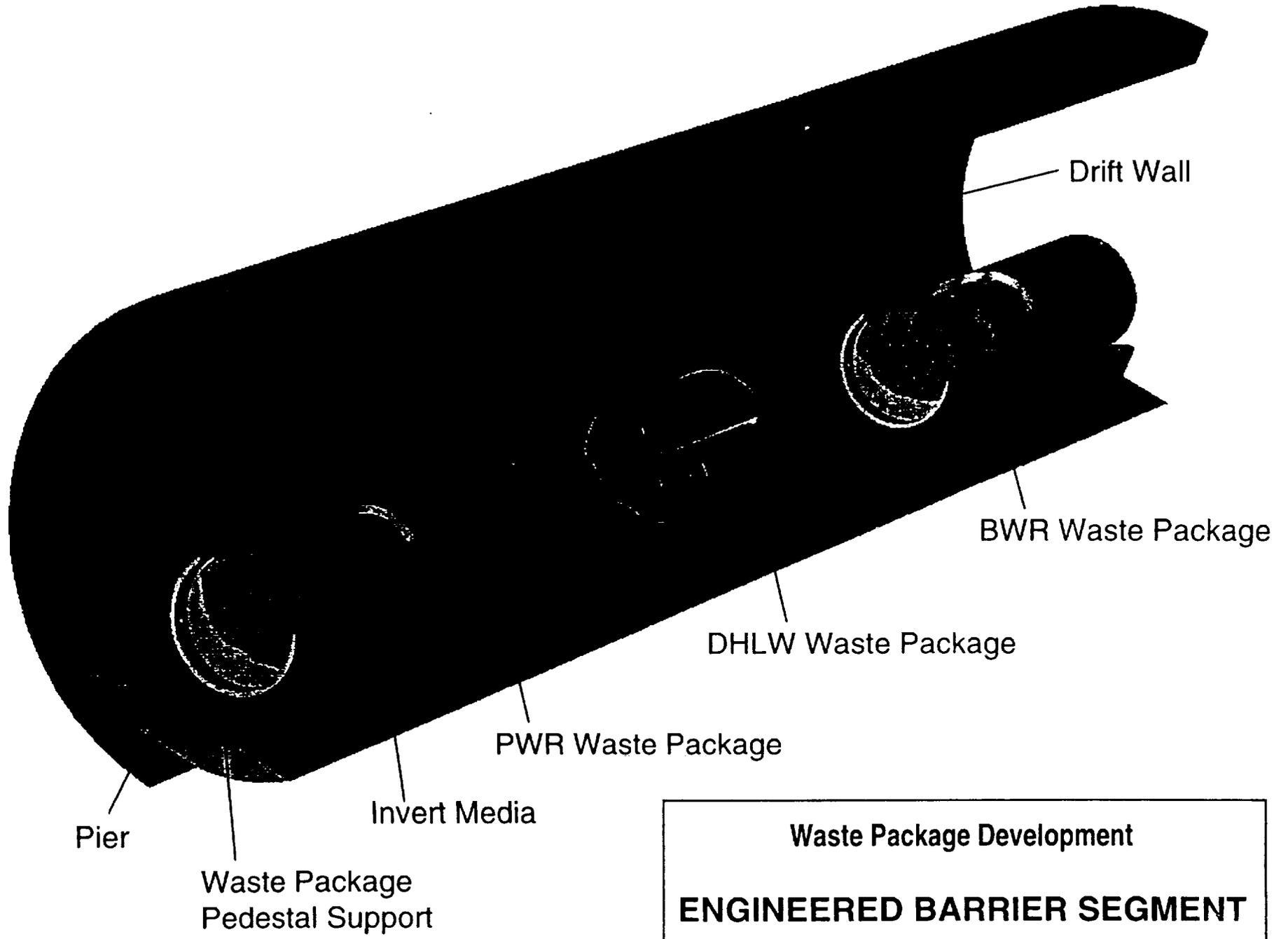
TRW Environmental Safety
Systems Inc.

ENGINEERED BARRIER SEGMENT DESIGN CONCEPTS

Presented By: Thomas W. Doering

Manager of Design, Waste Package Development

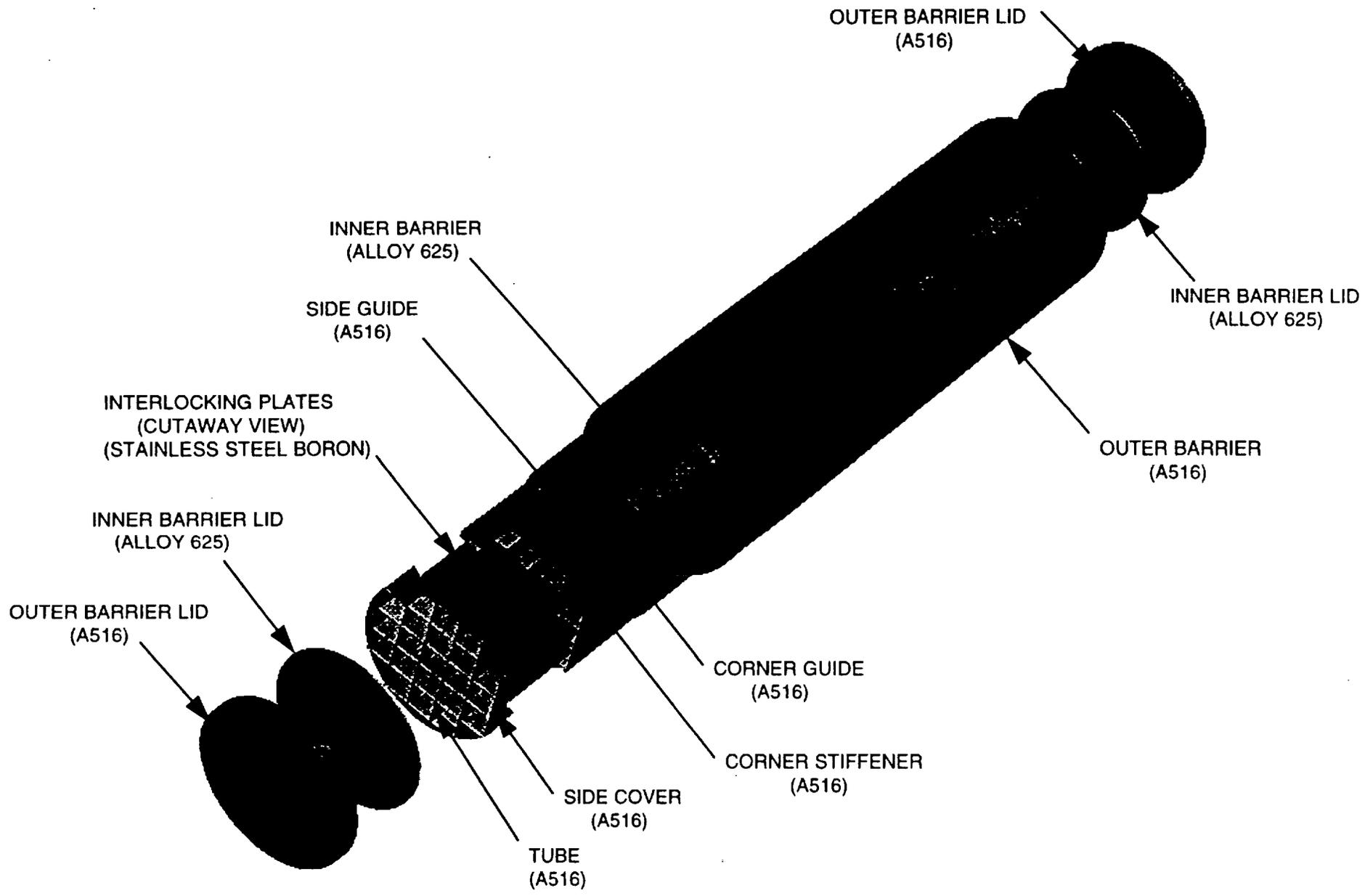
March 1997



Waste Package Development
ENGINEERED BARRIER SEGMENT

Engineered Barrier Segment

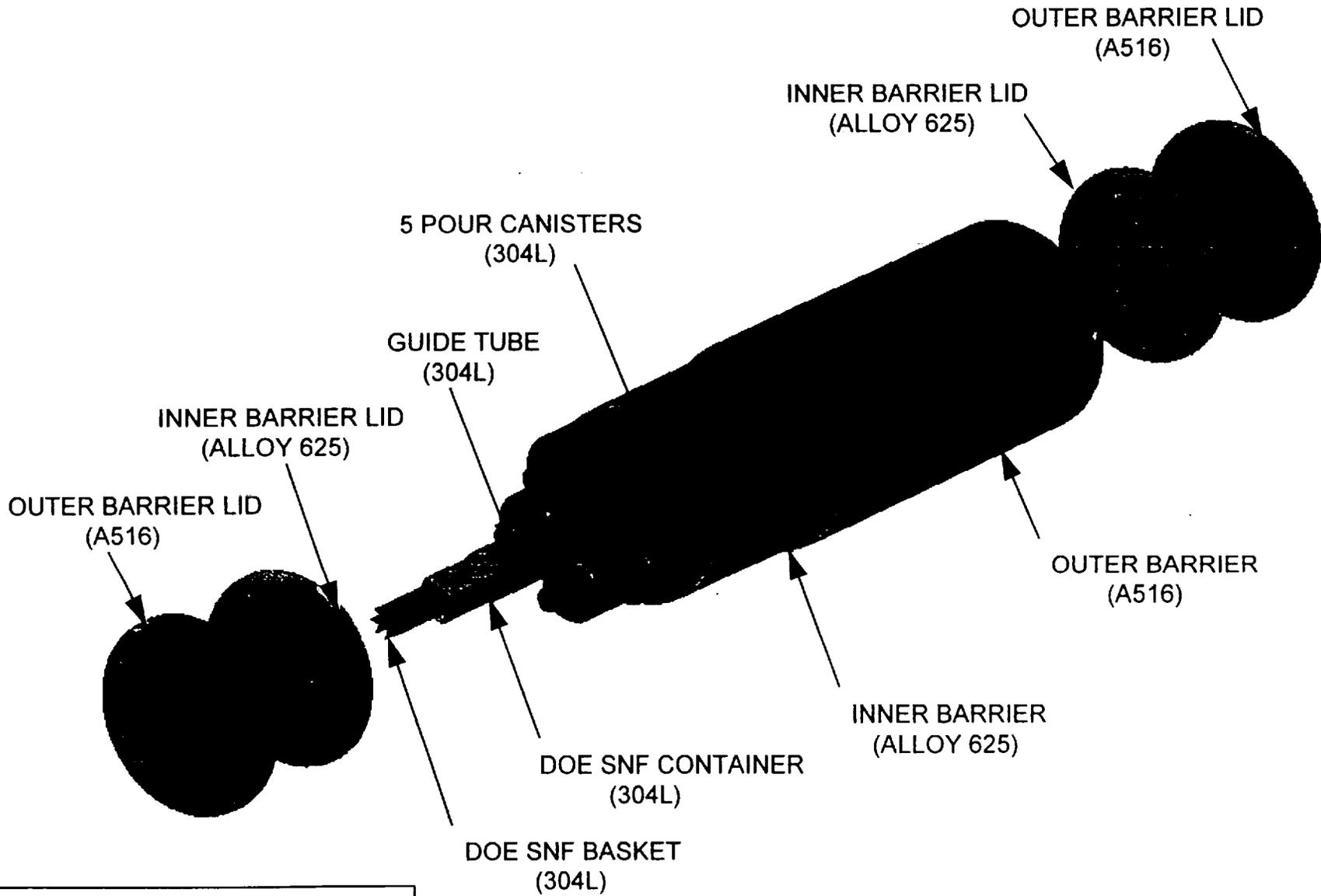
- Waste Package Design:
 - Uncanistered Waste Container
 - Canistered Waste Container
 - Defense High Level Waste (DHLW)- Waste Container
 - Co-Disposal DHLW - Waste Container
- EB Segment Additional Barriers
- Waste Package Support System



21 PWR UCF Waste Container

21-PWR Waste Container

- Geometry Description:
 - 21 PWR Uncanistered SNF Container (UCF)
 - 21 Fuel Assemblies/package
 - 21 Tubes: A516
 - Criticality Control Plates: SS-Boron (316B6A)
 - Inner Barrier: 20 mm - of Alloy 625
 - Outer Barrier: 100 mm of - A 516



LENGTH = 3890 mm
DIAMETER = 2070 mm
TARE WEIGHT = 36,429 kg
LOADED WEIGHT = 47,339 kg
EXCLUDES DOE SNF, BASKET,
CONTAINER , AND GUIDE TUBE

**Waste Package Development
DHLW/DOE SNF WASTE CONTAINER**

DHLW - Waste Container

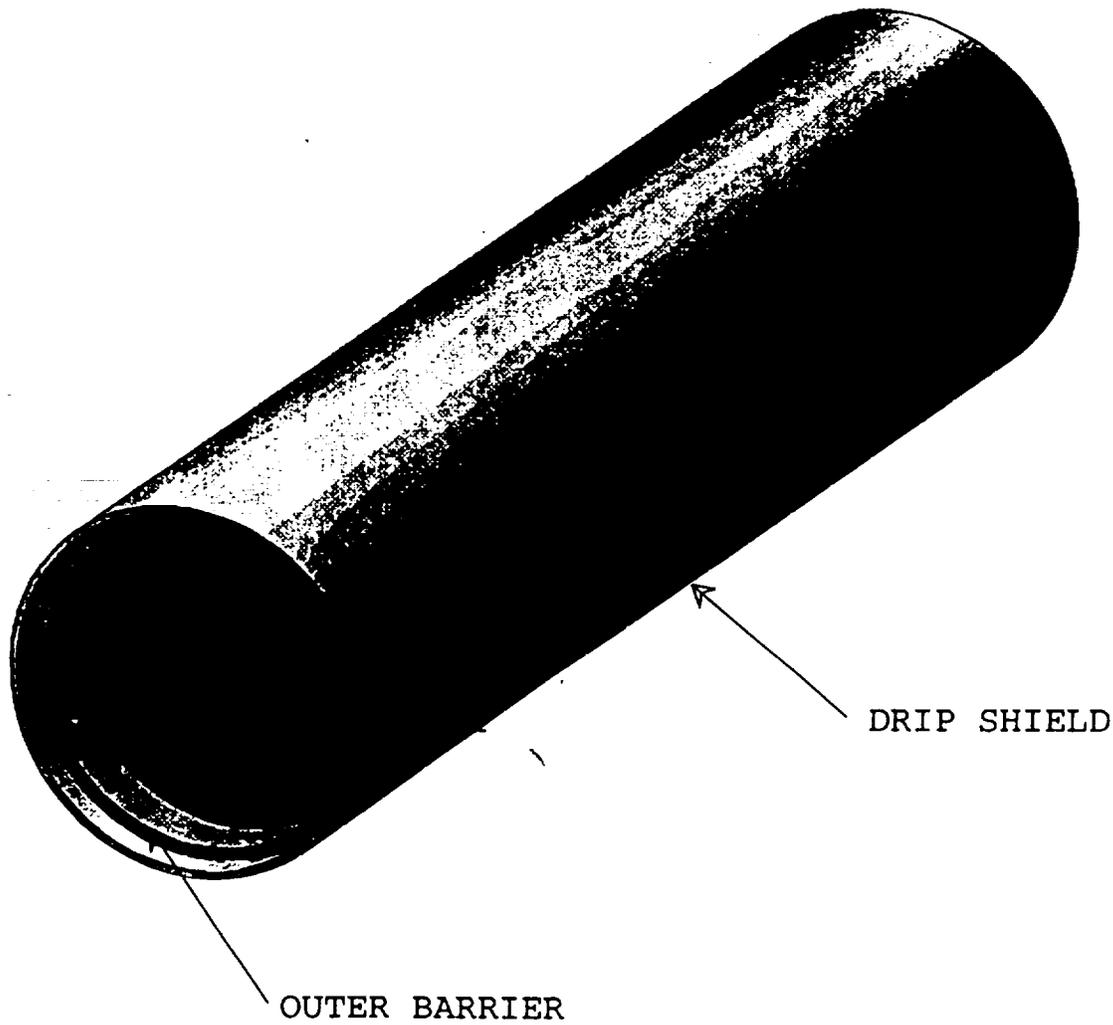
- Geometry Description:
 - DHLW - Waste Container
 - 5 Glass Pour Canisters/Package
 - Pour canister support: A 516
 - Criticality Control Plates: N/A
 - Inner Barrier: 20 mm - of Alloy 625
 - Outer Barrier: 100 mm of - A 516
 - Co-Disposal option: Addition of canistered DOE SNF in center region.

Additional Barrier

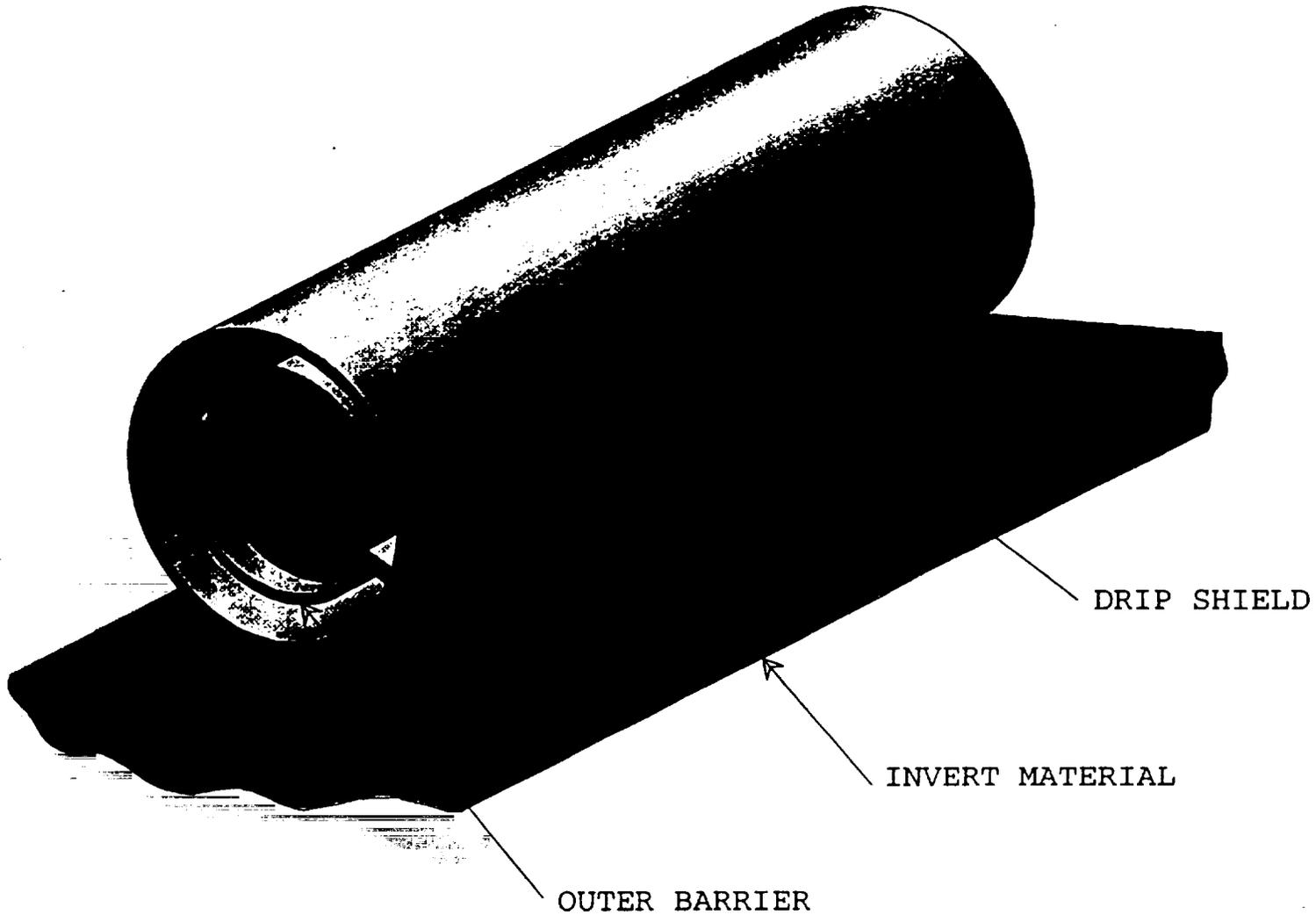
- Backfill
 - Single layer
 - Multi layer
 - Different rock types
- Drip Shield
 - Integral to waste container
 - Separate to waste container

