CNWRA 2001-02
Revision 1

RESPONSE TO THE EXTERNAL PEER REVIEW OF THE TOTAL-SYSTEM PERFORMANCE ASSESSMENT VERSION 3.2 CODE

Prepared for

U.S. Nuclear Regulatory Commission
Contract NRC–02–02–012

Prepared by

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

September 2001
Revised February 2003

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Response to the External Peer Review of the Total-System Performance Assessment Version 3.2 Code

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ABSTRACT

The U.S. Nuclear Regulatory Commission (NRC) undertook a formal independent peer review of the total system performance assessment methodology as embodied in the Total-system Performance Assessment (TPA) Version 3.2 Code in the summer of 1999. This peer review, organized by the Center for Nuclear Waste Regulatory Analyses (CNWRA), was conducted by eight scientists and engineers from outside the NRC high-level waste program who have expertise in material science, volcanology, hydrology, rock mechanics, geochemistry, radiation health physics, scenario analysis, and performance assessment. Each external peer reviewer provided an independent report documenting the strengths and weaknesses of the TPA code and the Total System Performance Assessment approach, evaluating the suitability of the TPA Version 3.2 Code for use in reviewing the U.S. Department of Energy License Application for the proposed Yucca Mountain repository. This report documents the response of the CNWRA and NRC staff to the comments of the external reviewers and describes modifications to the TPA code that have been made or are under consideration for inclusion in future versions of the code. Each suggestion put forward by the reviewers for improving the technical bases for the model abstractions, data used in the TPA Version 3.2 Code, and for improving the level of documentation used to support the TPA Version 3.2 Code has been responded to individually. The results of the external review, as summarized in this report and documented in full in the appendixes, have been used to a limited extent to assist in developing version 4.0 of the TPA code and will be used more