Additional Barriers

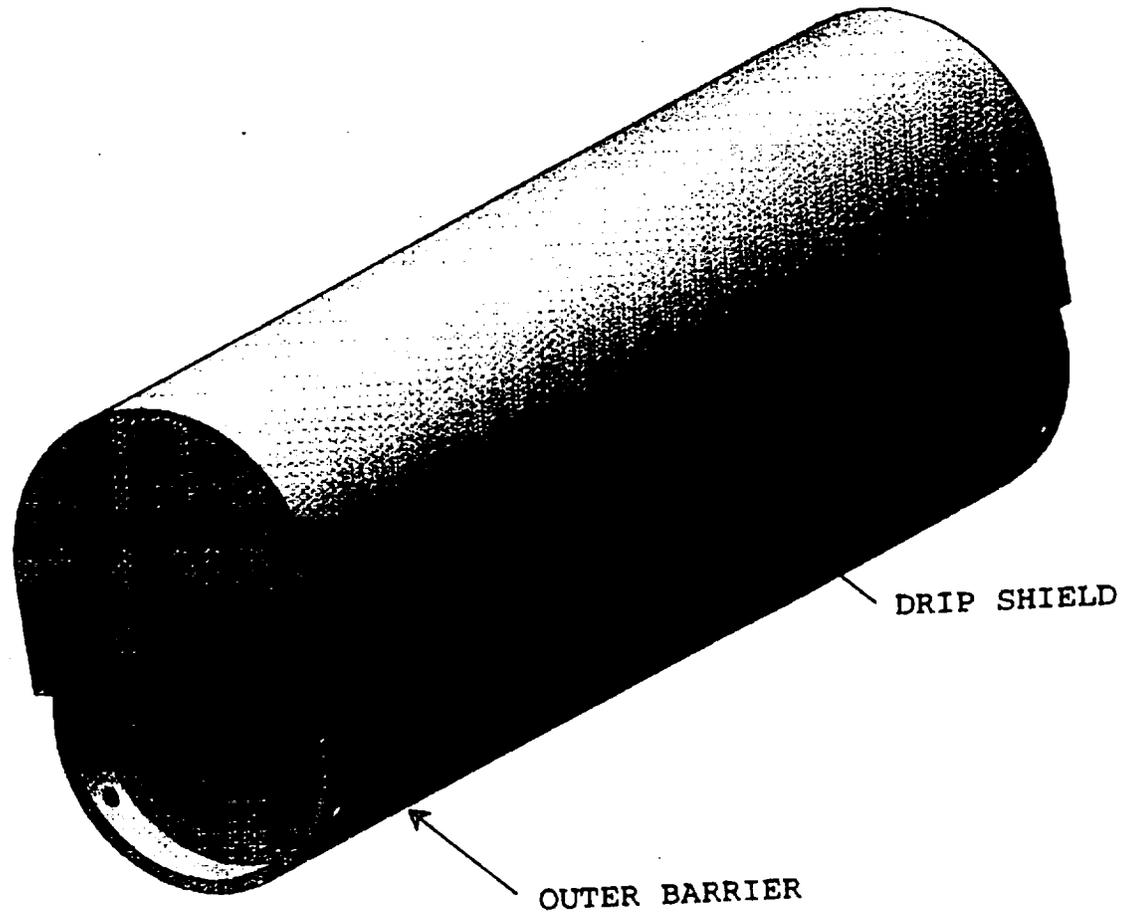
- Function:
 - Minimize the moisture contact
 - Above the waste container
 - Back fill
 - Drip Shield
 - Below the waste container
 - Invert material



DRIP SHIELD
ADDITIONAL METALIC/CERAMIC OUTER BARRIER



BUNKER DRIP SHIELD
TRANSPORTABLE

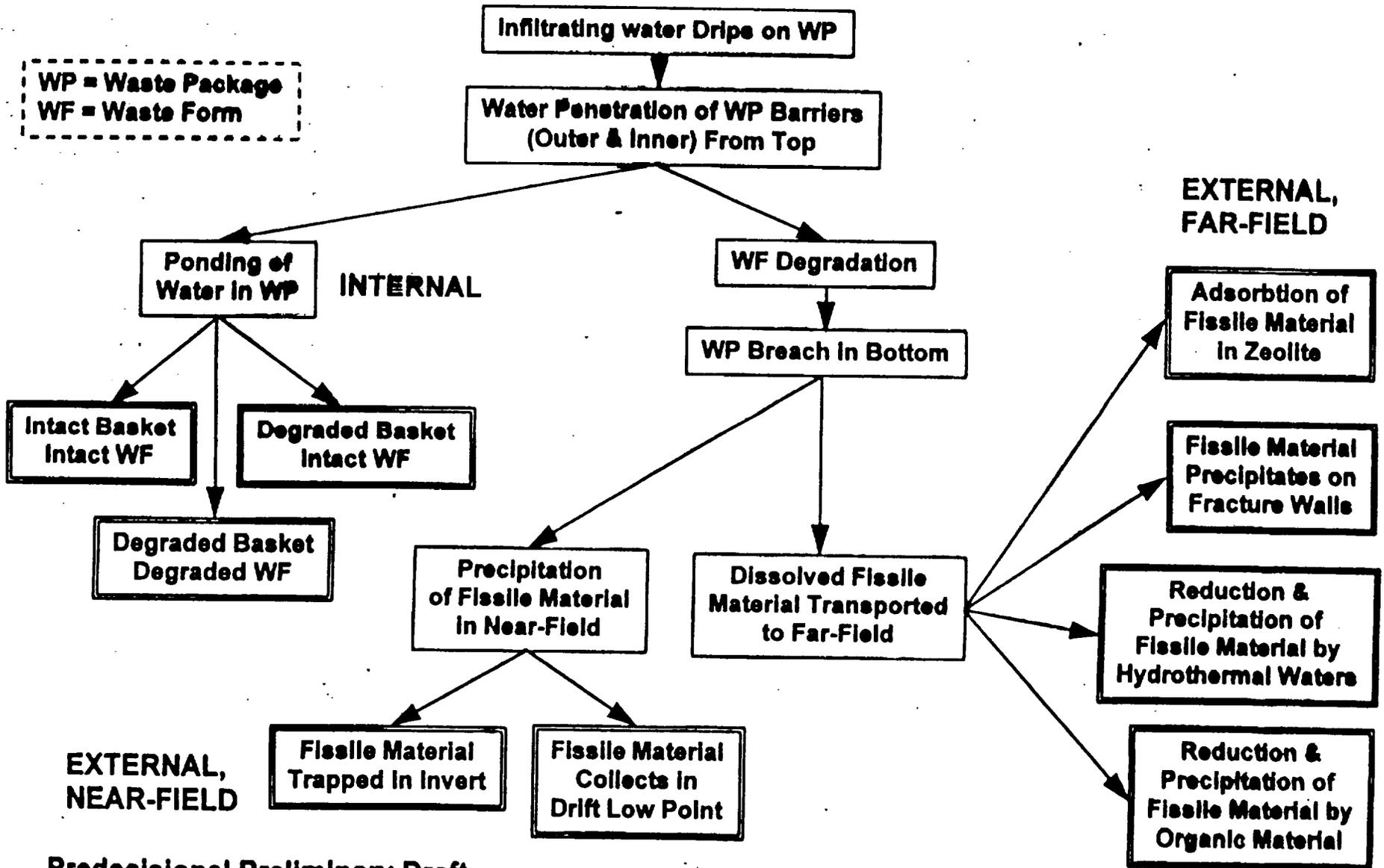


WASTE PACKAGE TUBE DESIGN
(21-BWR) WITH DRIP SHIELD

Post-Closure Criticality: System and Process Considerations

Peter Gottlieb
CRWMS M&O
Waste Package Development
3/18/97

Flowchart Defining Criticality Scenarios/Configurations

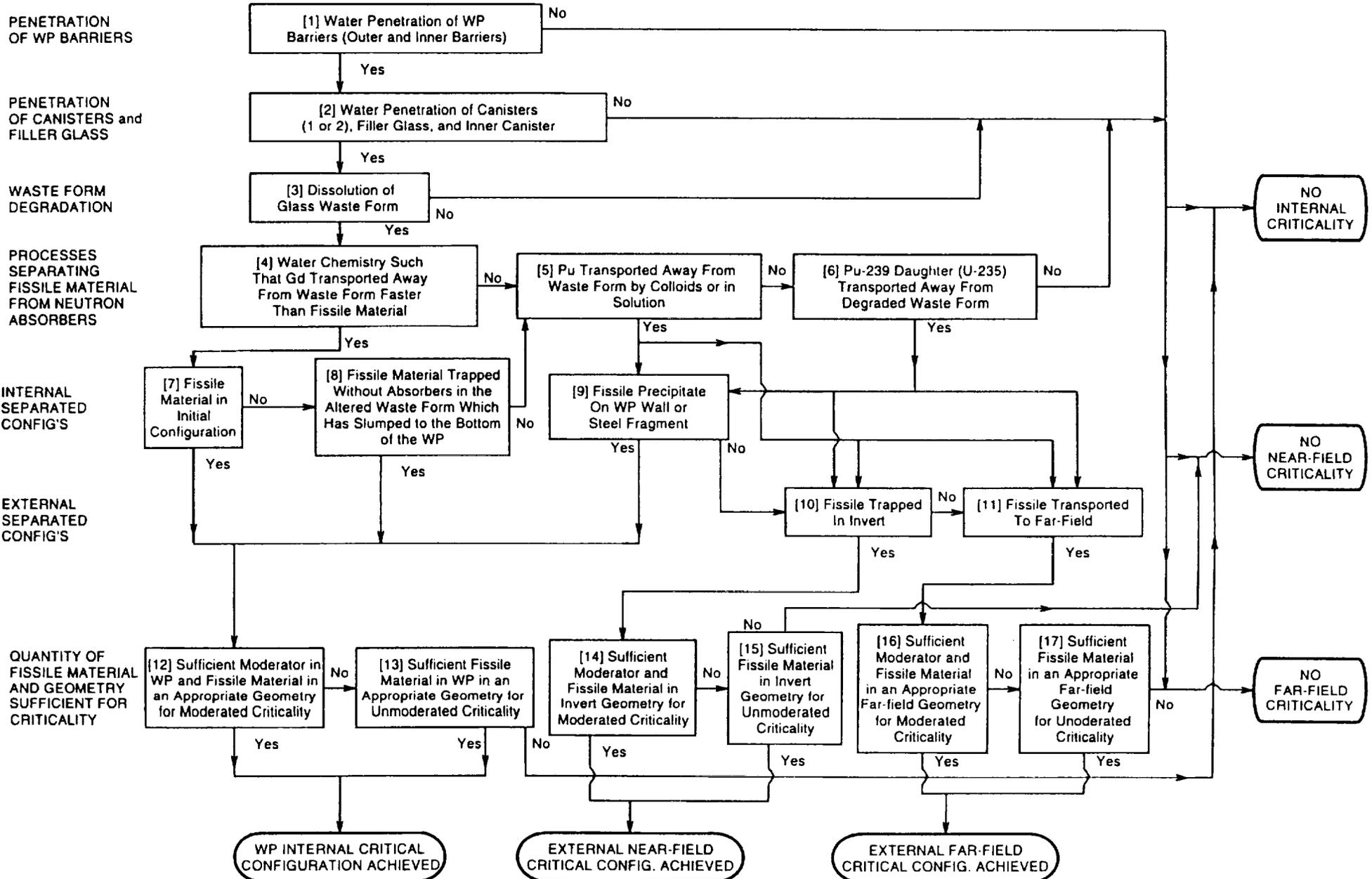


Attachment IV - Page 40

Predecisional Preliminary Draft

LV.WPD.PG.10/99.NRC/E

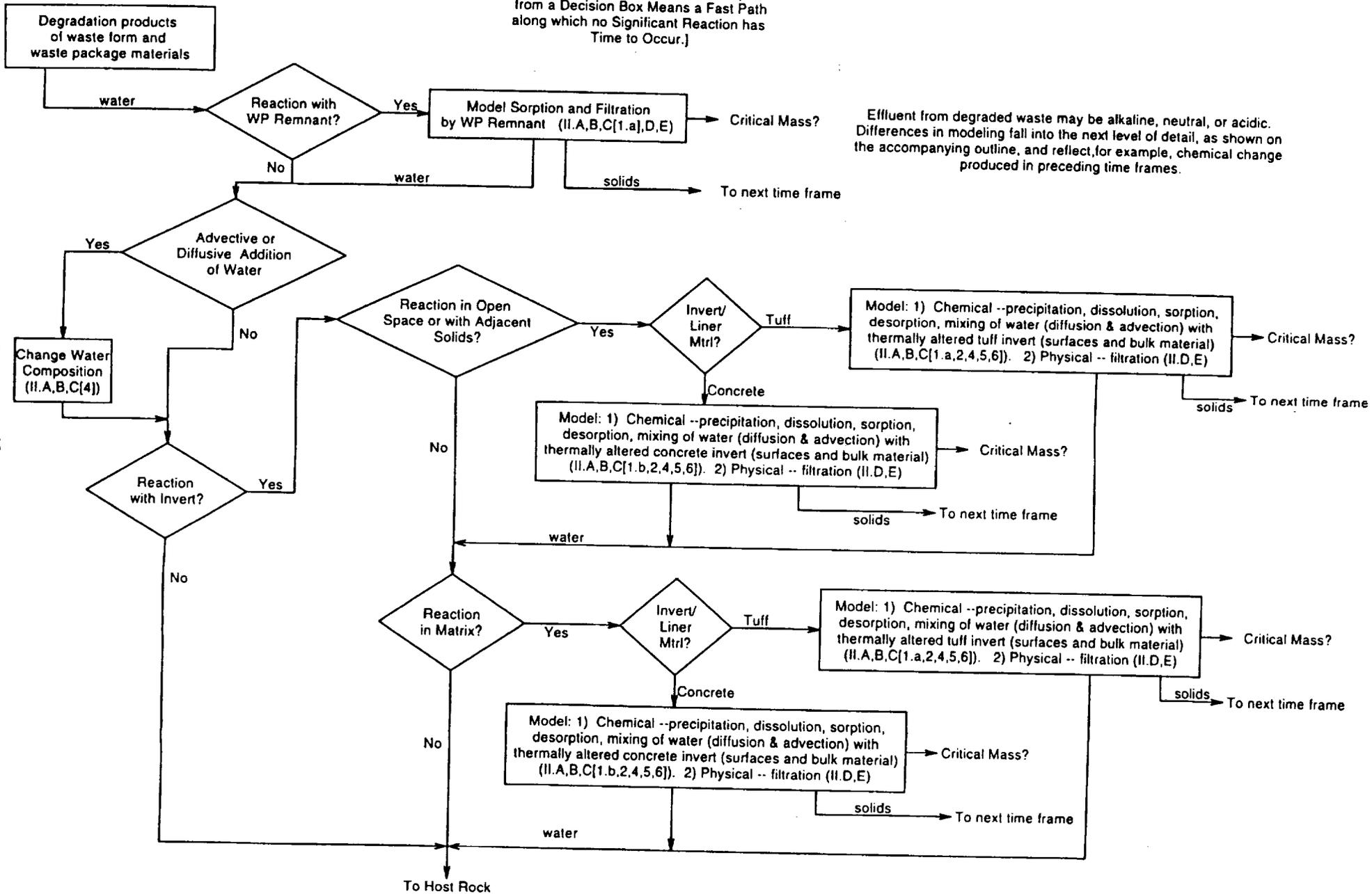
SYSTEM PERSPECTIVE OF EVENT/PROCESS SEQUENCES WHICH COULD LEAD TO CRITICALITY: APPLIED TO THE IMMOBILIZED PU WASTE FORM



Attachment IV - Page 41

FISSILE TRANSPORT LOGIC
Corrosion Products and Invert

[Except for Mixing of Waters, "No" path from a Decision Box Means a Fast Path along which no Significant Reaction has Time to Occur.]



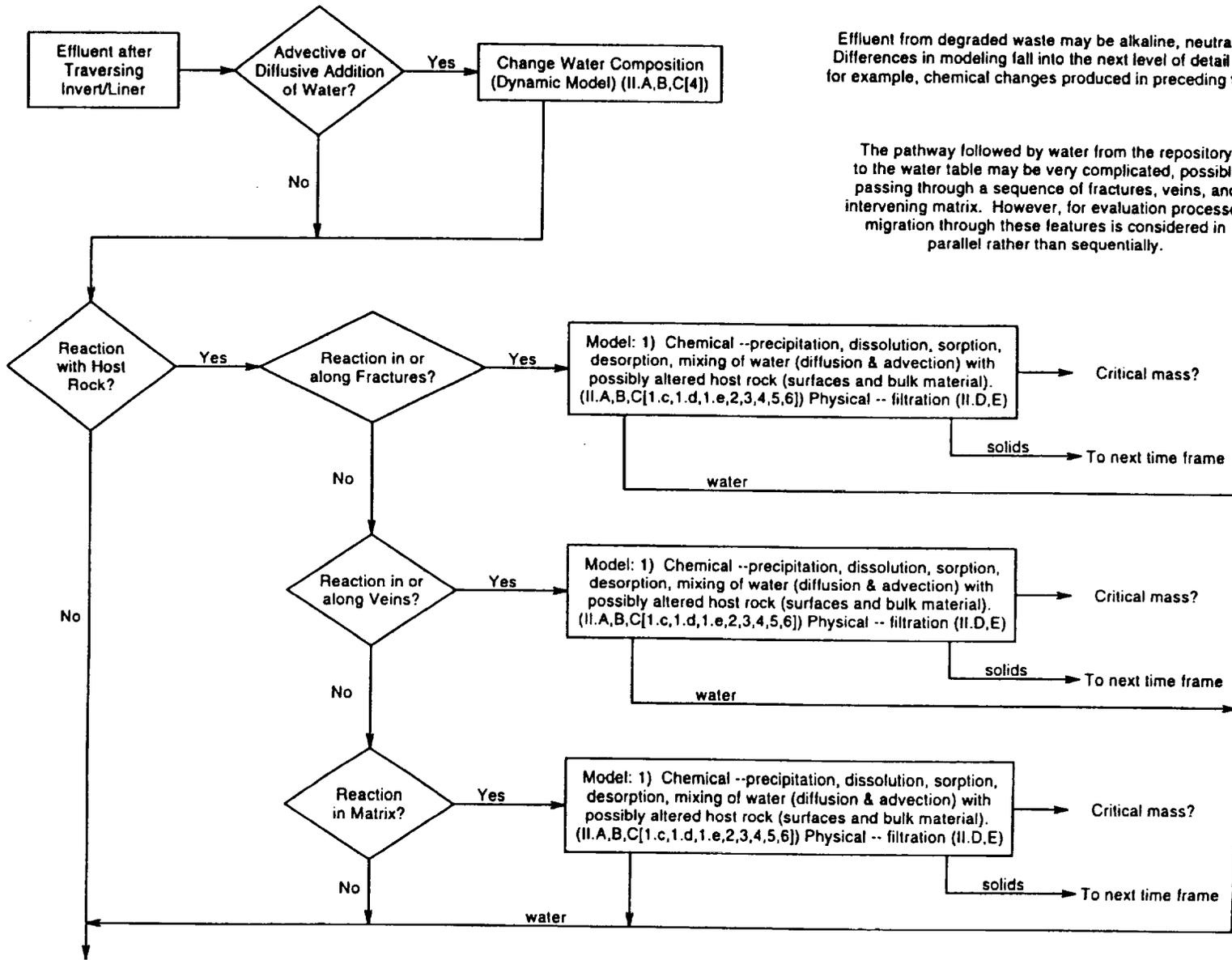
FISSILE TRANSPORT LOGIC
Host Rock*

[Except for Mixing of Waters, "No" path from a Decision Box Means a Fast Path along which no Significant Reaction has Time to Occur.]

* The same logic applies also to the underlying vitrophyre and Calico Hills

Effluent from degraded waste may be alkaline, neutral, or acidic. Differences in modeling fall into the next level of detail and reflect, for example, chemical changes produced in preceding time frames.

The pathway followed by water from the repository to the water table may be very complicated, possibly passing through a sequence of fractures, veins, and intervening matrix. However, for evaluation processes migration through these features is considered in parallel rather than sequentially.



	Compo.	Fissile bearing form	Environment/Models
Preclosure Internal	<ul style="list-style-type: none"> WP loaded with DBF and flooded (absorbers intact) Basket collapse from structural design basis event (if possible) Misloading of assembly types which exceeds criticality design basis 	<ul style="list-style-type: none"> Fissile content (U and Pu) Burnup credit (commercial SNF) <ul style="list-style-type: none"> Reduced fissile content Fission product absorbers Actinide absorbers 	<ul style="list-style-type: none"> Neutron absorber in basket (for SNF) External environment determined from DBE analysis <ul style="list-style-type: none"> Deterministic: design basis events (freq > 10⁻⁶) No significant degradation/corrosion
Postclosure Internal	<p>Commercial SNF:</p> <ul style="list-style-type: none"> Intact basket, intact fuel (not critical) Basket mostly corroded; iron oxide remaining in WP, but most B removed; intact fuel Complete basket collapse with intact assemblies touching; most iron oxide remaining; little-to-no boron remaining; intact fuel. Completely degraded basket and degraded waste form; most iron oxide remaining 	<ul style="list-style-type: none"> Same initial composition as preclosure. Degradation components precipitate/collect in various locations <ul style="list-style-type: none"> Fissile elements Neutron absorbers 	<ul style="list-style-type: none"> WP breached and containing sufficient water for moderation. Corrosion of WP components consistent with PA models. Environmental parameters such as water drip rate, # WPs contacted, humidity, temperature, water chemistry consistent with TSPA.
	<p>DOE SNF (Co-disposed w/ DHLW), similar to commercial SNF with the following exceptions:</p> <ul style="list-style-type: none"> SNF may degrade before the basket (particulate release) Glass from co-disposal may enhance clay formation, which may attract/concentrate fissile elements and water Possibility of rapid insertion induced by seismic event? Rubble pile (mainly for co-disposed WFs) 	<ul style="list-style-type: none"> Variety of fuel types leads to range of initial compositions. Primary analysis of extreme and/or bounding cases. Many cases of high enriched SNF (HEU) 	<ul style="list-style-type: none"> Corrosion of WP components consistent with PA models. Environmental parameters consistent with TSPA.
Postclosure External Near-field	<p>Fissile/moderator collection locations:</p> <ul style="list-style-type: none"> Fractures in aggregate/gravel rock Voidspace between rock pieces Internal rock spaces (zeolites) Backfill or sand filter 	<ul style="list-style-type: none"> Physical/chemical forms of fissile encapsulation: particulates, colloids, elements in solution. HEU, LEU, Pu pH of solution modified by WP degradation products and engineering material environment 	<ul style="list-style-type: none"> Engineered materials surrounding waste pkg <ul style="list-style-type: none"> Zeolites naturally in crushed tuff invert Zeolites from transformed liner cement Particulates collected in voidspace and fractures Colloids collected in fractures and on surfaces
Postclosure External Far-field	<p>Fissile/moderator collection locations</p> <ul style="list-style-type: none"> Perched water Deposits in fractures Zeolites or lithophysal cavities Unsaturated vs saturated zones Very far field (e.g. Playa Lakes) <p>Geometry influencing processes</p> <ul style="list-style-type: none"> Dispersion (fracture or matrix) Focusing by fractures and impermeabilities Fast paths 	<ul style="list-style-type: none"> HEU, LEU, Pu pH and other solution parameters further modified by geochemistry 	<ul style="list-style-type: none"> Environmental parameters and process selections consistent with TSPA. Plume dispersion and fracture focusing consistent with PA models Zeolite adsorption processes in CHn Geologic reducing zones (organic, other?) Reducing processes of hydrothermal waters Oxygen depleted water/zones (e.g. below water table)

ATTACHMENT V

Viewgraphs of Presentation for Issue Prioritization and Screening

R. Barnard: Post-Closure Criticality - Issues and Priorities

Post-Closure Criticality

Issues and Priorities

R. W. Barnard
Sandia National Laboratories
March 18, 1997



Impetus for Addressing Post-Closure Criticality

- Repository total-system containment requirements
 - what is the impact of criticality on total-system performance (remember 40 CFR 191?)
- NRC design criteria for a geologic repository
 - criticality control is specified in 10 CFR 60.113(h)



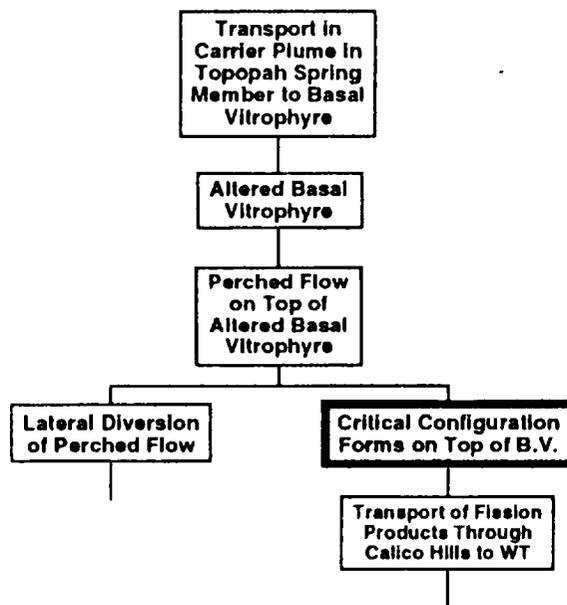
Issues Development

- Identification of Scenarios
 - in-package criticality
 - near-field criticality
 - Far-Field Criticality
- Prior PA and WP development work
 - "Strawman" proposal
- Workshop
 - identification of sub-issues
 - review and prioritization of sub-issues



3

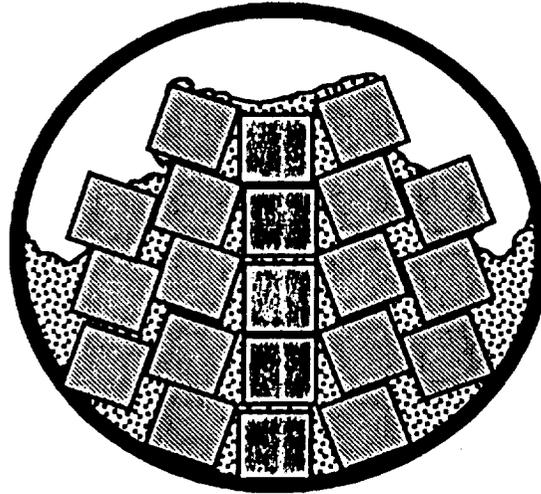
Far-Field Criticality



4

In-Package Criticality Issues

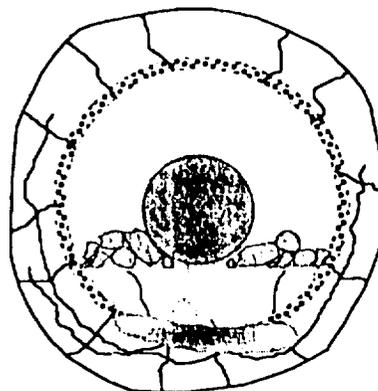
- Processes that can lead to critical configurations for various degrees of degradation of:
 - internal basket
 - fuel assemblies



5

Near-Field Criticality Issues

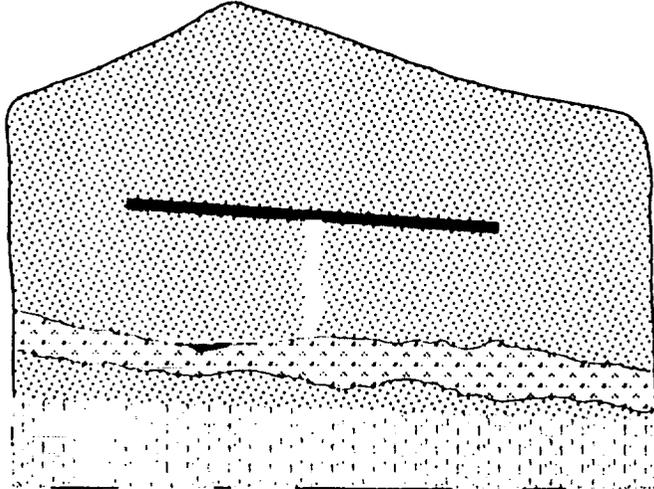
- Process that can lead to critical configurations in the drift or invert
- Environmental conditions
- Types and amounts of waste
- Types of critical configurations



6

Far-Field Criticality

- Processes for criticality in Yucca Mountain tuff
- Processes for criticality elsewhere
- Environmental conditions
- Types of critical configurations



7

Issues Prioritization Process

- To rank issues, complete the following sentence:

In-Package Criticality Issue	Source-Term Inventory
To what degree does the Near-Field Criticality Issue affect	RN release rate
Far-Field Criticality Issue	Dose

Answer with:

5	"Extremely"
3	for "Moderately"
1	"Slightly"

For each table of participants, arrive at average or consensus values for each sub-Issue using the above criteria. Round the numbers to the above values. Total the values for each sub-Issue over the three criteria given above.



8

Performance-Related Criteria

- Source-Term Inventory
 - isotopic abundances
 - decay ages
 - physical form of radionuclides available for transport
 - chemical form of radionuclides available for transport
- Radionuclide release rate (independent of changes in inventory characteristics)
 - from EBS
 - distribution (temporal and spatial) of transport to water table and beyond
- Dose (at boundary of YM controlled area and/or at Franklin Lakes Playa)
 - peak magnitude
 - rate of rise
 - duration
 - time of first arrival



9

Summary

- Remember the PA perspective for this workshop:
 - When applying the criteria, emphasis should be on the magnitude/extent/impact of a potential criticality — not on whether it will happen
 - Sensitivity/Testing studies should be chosen for their impact on the overall TSPA results



10

ATTACHMENT VI

Viewgraphs of Panel Presentations and Tables of Issue Prioritization for Session I

- J. McNeish: Session I: Issues Discussion TSPA Perspective on In-Package Criticality Representation
- W. Davis: Disposal Criticality Workshop: Internal Criticality Analyses for Commercial SNF
- J. Massari: Internal Criticality Consequences (Source Term)
- C. Stockman: Most Likely Series of Events for Commercial Fuel
- E. Siegmann: Criticality in TSPA-VA
- Henry Loo/Paul Sentieri: TSPA-VA Disposal Criticality Abstraction/Testing Workshop
- R. Beyer: Concrete Reflection with PWR-1 Seed 2 Modules

Session I: Issues Discussion TSPA Perspective on In-Package Criticality Representation

Jerry McNeish
CRWMS M&O/INTERA (DE&S)

Criticality Abstraction Workshop
18 March 1997
Las Vegas, NV

B&W Federal Services
Duke Engineering & Services, Inc.
E. R. Johnson Associates, Inc.
Fluor Daniel, Inc.
Framatome Cogema Fuels
Integrated Resources Group
INTERA, Inc. (DE&S)

JK Research Associates, Inc.
Kiewit/Parsons Brinkerhoff
Lawrence Berkeley National Laboratory
Lawrence Livermore National Laboratory
Logicon RDA
Los Alamos National Laboratory
Mortenson-Krudean Corporation

SAIC
Sandia National Laboratories
TRW Environmental Safety Systems Inc.
Woodward-Clyde Federal Services
Winston & Strawn
Cooperating Federal Agency
U.S. Geological Survey

Outline of Presentation

- Previous Performance Assessment representation of in-package criticality
- Approach to represent in-package criticality in TSPA-VA
- Key issues and uncertainties

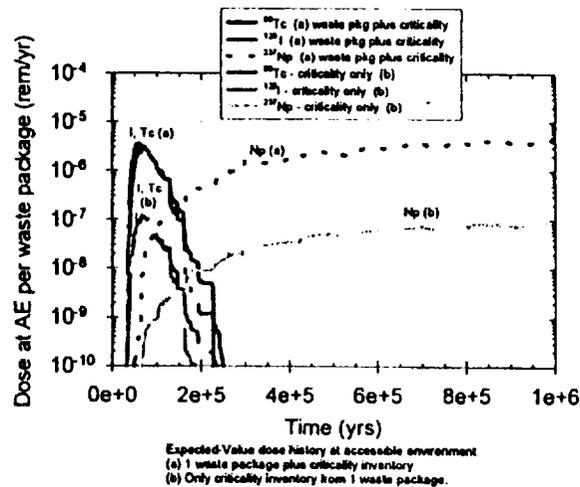
Example Performance Assessment Calculation

- Assumed a case from TSPA-1995 as the starting point
- Assumed steady-state internal criticality event in one waste package starting at 15,000 yrs and ending at 25,000 yrs
- Inventory due to the criticality increased 4% for ^{129}I and ^{99}Tc and 2% for ^{237}Np in the affected waste package
- This additional source term was included and repository performance (dose at AE) was evaluated

Civilian Radioactive Waste
Management System
Management & Operating
Contractor

Criticality JMM 3/19/97 p 5

Example TSPA Results: Consequence of Internal Criticality



Potential In-Package Criticality Abstractions for TSPA-VA

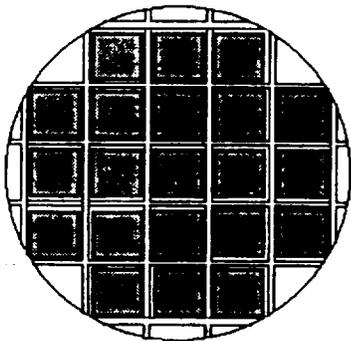
- **Develop set of scenarios which bound performance effects of internal criticality**
 - **Product: Key scenarios for TSPA-VA**
- **Evaluation of depleted uranium effect on criticality**
 - **Product: Factor by which to retard transport of ²³⁵U**
- **Evaluation of degradation/transport of absorbers from basket**
 - **Product: Response surface of rate of removal as f(percolation flux, WP degradation)**

Disposal Criticality Workshop: Internal Criticality Analyses for Commercial SNF

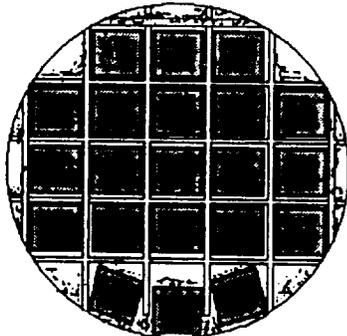
Wesley Davis

WP Degraded Internal Configurations (Schematic)

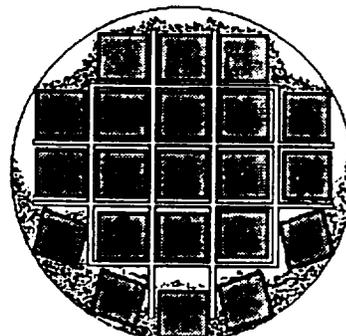
(all failure times based solely on general corrosion data and models and should be considered preliminary)



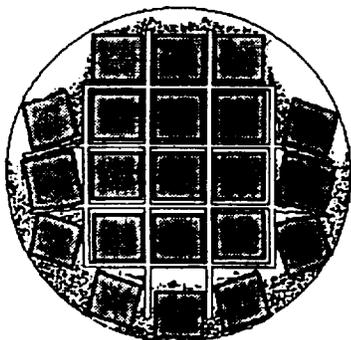
Initial Configuration



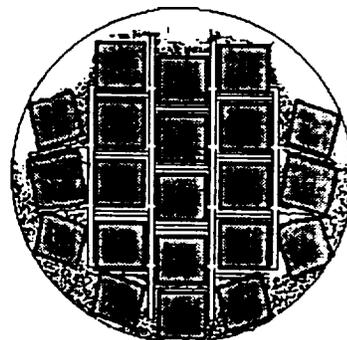
Side Guide Failure
60 to 340 years after WP breach



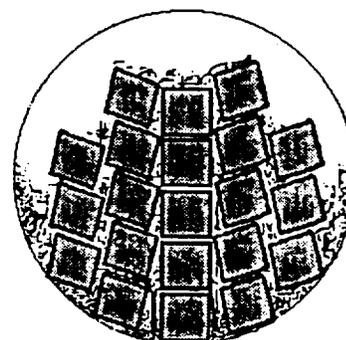
Corner Guide Failure
100 to 500 years after WP breach



Long Criticality Control Plates
Bend at Ends
2000 to 8500 years after WP breach



Complete Basket Collapse
2000 to 18000 years after WP breach
(remainder of plates still between assemblies)



Complete Basket Degradation
5700 to 24000 years after WP breach

Major Assumptions for Degraded Scenarios Involving Commercial SNF

- Design Basis Fuel - 3% Initial Enrichment, 20 GWD/MTU with Borated (1.6 wt%) SS Basket
- Carbon Steel will oxidize completely before significant corrosion of SS
- Basket Structure Collapsed by Removing Void Space and Trapping Remaining Plate Thickness Between Assemblies
- Fe_2O_3 will remain evenly distributed in and around assemblies
- No boron leaching from intact Borated SS
- Fuel Assemblies remain relatively intact
- Conservative Fuel Compositions Correspond to Secondary Peak (~10,000 years)

Scenarios Developed

- **Progressive Degradation of Borated SS Plate in Basket**
- **Basket Completely Degraded, Uniform Fe_2O_3 and Boron Distribution**
- **Basket Completely Degraded, Nonuniform Fe_2O_3 and Boron Distribution**
- **Assembly Collapse, Control Rod Effects and Partial Flooding of WP**

Progressive Degradation of SSB Plate in Basket

- **Approximately 33% of the void volume within the WP could be filled with Fe_2O_3 if all steel oxidized**

Indication of Relative Absorbing Effectiveness of Fe_2O_3 vs. Boron

- **Subcritical w/ 10% of Borated SS and 75% of Fe_2O_3 Evenly Distributed (No Boron in Fe_2O_3)**
- **Subcritical w/ 10% of Borated SS, 30% of Fe_2O_3 and 8% of Boron in solution**

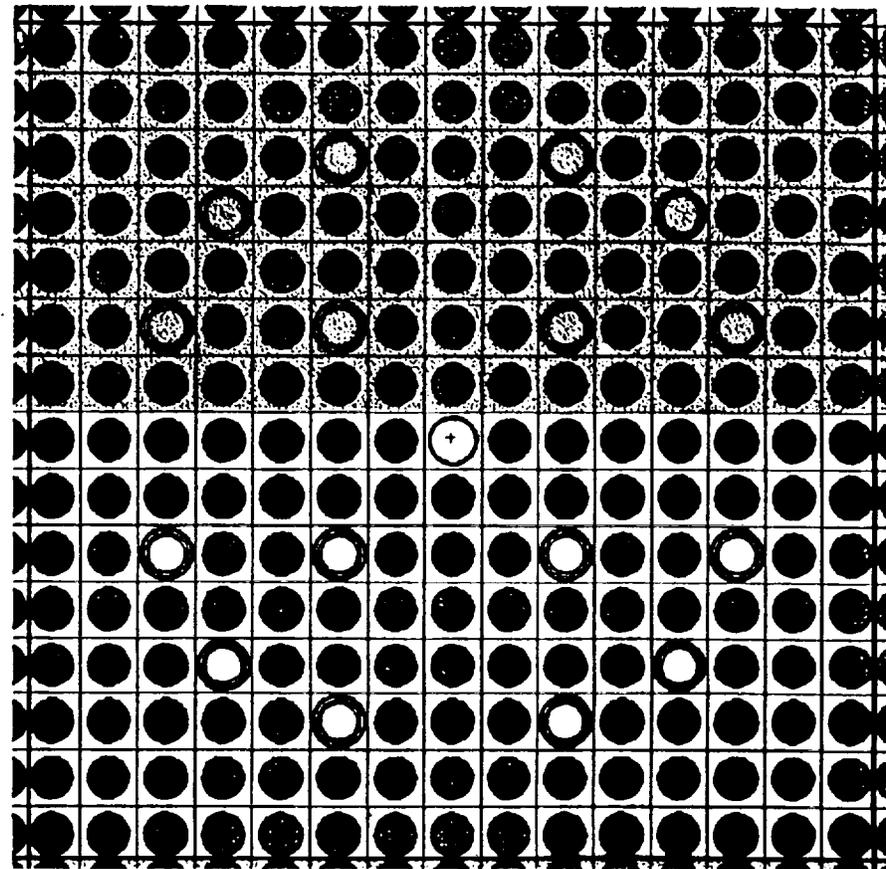
Basket Completely Degraded, Uniform Fe₂O₃ and B Distribution

**Indication of Relative Absorbing Effectiveness
of Fe₂O₃ vs. Boron**

- **Subcritical w/ 90% Fe₂O₃ and 6% Boron**
- **Subcritical w/ 60% Fe₂O₃ and 14% Boron**
- **Subcritical w/ 30% Fe₂O₃ and 18% Boron**

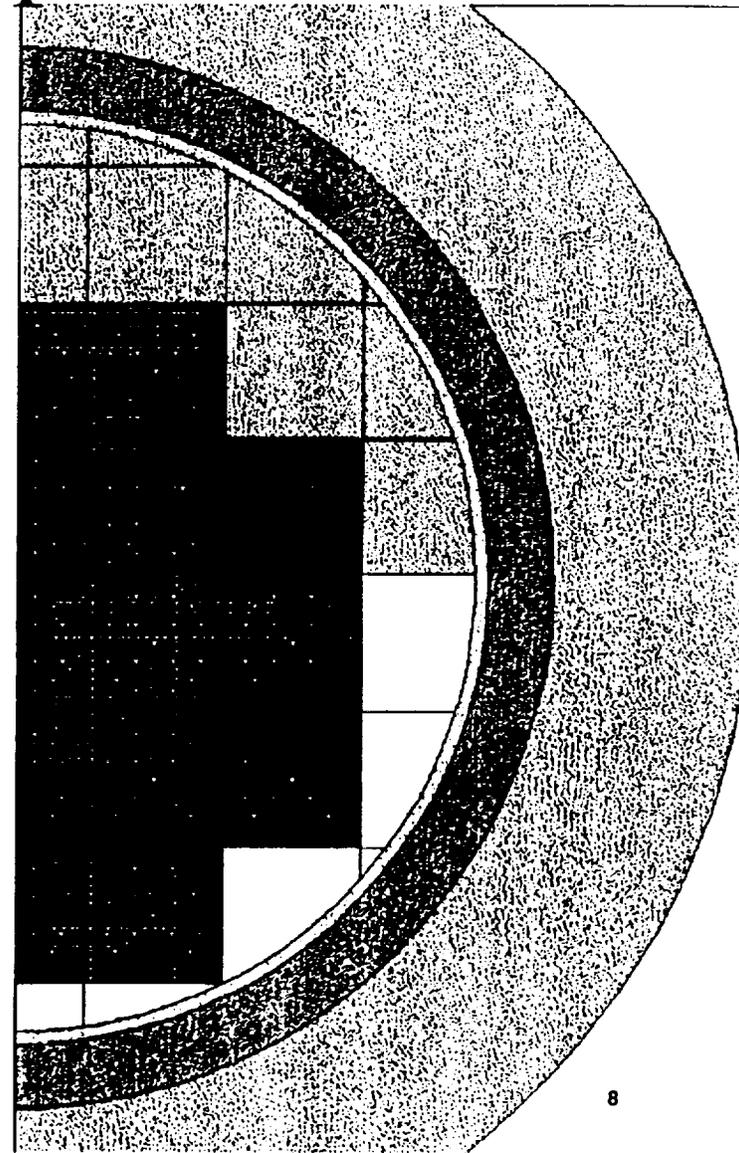
Sensitivity of k_{eff} to Distribution of Fe_2O_3 and Trapped Boron

- Nominal: Uniform Distribution within Fuel Assembly Void Space
- Variation: Stratification Within Assembly
- Extreme Stratification Results in a delta k_{eff} of .005



Sensitivity of k_{eff} to Distribution of Fe_2O_3 and Trapped Boron cont.

- Nominal: Uniform Distribution in Waste Package Void Space
- Variation: Stratification Within WP
- 1/3 - 2/3 Distribution of Fe_2O_3 w/ uniform B Results in No Change
- Extreme Stratification (0 - 1) w/ B Removed from the Upper 38% of Fuel Can Result in > 0.1 delta in k_{eff}



Assembly Collapse, Control Rod Effects and Partial Flooding of WP

- Collapse in One Dimension Results in about 2% decrease in k_{eff}
- Collapse in Two Dimensions Results in about 15% decrease in k_{eff}
- Subcritical w/ 9 to 10 B_4C control rods/assembly, no Fe_2O_3 and no Boron
- Critical w/ Lower Row plus 1/2 Second Row Flooded, no Fe_2O_3 and no Boron

PA CRITICALITY WORKSHOP

Internal Criticality Consequences (Source Term)

**Presented By
John Massari,
Waste Package Development, CRWMS M&O**

March 18, 1997

Configuration supporting a steady state internal WP criticality

- Steady State Conservative/Bounding of Transient Cycling

- First Step:

Find water temperature (T) where $m_{\text{evap}} = m_{\text{drip}}$

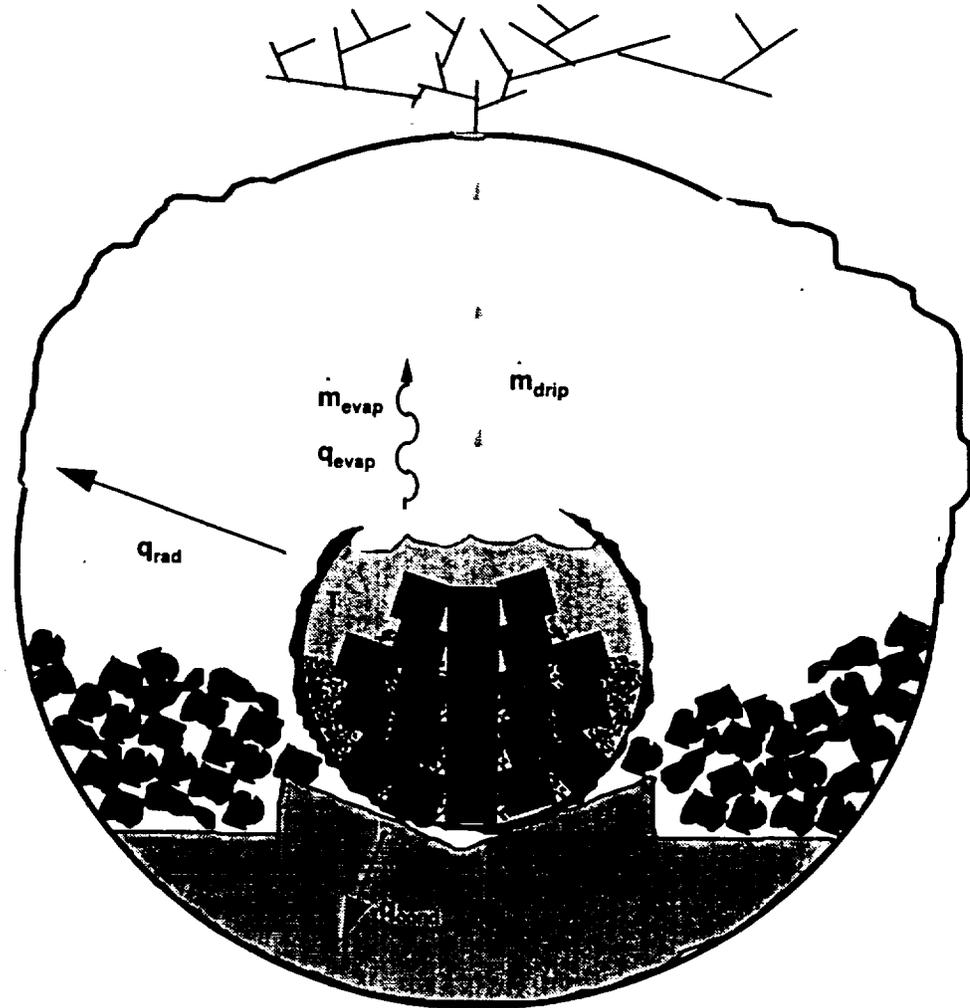
- max. m_{drip} from TSPA-95 = 191 liters/yr
- T = 57°C at 96% relative humidity
- Assumes no local recondensation of evaporating water

- Second Step:

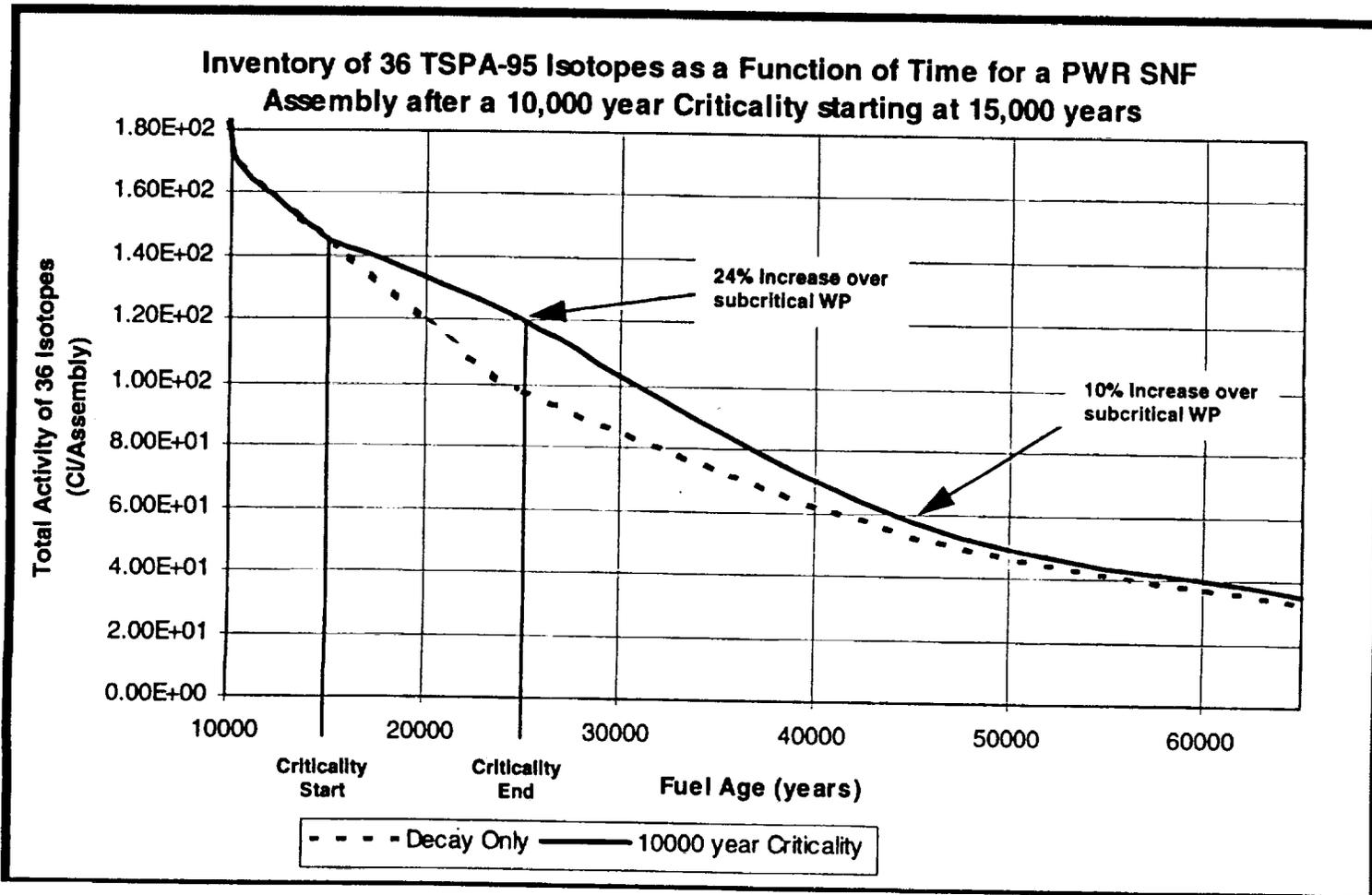
Determine steady state power necessary to support water temperature given heat dissipation by evaporation, radiation, and conduction.

- Power = $q_{\text{evap}}(T) + q_{\text{rad}}(T) + q_{\text{cond}}(T)$
= 2.2 kW

- Durations of 1000, 5000, and 10000 years considered.



Illustrations of increased radionuclide inventory:



Most likely series of events for commercial fuel:

- 1) Dripping on waste package causes penetration of waste package
- 2) Penetration(s) are small so that most dripping water does not enter waste package but causes continued degradation of waste package
- 3) Water vapor and small amounts of water enter waste package and cause stress corrosion cracking of borated steel basket, but carbon steel square tubes within the basket hold it in place
- 4) Water does not accumulate to any extent before holes in the bottom of the WP allow drainage
- 5) Generalized corrosion of carbon steel tubes proceeds resulting in eventual basket collapse
- 6) Collapsing basket damages the zircaloy clad fuel rods and fuel is exposed to alteration.
- 7) Uranium and Plutonium slowly leave the waste package either in dissolved or colloidal form through small opening in corrosion resistant material. Boron from the borated steel can only leave as small metal boride particles.
- 8) At late time when carbon steel is all oxidized and corrosion resistant material is severely pitted or cracked, more water may enter the packages and larger particles of fuel or basket corrosion products may leave container through larger openings.

In-package criticality is not likely for commercial fuel because:

- 1) Boron is expected to remain mainly within the borated steel and steel corrosion products and these are expected to remain mainly with the fuel as the basket collapses
- 2) Water is expected to enter the package slowly, and holes will develop in the bottom decreasing the likelihood of the bathtub condition
- 3) Zircaloy is expected to keep the fuel within the basket, at least until the basket collapses

In-package criticality could be more likely for other DOE fuels because:

- 1) Some fuels are highly enriched
- 2) Some cladding is disrupted or made of less corrosion resistant materials and fuel could spill from the basket to the bottom of the waste package where there is less borated steel

These problems can be mitigated by:

- 1) Co-disposal of small amounts of highly enriched materials with large amounts of other materials so that a critical mass cannot be assembled within the package
- 2) Use of depleted uranium with the highly enriched uranium spent fuels (in the low flow cases, this could help with ^{239}Pu as well, because ^{239}Pu decays with a half-life of 24,000 years to ^{235}U)
- 3) Filling package void space with materials that are poorer moderators than water
- 4) Adding a borated steel liner, or otherwise increasing the amount of borated steel within the package

Unanswered questions:

- 1) How fast do metal borides within the borated steel alter and release their boron?
- 2) What is the maximum amount of water that could flow over and into an individual waste package?
- 3) Will an even more corrosion resistant material such as C22 be used for the corrosion resistant layer and will this increase the likelihood of the bathtub scenario?

Careful design should be able to keep the probability of a criticality within the package to less than 10^{-6} /year

Criticality in TSPA-VA

Attachment VI - Page 17

Eric Siegmann
CRWMS M&O/INTERA (DE&S)
Disposal Criticality Workshop
March 18, 1997
Las Vegas, , NV

B&W Federal Services
Duke Engineering & Services, Inc.
E. R. Johnson Associates, Inc.
Fluor Daniel, Inc.
Framatome Cogema Fuels
Integrated Resources Group
INTERA, Inc.

JK Research Associates, Inc.
Kiewit/Parsons Brinkerhoff
Lawrence Berkeley Laboratory
Lawrence Livermore National Laboratory
Logicon RDA
Los Alamos National Laboratory
Morrison-Knudsen Corporation

SAIC
Sandia National Laboratories
TRW Environmental Safety Systems Inc.
Woodward-Clyde Federal Services
Winston & Strawn
Cooperating Federal Agency:
U.S. Geological Survey

Criticality

- 1) Nuclear physics calculation well understood, criticality is possible.
(At least 4 studies)

- 2) Material Transport needs to be adequately addressed.

- 3) Current analytical capabilities are questionable (Pocos de Caldas bench marks, 11 of 12 cases severely off from measurements)

Oklo Natural Reactors (16 reactors)

– Information from Oversby, V.M., SKB TR 96-07

Reactor Conditions (Zone 2)

- 1) At reactor start, UO₂ concentrations 50% (3.68% U²³⁵), 20% SiO₂, 30% clay, Void fraction = 10%. At end, 50% UO₂, 50% clay, H₂O replace SiO₂
- 2) Core Lens Shaped, 60 cm. height, 10 M Diameter (slab geometry).
- 3) Cores had a negative temperature coefficient, under moderated.
- 4) Neutron poisons were about 50 ppm B¹⁰ equivalent, needed as burnable poison for desired burnup.
- 5) Tectonics increased water content for criticality, water circulated but did not boil
- 6) Reactor operated 800,000 years duration, fluence 1E²¹ n/cm²

Attachment VI - Page 19

TSPA-VA Disposal Criticality Abstraction/Testing Workshop

March 18-20, 1997

DOE-owned SNF Issues

Henry Loo/Paul Sentieri
Lockheed Martin Idaho Technologies Co.



DOE Fuel Characteristics

- Wide U-235 enrichment
- Contain other fissile materials such as U-233
- Higher concentration of Pu-239 contents than commercial
- DOE fuels have variable integrity
 - Varying corrosion/solubility due to matrix materials, cladding integrity, and fuel conditions



DOE Fuel Package Variations From Commercial Fuel

- Co-disposal options with borosilicate glass
- Thermal output of the waste package much less than 14.2 kW

Internal Criticality Issues

- Impact of HEU
- Impact of silica from glass on U solubility/reconcentration
- Impact of corrosion products on water displacement and neutron absorber retention
- Impact of different neutron absorber materials such as Hf and Gd



Near Field Criticality

- Impact of HEU
- Impact of silica from glass on U reconcentration near the container
- Consideration of placing DU in drift of the repository
- If other material such as zeolite is placed in the drift to absorb radionuclides, the potential of concentrating of fissile materials should be considered



Probability and Consequences

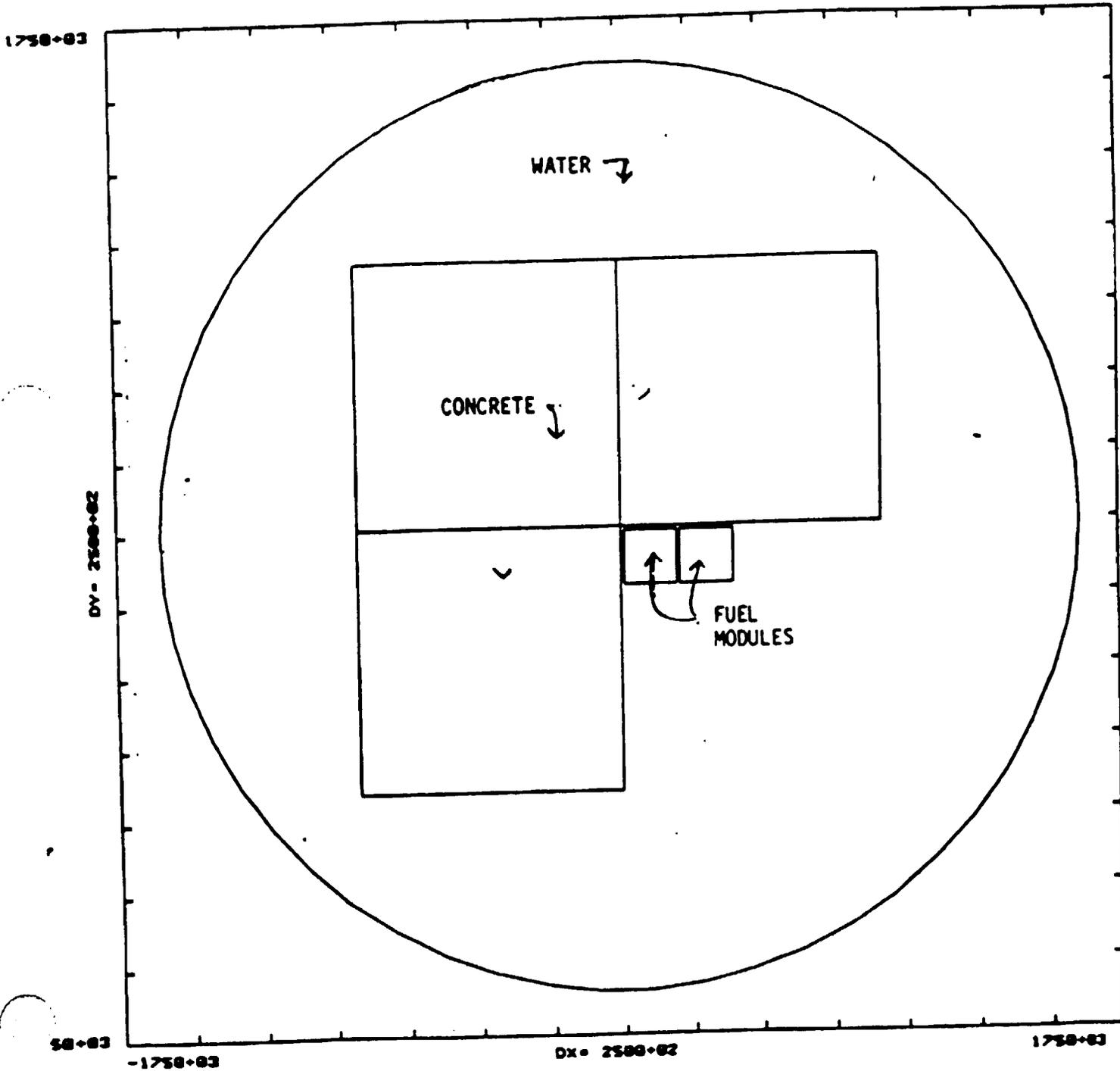
- Continuous low power reactor may be too conservative, should consider dynamic models that takes neutron kinetics and hydrodynamics that would lead to shutdown of the reactions
- Due to the large uncertainties associated with the various input parameters and the physical configuration of the system, use of RELAP for applications outside of the reactor core, especially in a repository environment, may not be the right tool



Concrete Reflection with PWR-2 Seed 2 Modules

R. F. Beyer

Radial Geometry for Two PWR-2 Seed 2 Fuel Modules with Concrete Reflection



Two PWR-2 Seed 2 Modules with Concrete Reflection

Case	Fuel - Concrete Separation (inches)	Fuel Module Separation (inches)	K_{eff}^* (± 0.01)
1. No concrete	-	0.50	0.925
2. Concrete	0.5	0.50	0.951
3. Concrete	0.5	0.25	0.954
4. Concrete	0.0	0.25	0.973

* With fission products and residual poison but without control rods.

Session 1 - In-Package Criticality

Group 1					
#	Sub Issue	Criterion 1	Criterion 2	Criterion 3	Total
1.1	Failure Model of waste package (bathtub, flow-through)	5	5	1	11
1.2	Extent of degradation of basket materials	3	3	1	7
1.3	Removal of absorbers from WP and/or basket (particularly bromides)	5	5	1	11
1.4	Extent of degradation of waste form (physical, chemical, cladding)	1	3	1	5
1.5	Physical form of fissile materials	1	3	3	7
1.6	Geometric configuration of fissile material	3	3	1	7
1.7	Location of criticality (WP volume, WP bottom, WP wall)	1	1	1	3
1.8	Chemical composition and other properties (including materials properties) of moderator and reflector	3	1	1	5
1.9	Start time of criticality event(s)	3	1	1	5
1.10	Duration of criticality event(s)	5	1	1	7
1.11	Mode (continuous or periodic) of criticality event(s)	1	1	1	3
1.12	Power release from criticality events	5	1	3	9
1.13	Depleted uranium inside waste package	1	3	1	5
1.14	Waste form characteristics	5	5	3	13
1.15	Mechanical shock	1	1	1	3
1.16	Effect of materials external to waste package	3	3	1	7

Session 1 - In-Package Criticality

Group 2					
#	Sub Issue	Criterion 1	Criterion 2	Criterion 3	Total
1.1	Failure Model of waste package (bathtub, flow-through)	5	5	1	11
1.2	Extent of degradation of basket materials	3	3	1	7
1.3	Removal of absorbers from WP and/or basket (particularly bromides)	5	5	1	11
1.4	Extent of degradation of waste form (physical, chemical, cladding)	3	3	1	7
1.5	Physical form of fissile materials	3	3	1	7
1.6	Geometric configuration of fissile material	3	3	1	7
1.7	Location of criticality (WP volume, WP bottom, WP wall)	1	1	1	3
1.8	Chemical composition and other properties (including materials properties) of moderator and reflector	3	3	1	7
1.9	Start time of criticality event(s)	1	1	1	3
1.10	Duration of criticality event(s)	5	3	1	9
1.11	Mode (continuous or periodic) of criticality event(s)	1	1	1	3
1.12	Power release from criticality events	1	1	1	3
1.13	Depleted uranium inside waste package	1	1	1	3
1.14	Waste form characteristics	3	5	1	9
1.15	Mechanical shock	1	1	1	3
1.16	Effect of materials external to waste package	3	3	1	7

Session 1 - In-Package Criticality

Group 3					
#	Sub Issue	Criterion 1	Criterion 2	Criterion 3	Total
1.1	Failure Model of waste package (bathtub, flow-through)	5	5	5	15
1.2	Extent of degradation of basket materials	1	1	1	3
1.3	Removal of absorbers from WP and/or basket (particularly bromides)	5	5	5	15
1.4	Extent of degradation of waste form (physical, chemical, cladding)	3	3	3	9
1.5	Physical form of fissile materials	3	3	3	9
1.6	Geometric configuration of fissile material	3	3	3	9
1.7	Location of criticality (WP volume, WP bottom, WP wall)	1	1	1	3
1.8	Chemical composition and other properties (including materials properties) of moderator and reflector	3	3	3	9
1.9	Start time of criticality event(s)	5	1	1	7
1.10	Duration of criticality event(s)	5	1	5	11
1.11	Mode (continuous or periodic) of criticality event(s)	1	1	1	3
1.12	Power release from criticality events	5	1	5	11
1.13	Depleted uranium inside waste package	3	3	3	9
1.14	Waste form characteristics	3	3	3	9
1.15	Mechanical shock	3	3	3	9
1.16	Effect of materials external to waste package	3	1	1	5

Session 1 - In-Package Criticality

Group 4					
#	Sub Issue	Criterion 1	Criterion 2	Criterion 3	Total
1.1	Failure Model of waste package (bathtub, flow-through)	1	5	5	11
1.2	Extent of degradation of basket materials	1	5	1	7
1.3	Removal of absorbers from WP and/or basket (particularly bromides)	1	5	1	7
1.4	Extent of degradation of waste form (physical, chemical, cladding)	1	5	1	7
1.5	Physical form of fissile materials	1	5	1	7
1.6	Geometric configuration of fissile material	1	5	1	7
1.7	Location of criticality (WP volume, WP bottom, WP wall)	1	1	1	3
1.8	Chemical composition and other properties (including materials properties) of moderator and reflector	1	3	1	5
1.9	Start time of criticality event(s)	1	1	1	3
1.10	Duration of criticality event(s)	1	1	3	5
1.11	Mode (continuous or periodic) of criticality event(s)	1	1	1	3
1.12	Power release from criticality events	1	1	1	3
1.13	Depleted uranium inside waste package	1	5	1	7
1.14	Waste form characteristics	1	5	5	11
1.15	Mechanical shock	1	3	1	5
1.16	Effect of materials external to waste package	1	1	1	3

Session 1 - In-Package Criticality

#	Sub-Issue	Group 1	Group 2	Group 3	Group 4	Total	S. D.*
1.1	Failure Model of waste package (bathtub, flow-through)	11	11	15	11	48	8.00
1.2	Extent of degradation of basket materials	7	7	3	7	24	8.00
1.3	Removal of absorbers from WP and/or basket (particularly bromides)	11	11	15	7	44	13.06
1.4	Extent of degradation of waste form (physical, chemical, cladding)	5	7	9	7	28	6.53
1.5	Physical form of fissile materials	7	7	9	7	30	4.00
1.6	Geometric configuration of fissile material	7	7	9	7	30	4.00
1.7	Location of criticality (WP volume, WP bottom, WP wall)	3	3	3	3	12	0.00
1.8	Chemical composition and other properties (including materials properties) of moderator and reflector	5	7	9	5	26	7.66
1.9	Start time of criticality event(s)	5	3	7	3	18	7.66
1.10	Duration of criticality event(s)	7	9	11	5	32	10.33
1.11	Mode (continuous or periodic) of criticality event(s)	3	3	3	3	12	0.00
1.12	Power release from criticality events	9	3	11	3	26	16.49
1.13	Depleted uranium inside waste package	5	3	9	7	24	10.33
1.14	Waste form characteristics	13	9	9	11	42	7.66
1.15	Mechanical shock	3	3	9	5	20	11.31
1.16	Effect of materials external to waste package	7	7	5	3	22	7.66
*	Standard Deviation x 4						

#	Sub-Issue	Groups				Total	S.D.*
		1	2	3	4		
1.1	Failure Model of waste package (bathtub, flow-through)	11	11	15	11	48	8.00
1.3	Removal of absorbers from WP and/or basket (particularly borides)	11	11	15	7	44	13.06
1.14	Waste form characteristics	13	9	9	11	42	7.66
1.10	Duration of criticality event(s)	7	9	11	5	32	10.33
1.5	Physical form of fissile materials	7	7	9	7	30	4.00
1.6	Geometric configuration of fissile material	7	7	9	7	30	4.00
1.4	Extent of degradation of waste form (physical, chemical, cladding)	5	7	9	7	28	6.53
1.8	Chemical composition and other properties (including materials properties) of moderator and reflector	5	7	9	5	26	7.66
1.12	Power release from criticality events	9	3	11	3	26	16.49
1.2	Extent of degradation of basket materials	7	7	3	7	24	8.00
1.13	Depleted uranium inside waste package	5	3	9	7	24	10.33
1.16	Effect of materials external to waste package	7	7	5	3	22	7.66
1.15	Mechanical shock	3	3	9	5	20	11.31
1.9	Start time of criticality event(s)	5	3	7	3	18	7.66
1.7	Location of criticality (WP volume, WP bottom, WP wall)	3	3	3	3	12	0.00
1.11	Mode (continuous or periodic) of criticality event(s)	3	3	3	3	12	0.00
* Standard Deviation x 4							

ATTACHMENT VII

Viewgraphs of Panel Presentations and Tables of Issue Prioritization for Session II

- D. Sassani: Session II: Issues Discussion Near-Field Criticality TSPA Perspective**
- R. Rechar: Criticality Evaluation**
- P. Gottlieb: Evaluation of External Criticality: Near Field Example: Deterministic Calculation**
- L. Sanchez: Nuclear Dynamics Consequence Analyses (NDCA)**
- R. VanKonynenberg: Behavior of Boron**

Session II. Issues Discussion Near-Field Criticality TSPA Perspective

David C. Sassani
March 18, 1997
M&O Performance Assessment

B&W Federal Services
Duke Engineering & Services, Inc.
Fluor Daniel, Inc.
Framatome Cogema Fuels
Integrated Resources Group
INTERA, Inc.
JAI Corporation

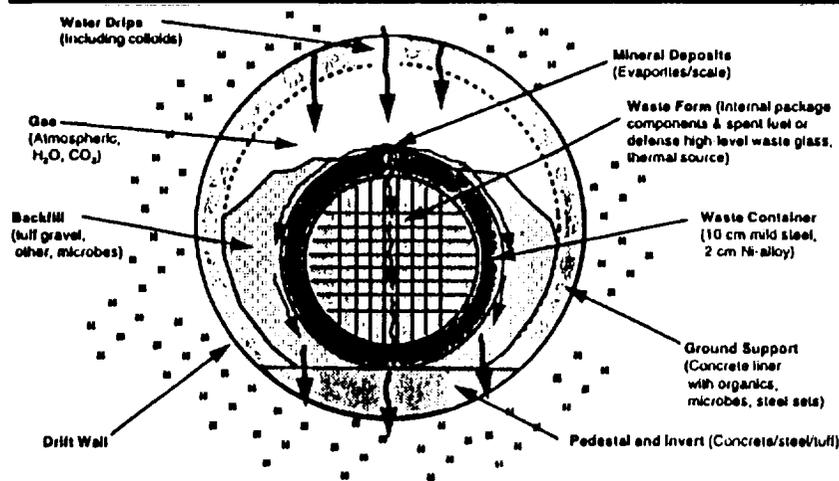
JK Research Associates, Inc.
Lawrence Berkeley Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
Morrison Knudsen Corporation
Science Applications International Corporation

Sandia National Laboratories
TRW Environmental Safety Systems Inc.
Woodward Clyde Federal Services
Winston & Strawn
Cooperating Federal Agency:
U.S. Geological Survey

Previous Treatment in TSPA

- Only In-Package Criticality Analyzed
 - Disposal Criticality Analysis Method Report, 1996
 - Changes to source-term
- Near-Field Scenario Defined by Wp Group
 - Degraded Mode Criticality Analysis Report, 1997
 - ^{235}U partially extracted by zeolites in invert
 - Not yet analyzed

Near-Field Environment Schematic



Civilian Radioactive Waste
Management System
Management & Operating
Contractor

Criticality Workshop TSPA Near Field © C. Beaman

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3/18/97

Possible Aspects for TSPA-VA

- **Bounding Likelihood of Critical Event in NFE**
 - Scenario development
 - Identify possible chemical paths to criticality
 - Mass balance constraints
 - Differential rates assessment
 - Accumulation/Separation of fissile elements vs. absorbers
- **Assessing the Changes to the NFE**
 - Thermal disturbance
 - Mechanical disturbance
 - Source term changes
 - Timescale of disturbances
 - Is the system self-perpetuating or self-limiting?

Civilian Radioactive Waste
Management System
Management & Operating
Contractor

Criticality Workshop TSPA Near Field © C. Beaman

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Sources of Uncertainty

- **Near-Field Environment Conditions**
 - Definition of transport pathways
 - fracture vs matrix
 - temporal variability
 - Along path chemistries are complex
 - Temperature gradients
- **Modeling Capabilities**
 - Multicomponent system
 - Conceptual models of phases containing fissiles
 - Relative changes compound uncertainties
 - Coupling of semi-empirical waste-form models to thermochemical models



Criticality Evaluation

Rob Rechar

Sandia National Laboratories

March 18, 1997

Processes of screening FEPs like mini PA but cannot always separate from overall PA



- **Screening process**
 1. **System characterization**
 2. **Scenario development**
 3. **Probability estimation**
 4. **Consequence analysis**
 5. **Regulatory comparison**
 6. **Sensitivity analysis(?)**
- **Screening processes can be repeated several times**
- **Criticality not easily separated from overall PA (e.g., plenty of fissile material)**
 - **Certain situations can be separated and examples given**
 - **Usually must examine geochemical processes to see if concentration large**

First major issue is the geochemical and hydrologic environment around the container



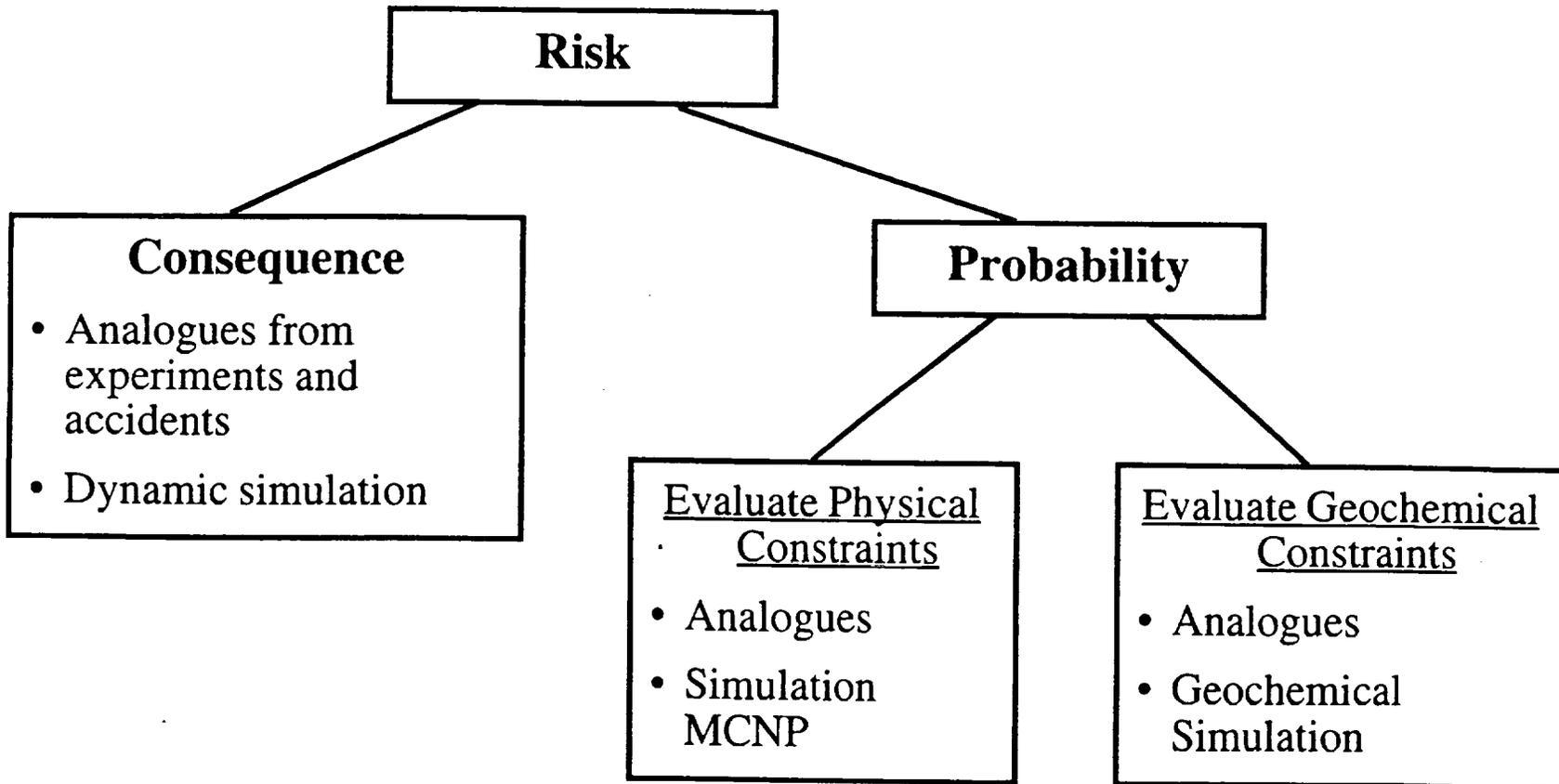
- **Influences**
 - **Degradation of container**
 - **Solubility of fissile material relative to neutron poisons such as other radioisotopes**
- **Once evaluated determines necessity for simulation way from container**

Several steps should be take to evaluate criticality event



- **Develop criticality criteria (mass, volume, concentration) for spherical and planar shapes for several mixtures of geologic media.**
- **Simulate degradation of containers and fuel with detailed models; from simulation**
 - **Monitor movement of fissile material**
 - **Evaluate probability of criticality at various locations**
- **Evaluate maximum consequences through dynamic neutronic modeling.**
- **Look for more analogues with container degradation and radioisotope movement.**
- **Work with NRC on interpretation of critical requirements.**

Evaluation of the risk from criticality can use several categories



Evaluation of External Criticality: Near Field Example: Deterministic Calculation

Peter Gottlieb
CRWMS M&O
Waste Package Development
3/18/97

External Criticality: Near-Field Example

Critical Mass Concentrating in Zeolite: Is it possible?

Concentration of zeolites in invert, liner and host rock (up to 50 wt%)

Maximum concentration of uranium in zeolite (wt%)

- Actually observed in mines: 0.7% in the Northern Reese River Valley
- Laboratory experiment: 1.0% resulting from treatment of zeolite with uranium saturated water
- Theoretical maximum: 1.49% resulting from replacement of all Ca^{++} with UO_2^{++}

Calculated $k_{\infty} = 0.88$ for ^{235}U enrichment = 1.9%, and the following assumptions

- Design basis fuel, which is more reactive than 98% of the expected deliveries of commercial SNF to the repository.
- ^{239}Pu decayed to ^{235}U (24,100 year half-life)
- Assumed maximum U concentration (1.49 wt%).
- Optimum water concentration (30 vol%).

NUCLEAR DYNAMICS CONSEQUENCE ANALYSIS (NDCA)

Lawrence C. Sanchez



**Nuclear Waste Management Program Center,
Sandia National Laboratories**

*A National Spent Nuclear Fuel Program (NSNFP) Project in in Collaboration with
Idaho National Engineering & Environmental Laboratory (INEEL)*

NUCLEAR DYNAMICS CONSEQUENCE ANALYSIS (NDCA) -- Nuclear Criticality



Nuclear Criticality is a concern for the disposal of DOE-owned spent nuclear fuels because many of these fuels have high fissile enrichment.

NDCA Project addresses the following:

- 1. Initial disposal storage criticality limits (i.e., static K_{eff} calculations which demonstrate that the criticality limit of 0.95 is being met for initial in-situ geometries).**
- 2. Identification of criticality values for degraded internal (in-situ) geometries at various time frames.**
- 3. Identification of criticality values for near-field geometry (fissile material that has been transported just outside of the internal geometry)**

NUCLEAR DYNAMICS CONSEQUENCE ANALYSIS (NDCA) -- Nuclear Criticality



NDCA Project addresses::

4. Identification of criticality values for far-field geometry (fissile material transported a considerable distance from the internal geometry undergoing a low reactivity; e.g., less than prompt critical).
5. Nuclear dynamics analysis corresponding to a far-field geometry undergoing a low reactivity (much less than prompt critical) nuclear excursion.

NUCLEAR DYNAMICS CONSEQUENCE ANALYSIS (NDCA) -- Nuclear Criticality



NDCA Project addresses:

6. Nuclear dynamics analysis corresponding to an internal geometry undergoing a high reactivity ($>$ prompt) nuclear excursion.
7. Nuclear dynamics analysis corresponding to a far-field geometry undergoing a low reactivity (much less than prompt critical) nuclear excursion.

NUCLEAR DYNAMICS CONSEQUENCE ANALYSIS (NDCA) -- Nuclear Criticality



Analysis Capabilities:

1. Processing of nuclear cross sections (key input used in Monte Carlo code/solution to Boltzmann Transport Equation).
 - a. processing of ENDF/VI evaluated nuclear x-sections for S (alpha, beta); i.e., scattering kernel.
 - b. processing of ENDF/VI evaluated nuclear x-sections for thermal treatment (Doppler broadening) at ambient (ground) and elevated temperature ranges.

NUCLEAR DYNAMICS CONSEQUENCE ANALYSIS (NDCA) -- Nuclear Criticality



Analysis Capabilities:

2. **Static Keff calculations (used for the generation of the key input parameters employed in the nuclear dynamics analysis of a nuclear excursion).**
 - a. **generation of atom number densities and geometry data for Monte Carlo neutral particle transport code, Boltzmann Transport Equation).**
 - b. **criticality evaluation (determine Keff)**
 - c. **buckling search (perform a series of criticality calculations to identify, for a given material composition, the geometry that yields a critical system, i.e., $K_{eff} = 1$).**
 - d. **Doppler Coefficient evaluation.**

NUCLEAR DYNAMICS CONSEQUENCE ANALYSIS (NDCA) -- Nuclear Criticality



Analysis Capabilities:

3. **Nuclear Kinetics Calculations (key nuclear physics modeling used in the analysis of a nuclear excursion).**
 - a. model (via reactor point kinetics) the kinetics (time behavior, without feedback dynamics) of a nuclear excursion.
 - b. benchmark on classical “rod drop” and “prompt jump” problems.

4. **Nuclear Dynamics (determine integrated energy released during an inadvertent underground nuclear excursion)**
 - a. uncoupled nuclear dynamics --small & large reactivity insertions (not coupled to groundwater transport code)
 - b. fully- coupled nuclear dynamics -- calculations used only to demonstrate that a nuclear excursion will shut down rapidly due to Doppler alone. (and not void coefficient)

NUCLEAR DYNAMICS CONSEQUENCE ANALYSIS (NDCA) -- Nuclear Criticality



Analysis Capabilities:

5. Transient Two-Phase Groundwater Thermal Hydraulics

- a. uncoupled thermal hydraulics analysis to identify the thermal recovery time of a fissile assembly after a nuclear excursion has occurred.

NUCLEAR DYNAMICS CONSEQUENCE ANALYSIS (NDCA) -- Nuclear Criticality



Computational Codes Under Development:

- **RKeff** -- Pre- and Post- Processor for (static) keff Calculations (MCNP and FEMP1D)
- **NARK** -- NucleAR Kinetics & Dynamics model for analyzing potential supercriticality events related to the disposal of fissile material in a geologic repository setting.

Code Characteristics:

Large FORTRAN77 Codes -- RKeff in excess of 20,000 lines, NARK in excess of 37,000 lines. (codes are written in platform-independent ANSI standard F77)

NUCLEAR DYNAMICS CONSEQUENCE ANALYSIS (NDCA) -- Nuclear Criticality



Rkeff Capabilities:

- Pre- and Post- Processor for MCNP and FEMP1D.
- Provides half-life, specific activity, and heatload based on ENDF/V data from ORIGEN2 decay libraries.
- Generates documented input files for buckling searches with MCNP for various user selections of:
 1. host rock material
 2. isotopic composition of fissile material
 3. precipitated fissile minerals
 4. host rock porosity
 5. % porosity field w/ fissile material
 6. host rock water saturation
 7. groundwater composition
 8. geometry type of fissile assembly
 9. geometry dimensions of fissile assembly
 10. reflector material surrounding fissile assembly

NUCLEAR DYNAMICS CONSEQUENCE ANALYSIS (NDCA) -- Nuclear Criticality



NARK Capabilities:

- **Kinetics/uncoupled dynamics in stand-alone mode**
- **Fully coupled nuclear dynamics when used with transient two-phase groundwater thermal hydraulics.**
- **Can analyze delayed & prompt critical nuclear excursions.**
 1. **fuel Doppler feedback mechanism**
 2. **moderator Doppler feedback mechanism**
 3. **void coefficient (desaturation)**
 4. **generates power (fissions) time-histories**
 5. **uses self-adaptive ODE numerical integrators for both stiff and non-stiff ODEs (thus, NARK can solve delayed and prompt nuclear excursions)**

BEHAVIOR OF BORON

Rich Van Konynenburg

Lawrence Livermore National Laboratory

Criticality Workshop

Las Vegas

March 18-20, 1997

**Reference neutron absorber material--
A978 boron-containing stainless steel**

**Consists of a dispersion of mixed metal
boride particles in an austenitic
stainless steel matrix**

**Boride particles are elongated and typically
a few microns in size. Composition is
 M_2B , where M is over half Cr, nearly half
Fe, and a small amount of Ni (and
perhaps Mo).**

**Stainless steel matrix is similar to Type 316
(18.5 wt% Cr, 13 wt% Ni, 2.2 wt% Mo,
0.04 wt % max C, balance Fe.**

**Preliminary measurements indicate that
matrix is noble with respect to borides.
Thus, corrosion behavior will likely be
dominated by corrosion of matrix.**

**Corrosion rate of stainless steel will depend
strongly on environment. Could be less
than 0.1 micron/year if benign. Could be
more than 1.0 micron/year if wet with
water having significant concentrations
of solutes such as chloride or oxalate.**

Metal borides will corrode to form metal (hydr)oxides and orthoboric acid or borates.

Orthoboric acid and borates in general have fairly high solubilities in water.

Boron is not significantly sorbed by iron oxides or by most natural minerals.

The fraction of boron that remains in solution during leach testing of HLW glass is higher than for any other element present.

Naturally occurring boron-containing minerals have significant solubilities in water.

Natural deposits of boron have resulted from evaporation of water containing dissolved boron. Major ones are not far from Yucca Mountain.

We should assume that after the borides corrode, the boron will dissolve in available water and will be transported away if the water moves away from the packages.

Session 2 - In-Package Criticality

Group 1					
#	Sub Issue	Criterion 1	Criterion 2	Criterion 3	Total
2.1	Seepage into Drift	5	5	3	13
2.2	Separation of fissile and absorbing materials	3	5	1	9
2.3	WP corrosion products	3	3	1	7
2.4	Design of invert materials (filtering and sorbing properties)	5	5	1	11
2.5	Total time of release of radionuclides	1	1	1	3
2.6	Start time of criticality in NF	1	1	1	3
2.7	Duration of criticality in NF	3	1	1	5
2.8	Mode (continuous or periodic) of criticality event	1	1	1	3
2.9	Physical/chemical form of fissile material (particulates, colloids, or elements in solution)	3	5	3	11
2.10	Depleted uranium in backfill	1	5	1	7
2.11	Focussing of effluent flow from WP	1	1	1	3
2.12	Waste form characteristics	3	5	3	11

Session 2 - In-Package Criticality

Group 2					
#	Sub Issue	Criterion 1	Criterion 2	Criterion 3	Total
2.1	Seepage into Drift	3	5	1	9
2.2	Separation of fissile and absorbing materials	5	5	1	11
2.3	WP corrosion products	3	3	1	7
2.4	Design of invert materials (filtering and sorbing properties)	3	5	1	9
2.5	Total time of release of radionuclides	1	1	1	3
2.6	Strart time of criticality in NF	1	1	1	3
2.7	Duration of criticality in NF	5	1	1	7
2.8	Mode (continous or periodic) of criticality event	1	1	1	3
2.9	Physical/chemical form of fissile material (particulates, colloids, or elements in solution)	5	5	1	11
2.10	Depleted uranium in backfill	3	3	1	7
2.11	Focussing of effluent flow from WP	3	3	1	7
2.12	Waste form characteristics	3	5	1	9

Session 2 - In-Package Criticality

Group 3					
#	Sub Issue	Criterion 1	Criterion 2	Criterion 3	Total
2.1	Seepage into Drift	3	5	3	11
2.2	Separation of fissile and absorbing materials	5	5	5	15
2.3	WP corrosion products	1	5	1	7
2.4	Design of invert materials (filtering and sorbing properties)	3	5	3	11
2.5	Total time of release of radionuclides	3	3	3	9
2.6	Start time of criticality in NF	3	1	1	5
2.7	Duration of criticality in NF	5	1	5	11
2.8	Mode (continous or periodic) of criticality event	3	1	3	7
2.9	Physical/chemical form of fissile material (particulates, colloids, or elements in solution)	5	5	5	15
2.10	Depleted uranium in backfill	3	5	3	11
2.11	Focussing of effluent flow from WP	5	5	5	15
2.12	Waste form characteristics	3	3	3	9

Session 2 - In-Package Criticality

Group 4					
#	Sub Issue	Criterion 1	Criterion 2	Criterion 3	Total
2.1	Seepage into Drift	1	5	5	11
2.2	Separation of fissile and absorbing materials	1	5	1	7
2.3	WP corrosion products	1	3	1	5
2.4	Design of inert materials (filtering and sorbing properties)	1	5	3	9
2.5	Total time of release of radionuclides	1	3	5	9
2.6	Start time of criticality in NF	1	1	1	3
2.7	Duration of criticality in NF	1	1	1	3
2.8	Mode (continuous or periodic) of criticality event	1	1	1	3
2.9	Physical/chemical form of fissile material (particulates, colloids, or elements in solution)	1	5	1	7
2.10	Depleted uranium in backfill	1	5	3	9
2.11	Focussing of effluent flow from WP	1	5	1	7
2.12	Waste form characteristics	1	5	5	11

Session 2 - In-Package Criticality

#	Sub-Issue	Group 1	Group 2	Group 3	Group 4	Total	S. D. *
2.1	Seepage into Drift	13	9	11	11	44	6.53
2.2	Separation of fissile and absorbing materials	9	11	15	7	42	13.66
2.3	WP corrosion products	7	7	7	5	26	4.00
2.4	Design of invert materials (filtering and sorbing properties)	11	9	11	9	40	4.62
2.5	Total time of release of radionuclides	3	3	9	9	24	13.86
2.6	Strart time of criticality in NF	3	3	5	3	14	4.00
2.7	Duration of criticality in NF	5	7	11	3	26	13.66
2.8	Mode (continous or periodic) of criticality event	3	3	7	3	16	8.00
2.9	Physical/chemical form of fissile material (particulates, colloids, or elements in solution)	11	11	15	7	44	13.06
2.10	Depleted uranium in backfill	7	7	11	9	34	7.66
2.11	Focussing of effluent flow from WP	3	7	15	7	32	20.13
2.12	Waste form characteristics	11	9	9	11	40	4.62
	* Standard Deviation x 4						

Session 2 - In-Package Criticality

Sub-Issue	Group1	Group 2	Group3	Group 4	Total	Tot.-S.D
2.1 Seepage into Drift	13	9	11	11	44	37.5
2.9 Physical/chemical form of fissile material (particulates, colloids, or elements in solution	11	11	15	7	44	30.9
2.2 Separation of fissile and absorbing materials	9	11	15	7	42	28.3
2.4 Design of inert materials (filtering and sorbing properties)	11	9	11	9	40	35.4
2.12 Waste form characteristics	11	9	9	11	40	35.4
2.10 Depleted uranium in backfill	7	7	11	9	34	26.3
2.11 Focussing of effluent flow from WP	3	7	15	7	32	11.9
2.3 WP corrosion products	7	7	7	5	26	22.0
2.7 Duration of criticality in NF	5	7	11	3	26	12.3
2.5 Total time of release of radionuclides	3	3	9	9	24	10.1
2.8 Mode (continous or periodic) of criticality event	3	3	7	3	16	8.0
2.6 Strart time of criticality in NF	3	3	5	3	14	10.0
* Standard Deviation x 4						

ATTACHMENT VIII

Viewgraphs of Panel Presentations and Tables of Issue Prioritization for Session III

- J. McNeish: Session III: Issues Discussion TSPA Perspective on Far Field Criticality Representation**
- P. Gottlieb: Evaluation of External Criticality Far Field Example: Probabilistic Calculation**
- D. Jolley: Stratigraphic Interfaces of Potential Concern to Far-Field Criticality**

Session III: Issues Discussion TSPA Perspective on Far Field Criticality Representation

Jerry McNeish
CRWMS M&O/INTERA (DE&S)

Criticality Abstraction Workshop
18 March 1997
Las Vegas, NV

B&W Federal Services
Data Engineering & Services, Inc.
E. R. Johnson Associates, Inc.
Fluor Daniel, Inc.
Framatome Cogema Fuels
Integrated Resources Group
INTERA, Inc. (DE&S)

JK Research Associates, Inc.
Kiewit/Parsons Brinkerhoff
Lawrence Berkeley National Laboratory
Lawrence Livermore National Laboratory
Logicon RDA
Los Alamos National Laboratory
Morrison-Knudsen Corporation

SAIC
Sandia National Laboratories
TRW Environmental Safety Systems Inc.
Woodward-Clyde Federal Services
Winston & Strawn
Cooperating Federal Agency:
U.S. Geological Survey

Outline of Presentation

- Approach to represent far field criticality in TSPA-VA
- Key issues and uncertainties

Potential Representation of Far Field Criticality in TSPA-VA (continued)

- Definition of location for potential criticality
- Source term from WP group
- Implement new source term in TSPA
 - determine leach rate
- Evaluate at probability of 1
- Evaluate change in peak dose at accessible environment

Civilian Radioactive Waste
Management System
Management & Operating
Contractor

Criticality JRM 3/16/97 p 3

Key Issues and Uncertainties with Representation of Far Field Criticality

- Location of criticality event
 - reducing zones
 - areas with significant porosity changes
- Determination of probability of occurrence
- Focusing mechanisms to reconcentrate the released radionuclides
- Timing of criticality event (>40,000 postclosure)

Civilian Radioactive Waste
Management System
Management & Operating
Contractor

Criticality JRM 3/16/97 p 3

Potential Far Field Criticality Abstraction for TSPA-VA

- Evaluation of location of criticality
 - Determine key potential locations for criticality
 - Product: Sensitivity analyses of effect on dose as f(location)

Evaluation of External Criticality Far Field Example: Probabilistic Calculation

Peter Gottlieb
CRWMS M&O
Waste Package Development
3/18/97

External Criticality: Far-Field Example

Probability of encounter with organic reducing zone

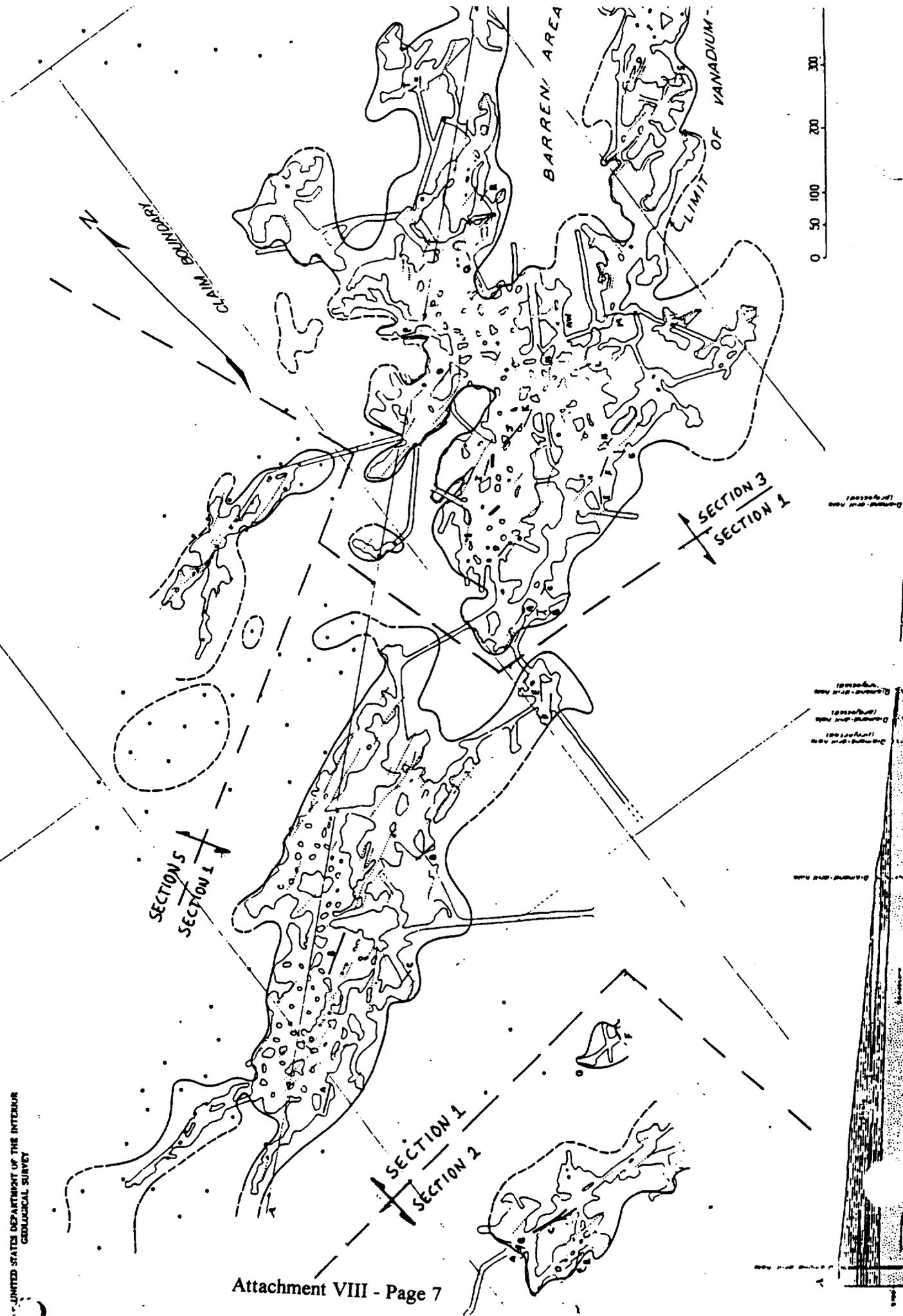
- Organic deposits are not likely in Yucca Mountain tuff, but one *relatively likely* mechanism:
 - Organic logs, analogous to those which supported high grade U deposits on the Colorado Plateau.
- Calculate minimum concentration of 1.9% enriched U which could be critical, in optimum concentration of water, which can fit in available porespace.
- Large/high concentrations of organic material could be supported by juxtaposition of logs (random?)
 - Use map of log locations in typical Colorado Plateau deposit
 - Measure distribution of: (1) Log lengths, (2) Nearest neighbor distances, (3) Next-nearest neighbor distances.
- Probability of encounter: $\Pr\{\text{log/size juxtaposition of sufficient size}\} \times \Pr\{\text{random WP outflow passes through the location}\}$
- Conservative cushions which can be removed for HEU SNF:
 - Consider spreading/dispersion of WP outflow (particularly in saturated zone).
 - Consider re-mobilization during the time required to build up a large U deposit (100,000 to 1,000,000 years).

PORTION OF LOG
LOCATION MAP

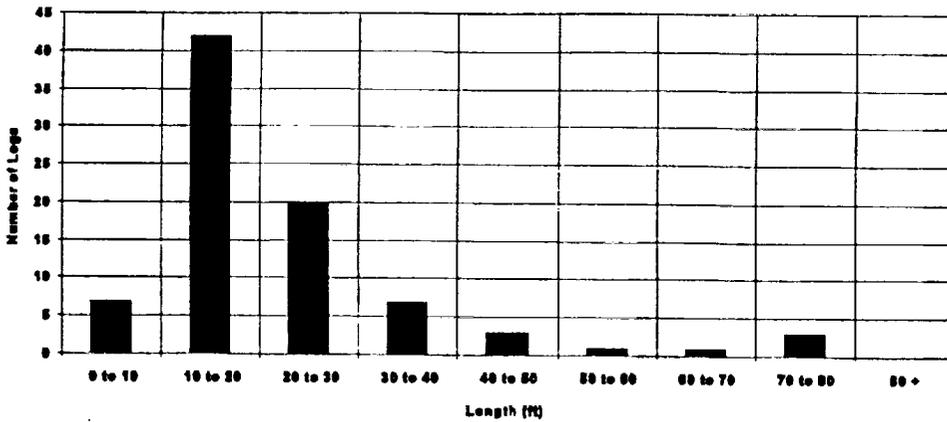
Attachment III

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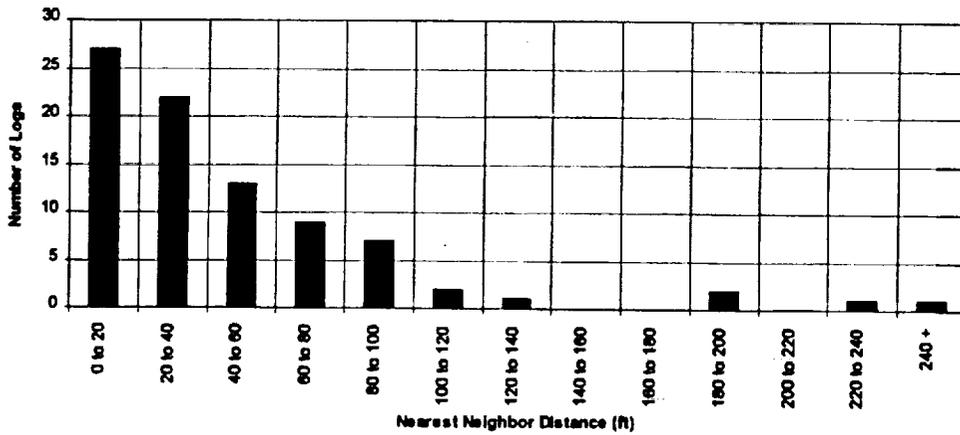
UNITED STATES DEPARTMENT OF THE INTERIOR
GEOLOGICAL SURVEY



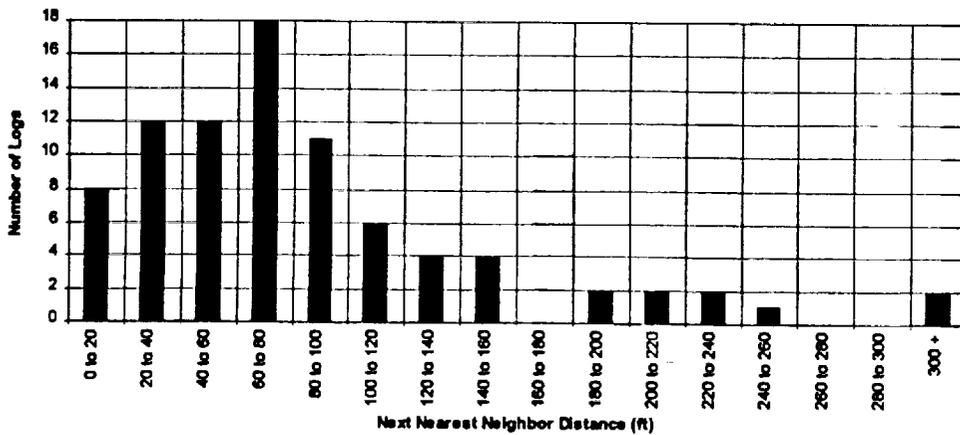
Statistics of Log Distributions



Distribution of fossil log lengths at the Club Mines.



Distribution of distance from log center to center of nearest log.



Distribution of distance from log center to center of next nearest log.

Stratigraphic Interfaces of Potential Concern to Far-Field Criticality

**Darren M. Jolley
March 18-20, 1997
INTERA Inc.
TSPA Criticality Workshop**

Far-Field Stratigraphic Concerns (cont.)

■ Unsaturated Zone

- Basil Vitrophyre (Tptpv3)
 - ♦ Porosity and Permeability Change (Example: ϕ changes from .13 to .05)
 - ♦ Perched water (UZ-1, UZ-14, NRG-7a, and SD-9)
 - ♦ Mineralogical changes (Glass, Smectite, and Zeolites)
- Two Major Zeolitic/Devitrified Tuff Interfaces (Tac and Tcp)
- Other Unique Interfaces (Tac)
 - ♦ Paleosols in bedded tuffs (Localized potential for organic matter [high uncertainty])
 - ♦ Basal Sandstone (0-18 ft.; medium to course grained and poorly sorted)

Session 3 - In-Package Criticality

Group 1					
#	Sub Issue	Criterion 1	Criterion 2	Criterion 3	Total
3.1	Location of criticality event (UZ or SZ)	3	3	3	9
3.2	Dispersion/dilution/mixing during transport to criticality location	3	3	1	7
3.3	Fracture focussing of radionuclides	3	5	1	9
3.4	Groundwater flow rate at criticality location	3	5	1	9
3.5	Homogeneous vs heterogeneous (fracture network) critical configurations	1	3	1	5
3.6	Organic concentrating environments (reduction or oxidation state)	3	5	1	9
3.7	Other stratigraphic or chemical concentrating mechanisms (sorption, colloids, filtration, etc)	3	5	1	9
3.8	Time of criticality events	1	3	1	5
3.9	Duration of criticality events	3	1	3	7
3.10	Mode (continuous or periodic) of criticality events	1	1	1	3
3.11	Reduction in moderation due to impurities in water	1	1	1	3
3.12	Type of fissile material transported (consider enrichment, depleted uranium as necessary)	3	5	1	9
3.13	Filtering mechanisms prior to the concentration point	1	1	1	3
3.14	Composition of plume	3	3	1	7

Session 3 - In-Package Criticality

Group 2					
#	Sub Issue	Criterion 1	Criterion 2	Criterion 3	Total
3.1	Location of criticality event (UZ or SZ)	5	3	5	13
3.2	Dispersion/dilution/mixing during transport to criticality location	3	5	3	11
3.3	Fracture focussing of radionuclides	3	3	3	9
3.4	Groundwater flow rate at criticality location	1	1	3	5
3.5	Homogeneous vs heterogeneous (fracture network) critical configurations	1	3	1	5
3.6	Organic concentrating environments (reduction or oxidation state)	3	5	3	11
3.7	Other stratigraphic or chemical concentrating mechanisms (sorption, colloids, filtration, etc)	5	5	3	13
3.8	Time of criticality events	1	1	1	3
3.9	Duration of criticality events	3	1	3	7
3.10	Mode (continuous or periodic) of criticality events	1	1	1	3
3.11	Reduction in moderation due to impurities in water	1	1	1	3
3.12	Type of fissile material transported (consider enrichment, depleted uranium as necessary)	3	5	3	11
3.13	Filtering mechanisms prior to the concentration point	1	3	1	5
3.14	Composition of plume	3	3	3	9

Session 3 - In Package Critical

Group 3					
#	Sub Issue	Criterion 1	Criterion 2	Criterion 3	Total
3.1	Location of criticality event (UZ or SZ)	5	5	5	15
3.2	Dispersion/dilution/mixing during transport to criticality location	5	5	5	15
3.3	Fracture focussing of radionuclides	5	5	1	11
3.4	Groundwater flow rate at criticality location	1	1	1	3
3.5	Homogeneous vs heterogeneous (fracture network) critical configurations	1	3	1	5
3.6	Organic concentrating environments (reduction or oxidation state)	5	5	5	15
3.7	Other stratigraphic or chemical concentrating mechanisms (sorption, colloids, filtration, etc)	3	3	3	9
3.8	Time of criticality events	1	1	1	3
3.9	Duration of criticality events	5	1	5	11
3.10	Mode (continuous or periodic) of criticality events	3	1	3	7
3.11	Reduction in moderation due to impurities in water	1	1	1	3
3.12	Type of fissile material transported (consider enrichment, depleted uranium as necessary)	5	5	5	15
3.13	Filtering mechanisms prior to the concentration point	5	5	5	15
3.14	Composition of plume	5	5	5	15

Session 3 - In-Package Criticality

Group 4					
#	Sub Issue	Criterion 1	Criterion 2	Criterion 3	Total
3.1	Location of criticality event (UZ or SZ)	1	5	3	9
3.2	Dispersion/dilution/mixing during transport to criticality location	1	5	5	11
3.3	Fracture focussing of radionuclides	1	5	3	9
3.4	Groundwater flow rate at criticality location	1	3	5	9
3.5	Homogeneous vs heterogeneous (fracture network) critical configurations	1	5	3	9
3.6	Organic concentrating environments (reduction or oxidation state)	1	5	3	9
3.7	Other stratigraphic or chemical concentrating mechanisms (sorption, colloids, filtration, etc)	1	5	3	9
3.8	Time of criticality events	1	1	1	3
3.9	Duration of criticality events	1	1	1	3
3.10	Mode (continuous or periodic) of criticality events	1	1	1	3
3.11	Reduction in moderation due to impurities in water	1	1	1	3
3.12	Type of fissile material transported (consider enrichment, depleted uranium as necessary)	1	5	1	7
3.13	Filtering mechanisms prior to the concentration point	1	3	3	7
3.14	Composition of plume	1	3	3	7

Session 3 - In-Package

#	Sub-Issue	Groups				Total	S.D.*
		1	2	3	4		
3.1	Location of criticality event (UZ or SZ)	9	13	15	9	46	12.00
3.2	Dispersion/dilution/mixing during transport to criticality location	7	11	15	11	44	13.06
3.6	Organic concentrating environments (reduction or oxidation state)	9	11	15	9	44	11.31
3.12	Type of fissile material transported (consider enrichment, depleted uranium as necessary)	9	11	15	7	42	13.66
3.7	Other stratigraphic or chemical concentrating mechanisms (sorption, colloids, filtration, etc)	9	13	9	9	40	8.00
3.3	Fracture focussing of radionuclides	9	9	11	9	38	4.00
3.14	Composition of plume	7	9	15	7	38	15.14
3.13	Filtering mechanisms prior to the concentration point	3	5	15	7	30	21.04
3.9	Duration of criticality events	7	7	11	3	28	13.06
3.4	Groundwater flow rate at criticality location	9	5	3	9	26	12.00
3.5	Homogeneous vs heterogeneous (fracture network) critical configurations	5	5	5	9	24	8.00
3.10	Mode (continuous or periodic) of criticality events	3	3	7	3	16	8.00
3.8	Time of criticality events	5	3	3	3	14	4.00
3.11	Reduction in moderation due to impurities in water	3	3	3	3	12	0.00
* Standard Deviation x 4							

Session 3 - In-Package Criticality

#	Sub-Issue	Groups				Total	S.D.*
		1	2	3	4		
3.1	Location of criticality event (UZ or SZ)	9	13	15	9	46	12.00
3.2	Dispersion/dilution/mixing during transport to criticality location	7	11	15	11	44	13.06
3.3	Fracture focussing of radionuclides	9	9	11	9	38	4.00
3.4	Groundwater flow rate at criticality location	9	5	3	9	26	12.00
3.5	Homogeneous vs heterogeneous (fracture network) critical configurations	5	5	5	9	24	8.00
3.6	Organic concentrating environments (reduction or oxidation state)	9	11	15	9	44	11.31
3.7	Other stratigraphic or chemical concentrating mechanisms (sorption, colloids, filtration, etc)	9	13	9	9	40	8.00
3.8	Time of criticality events	5	3	3	3	14	4.00
3.9	Duration of criticality events	7	7	11	3	28	13.06
3.10	Mode (continuous or periodic) of criticality events	3	3	7	3	16	8.00
3.11	Reduction in moderation due to impurities in water	3	3	3	3	12	0.00
3.12	Type of fissile material transported (consider enrichment, depleted uranium as necessary)	9	11	15	7	42	13.66
3.13	Filtering mechanisms prior to the concentration point	3	5	15	7	30	21.04
3.14	Composition of plume	7	9	15	7	38	15.14
*	Standard Deviation x 4						

ATTACHMENT IX

Viewgraphs of Guidelines for Abstraction/Testing Plan Development

- J. McNeish: Abstraction Plan Development in Working Groups**
- R. Barnard: Inputs from Other Workshops**
- D. Thomas: Planned/Ongoing Activities Supporting Disposal Criticality: WBS 1.2.2**
- P. Cloke: Abstraction Process for Internal Criticality (An Example)**
- R. Barnard: Development of Analysis Plans**

Abstraction Plan Development in Working Groups

Jerry McNeish
M&O/INTERA (DE&S)
19 March 1997

SAW Federal Services
Duke Engineering & Services, Inc.
E. R. Johnson Associates, Inc.
Fluor Daniel, Inc.
Fremont-Corpus Christi
Integral of Resources Group
INTERA, Inc. (DE&S)

TR Research Associates, Inc.
Kiewit/Parsons Behr/Kellogg
Lawrence Berkeley National Laboratory
Lawrence Livermore National Laboratory
Logicon RDA
Los Alamos National Laboratory
Monsanto-Kendron Corporation

SAIC
Sandia National Laboratories
TRW Environmental Safety Systems Inc.
Woodward-Clyde Federal Services
Winters & Strawn
Cooperating Federal Agency:
U.S. Geological Survey

Overview of Presentation

- Reiteration of Goals of Workshop
- What can PA use from Criticality Abstractions?
- Guidelines for abstraction plan working groups

Goals of Abstraction/Testing Workshop

- **Identification of Issues:** Identify and group the important issues with respect to *long-term performance*.
 - **Prioritization of Issues:** Prioritize the issues as to which are most important to address in the abstraction proposals.
 - **Develop Abstraction Plan:**
 - abstraction should produce reasonably accurate "bounding" behavior.
 - abstraction should be computationally efficient
 - heterogeneity and variability should be properly incorporated
 - spatial-temporal discretization should be adequately represented
-

Goals of Abstraction/Testing Workshop (continued)

- **Treatment of Uncertainty:** Ensure that appropriate parameter and behavioral uncertainty is included in abstractions; discuss how to quantify.
 - **Develop Testing Methodology:** Validate the abstraction through comparison with complex model.
 - **Coupling of Abstraction:** Ensure appropriate coupling with abstractions from other workshops.
 - **Scheduling/resources:** Coordinate with existing worksopes.
-

What Can PA use from Criticality Abstractions?

■ In-Package Criticality

- Criticality modified source term at specific time and location for specific scenarios [simplified source term]
- Criticality modified temperature as $f(\text{time, location})$ [response surface]

■ Near Field Criticality

- Simplification of criticality modified near field geochemistry [simple geochemical model]
- Criticality modified source term at specific time and location for specific scenarios [simplified source term]

What Can PA use from Criticality Abstractions? (continued)

■ Far Field Criticality

- Criticality modified source term at specific time and location for specific scenarios [simplified source term]
- Sensitivity analysis of effect of criticality location on performance [simple model of effect]

Format for Draft Abstraction/Testing Plans

1. **Title**
2. **Objective(s)**
3. **Hypothesis(es)** - This should make explicit connection to performance criteria.
4. **Product(s)** for TSPA-VA
 - a) Type of abstraction (e.g., response surface, distributions).
 - b) How to implement the product(s) in TSPA analyses.
5. **Issues covered by Product(s)**
 - a) Issues addressed and rationale.
 - b) Issues excluded and rationale.
6. **Abstraction/Testing Plan**
 - a) *Approach* - How will the abstraction be accomplished?
 - b) *Metrics* - Criteria to determine when abstraction is complete (e.g., the abstracted results are sufficiently comparable to process-level model results).
 - c) *Existing workscopes* - What portion of plan is covered by existing non-1.2.5 work?
 - d) *Information sources* - Previous analyses, other data sources, etc.
 - e) *Programs* to be utilized.
 - f) *Roles and responsibilities* of team - Identify people, affiliations, and tasks, in particular choose a lead member to act as interface to ACT for proposal development and implementation.
 - g) *Schedule* - Include 5/97 status and completion by 8/97.
 - h) *Other...*
7. **Model Assumption(s) and Uncertainty(ies)**
8. **Potential Follow-up Work**
9. **Inputs/feedbacks** to/from other WBS elements
10. **Potential Problems**
 - a) *Programmatic* - Resources, conflicts, schedule, etc.
 - b) *Technical* - Data availability, information needs, computational, etc.

Inputs from Other Workshops

R. W. Barnard
Sandia National Laboratories
March 19, 1997



Ties to Criticality Issues

In-Package Criticality

- In-package criticality is strongly influenced by
 - Waste-package degradation
 - failure of waste package marks start of processes leading to criticality
 - Near-field environment
 - pH, dissolved species of water; temperature affect rates of corrosion and other degradation processes
 - Waste-form degradation
 - engineered criticality-control measures can be degraded



2

Ties (Continued)

Near-Field Criticality

- Near-field criticality is affected by
 - Waste-form mobilization
 - fissile material moved from the waste package can accumulate in the drift
 - fissile material may be transported as solutes or colloids
 - Near-field environment
 - temperature, chemistry, mechanical stresses can all influence the formation of potential critical configurations
 - Thermohydrologic effects
 - water availability and flow when the repository is hot



3

Ties (Continued)

Far-Field Criticality

- Far-field criticality is influenced by
 - UZ flow and transport
 - sorption or filtration processes can cause accumulations of fissile materials
 - flow channeling and lateral diversion may cause accumulations
 - SZ flow and transport
 - organic deposits may provide reducing environment for depositing fissile materials
 - Near-field environment
 - residual effects from thermal excursions can alter hydrologic properties



4

Applicable Products from Workshops

(Analysis plans from completed workshops)

- Waste-Package Degradation
 - Processes for corrosion
 - outer barrier (corrosion-allowance material)
 - general corrosion
 - microbial-induced corrosion
 - inner barrier (corrosion-resistant alloy)
 - corrosion at exposed "patches"
 - Processes are influenced by near-field environment



5

Important Processes for Criticality From WPD Studies

- Outer-barrier corrosion
 - Models for aqueous corrosion will assume rate is a function of
 - temperature
 - pH
 - water chemistry
 - contact time
- Inner-barrier corrosion
 - Localization of corrosion at welds



6

NFE and T/H Analysis Plans

- The near-field environment analysis plans include
 - Characterization of the groundwater that can:
 - react with the waste package
 - transport radionuclides through the EBS
 - Investigation of colloid-facilitated radionuclide transport
 - this is an augmentation to the UZ-transport colloid analysis
 - will also include Pu colloids
- The thermohydrology workshop will investigate:
 - Drift-scale temperature, relative humidity, liquid saturation, flux
 - Seepage into drifts under “hot” conditions



7

Important Processes for Criticality from NFE Studies

- Model of water compositions
 - Time-dependent ranges of parameters for corrosion models
 - pH, Cl, F, SiO₂, CO₃, etc.
 - will consider various degrees of equilibration with concrete, tuff, steel
- Presence of colloids
 - Intrinsic Pu colloids
 - Pu sorbed on other colloids (e.g., iron oxides)



8

Important Processes for Criticality from T/H Studies

- Drift-scale T/H properties as a function of location
 - Temperature
 - Liquid saturation
 - Liquid-phase flux
- Seepage into drifts
 - Models for water seepage onto hot waste packages



9

Waste-Form Degradation and Mobilization Analysis Plans

- Spent-fuel dissolution
 - Determine time-dependent distributions
- Post-dissolution water chemistry and precipitated phase formation
 - Determine dissolved and transportable species



10

Important Processes for Criticality from WFD&M Studies

- Waste-form degradation
 - Time-dependent distributions for canister perforation
 - Alteration of DHLW glass and release of corrosion products
- Water chemistry
 - Develop a dissolution model
 - Determine rate of precipitated-phase formation
 - Alterations of water chemistry that could cause further interactions



11

Flow and Transport Workshops Analysis Plans

- UZ transport
 - Colloid-facilitated radionuclide transport
 - consider both fracture flow and coupled matrix–fracture flow
 - Sorption models for radionuclide transport
 - Review of environmental data on geochemistry
- UZ flow
 - Investigating perched-water models
- SZ flow
 - (coming up)



12

Important Processes for Criticality from UZT Studies

- Transient-flow transport
 - Effects of long-term changes in flow rates on transport
 - ^{237}Np (sorbing) and ^{99}Tc (nonsorbing) species
- Sorption models
 - Using K_d 's vs more sophisticated models
- Colloid transport
 - Transport by colloids in fractures with no matrix interaction



13

Important Processes for Criticality from UZ Flow Studies

- Perched water
 - Physical and stratigraphic controls on perched-water formation
 - Model the volume and residence times of perched water bodies



14

Summary

- TSPA-VA abstraction activities are developing models for the geologic processes for radionuclide transport
 - We must apply them to our modeling of potentially critical configurations
 - Many of the PI's from the other workshops are here
- The "rest of the story" — neutronics calculations — to follow



TSPA-VA Disposal Criticality Abstraction/Testing Workshop
Planned/Ongoing Activities
Supporting Disposal Criticality:
WBS 1.2.2

Daniel A. Thomas
March 19, 1997

FACR1WS PPT

WBS 1.2.2 Activities:

- **Burnup Credit for Commercial SNF**
 - Model Validation: isotopics/criticality
- **Material Degradation**
 - Barrier Materials (A516, A625, C22, ...)
 - Basket Materials (CS, SS)
- **Waste Form Degradation**
 - SNF
 - DHLW
- **Mechanical Degradation**
 - Rock Fall
 - Seismic

WBS 1.2.2 Activities: (Continued)

Probabilistic Evaluation Methodology

- **Variations**
 - Present and near term (up to a few hundred years following emplacement) values of well understood environmental parameters which will vary over the repository (e.g. water composition, temperature).
 - Criticality properties of the waste forms (e.g. burnup, enrichment)
- **Uncertainties**
 - Present and near term values of less well understood parameters (e.g. infiltration rate, ground water travel times)
 - Long-term behavior of parameters which are known to have varied over recent geologic/climatologic time (e.g. infiltration rate, level of water table)
 - Long-term properties of engineering materials (e.g. corrosion rate of SS-B)
 - Loading of individual waste packages, particularly commercial SNF
- **Use of probability distributions (pdf, CDF)**
 - Select the form of distributions most appropriate to the physical process (e.g. uniform distribution for quasi cyclic processes, normal distribution for parameters which may have well understood average values)
 - Select most likely value of parameter being modeled, and match this to the mean, or mode, of the selected distribution.

WBS 1.2.2 Activities: (Continued)

■ Probabilistic Configuration Determination Examples

- **Internal**
 - ♦ Sensitivity analyses for geometries
 - ♦ Sensitivity analyses for Fe₂O₃ & Boron
 - ♦ Applications to WP/EBS designs
- **External**
 - ♦ Sensitivity analyses
 - ♦ Engineering materials
 - ♦ Retardation and filtration
 - ♦ Hydrologic stagnation & focusing mechanisms

WBS 1.2.2 Activities: (Continued)

- **Criticality Consequence Model**
 - Primarily increase in radionuclide inventory
 - Internal
 - ♦ Steady state vs periodic
 - External
 - ♦ Methodology Development (NARC)
 - ♦ Possibility of additional consequences (autocatalitic, venting explosion)
- **DOE SNF and Pu Disposition**
 - Evaluations planned for 9 types, intent is to include 2 for TSPA-VA (AI clad, Shippingport)
 - Support evaluations for Pu disposition

WBS 1.2.2 Activities: (Continued)

- **Documenting Methodology**
 - Disposal Criticality Analysis Methodology
Technical Reports
 - ♦ Rev. 00 Technical Report, August 1996
 - ♦ Rev. 01 Technical Report, September 1997
 - Disposal Criticality Analysis Methodology
Topical Reports
 - ♦ Preliminary Topical Report, 1998

WBS 1.2.2 Activities: (Continued)

- **Applying Methodology to WP/EBS Designs**
 - **Commercial SNF WPs**
 - ♦ **Alternatives**
 - ♦ **Control Rods**
 - ♦ **Filler materials (Iron shot, DU)**
 - **DHLW and DHLW/DOE**
 - **WP support/invert design**
 - **Backfill, drip shields, and other additional barriers**

Abstraction Process for Internal Criticality (An Example)

**Paul L. Cloke
March 18, 1997**

B&W Federal Services
Duke Engineering & Services, Inc.
Fluor Daniel, Inc.
Framatome Cogema Fuels
Integrated Resources Group
INTERA, Inc.
JAI Corporation

JK Research Associates, Inc.
Lawrence Berkeley Laboratory
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
Morrison-Knudsen Corporation
Science Applications International Corporation

Sandia National Laboratories
TRW Environmental Safety Systems Inc.
Woodward-Clyde Federal Services
Winston & Strawn
Cooperating Federal Agency:
U.S. Geological Survey

PARAMETERS INCLUDED IN COMPLETE MODEL

Chemical

- J-13 Water Composition (14 measured elemental concentrations + pH)
- 21 More Elements Present in the Metal Barriers and Waste Forms
- Chemical Compositions of 304L Stainless Steel, Alloy 625, DHLW, Waste Glass, and either La-BS Pu Glass or Pu Rich Ceramic
- Reaction Rates for These 4 Components of the Waste Package

Physical

- Volume of Each Component of the Waste Package
- Surface Area of Each Component of the Waste Package
- Internal Surface of Waste Forms (i.e., Factor for Waste Fracturing)
- Infiltration Rate of J-13 Water

DOMINANT FACTORS CONTROLLING CHEMISTRY INSIDE WASTE PACKAGES (FOCUS ON PLUTONIUM WASTE FORMS)

Chemistry dominated by:

- Reaction with glass containing alkali and/or alkaline earths**
- Reaction with Cr/Mo alloys**
- Absorption of atmospheric CO₂**
- Oxidizing environment (atmospheric O₂ & radiolysis)**

Rate parameters:

- Flow through rate of water resulting in dilution and flushing**
- Waste form dissolution rates at long times**
- Metal corrosion rates**

DOMINANT FACTORS CONTROLLING CHEMISTRY INSIDE WASTE PACKAGES (FOCUS ON PLUTONIUM WASTE FORMS)

(Continued)

Thermodynamic data

- Above 25 ° C**
- For lanthanides & other neutron absorbers**
- Solids observed to form and not in current data base**

Attachment IX - Page 21

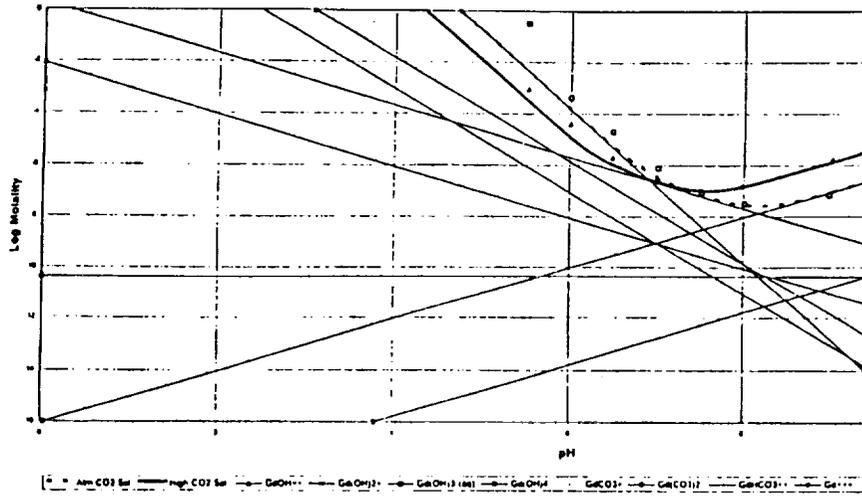


Figure C-1. Plot of idealized concentration of dissolved Gd species in equilibrium with $GdO(OH)_2$ (solid), corresponding total idealized Gd solubility, and EQ6 calculations of solubility. Heavy dashed line is for normal atmospheric partial pressure of CO_2 , and heavy solid line is for CO_2 partial pressure of 1.43×10^{-3} atm. Symbols at the ends of straight lines are provided only to enable the reader to identify lines for each aqueous species by use of the legend. They are not model results.

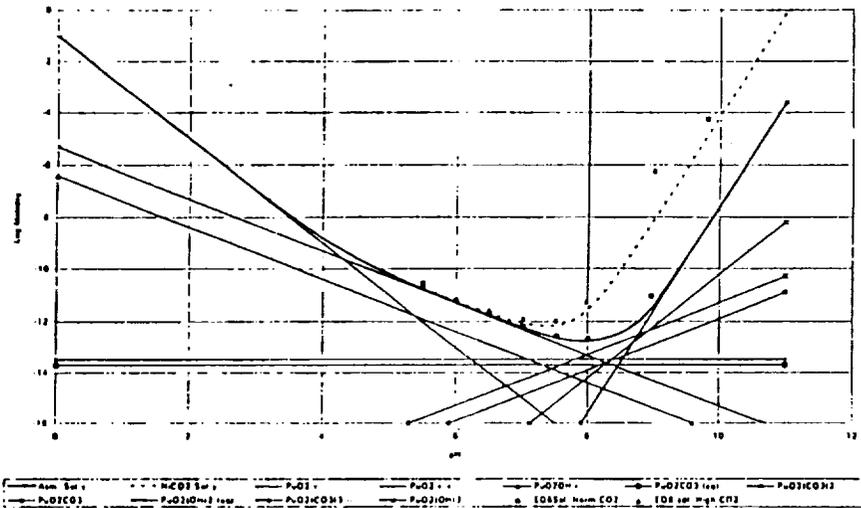


Figure C-2. Plot of idealized concentration of dissolved Pu species in equilibrium with PuO_2 (solid), corresponding total idealized Pu solubility, and EQ6 calculations of solubility. Heavy solid line is for normal atmospheric partial pressure of CO_2 , and heavy dashed line is for CO_2 partial pressure of 1.43×10^{-3} atm. Symbols at the ends of straight lines are provided only to enable the reader to identify lines for each aqueous species by use of the legend. They are not model results.

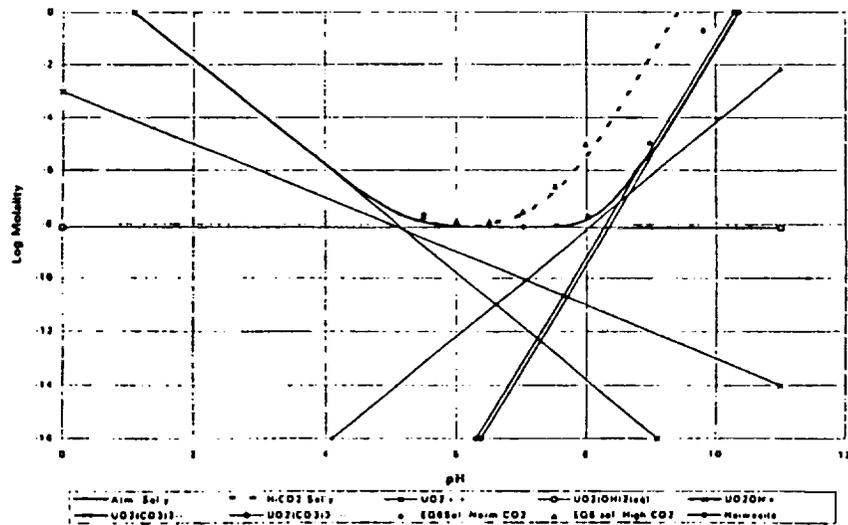


Figure C-3. Plot of idealized concentration of dissolved U species in equilibrium with solidite (except for $pH > 9$, when the solid is uranyl hydroxide), corresponding total idealized U solubility, and EQ6 calculations of solubility. Heavy solid line is for normal atmospheric partial pressure of CO_2 , and heavy dashed line is for CO_2 partial pressure of 1.43×10^{-3} atm. Symbols at the ends of straight lines are provided only to enable the reader to identify lines for each aqueous species by use of the legend. They are not model results.

CHEMICAL SPECIES CONSIDERED

631 Active Aqueous Species

589 Active Pure Minerals

57 Active Gases

8 Active Solid Solutions

RESULTS OF ABSTRACTION TO GET IMPORTANT CHEMICAL SPECIES

Gadolinium Species

- 1 Solid and 8 Aqueous Species

Plutonium Species

- 1 Solid and 9 Aqueous Species

Uranium Species

- 2 Solid and 5 Aqueous Species

Development of Analysis Plans

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Sandia National Laboratories
March 19, 1997

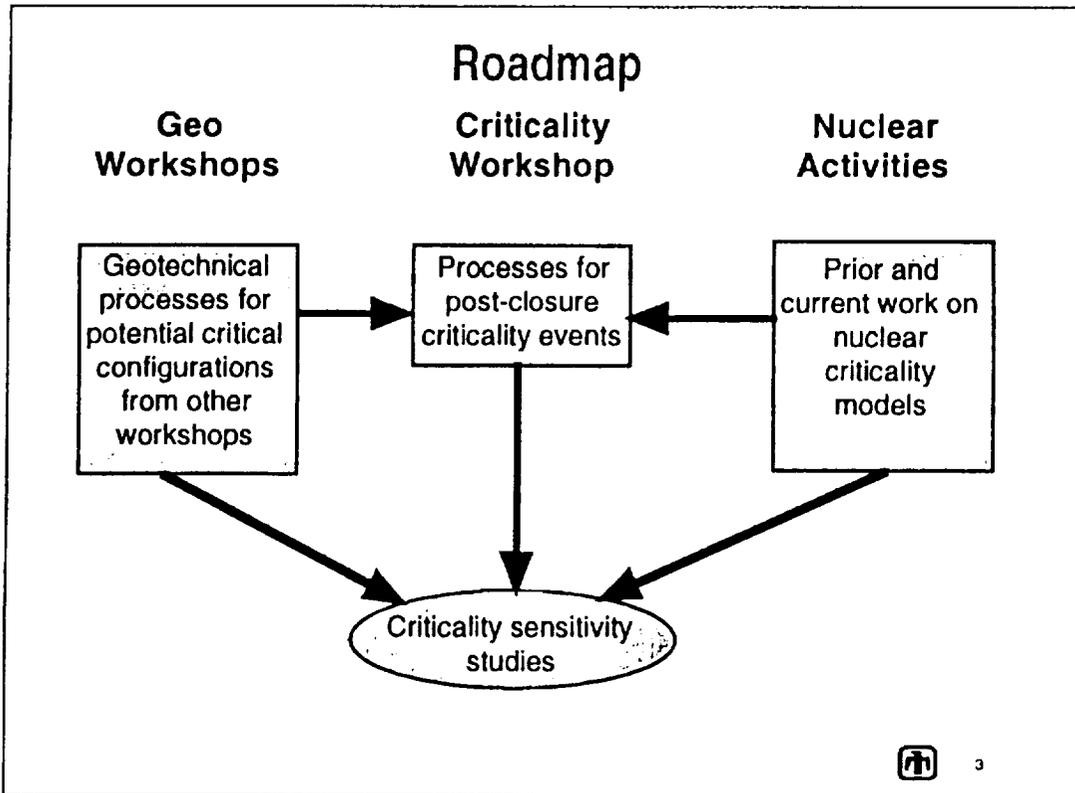


Overview

- We have identified and discussed the issues important to criticality
- We have prioritized the issues according to their impact on TSPA
- We have heard about other activities that can provide information on the constituent processes for our criticality models



2



- ## Mission
- Select the most important few issues for post-closure criticality
 - e.g., two scenarios from in-package criticality; one from far-field
 - Develop plans to identify and model the essential features of these issues
 - e.g., change in source term from a criticality event
 - Develop plans to identify the most important uncertainties in the models
 - e.g., changes in moderation due to groundwater chemistry
 - Identify the abstracted model that will come from these investigations
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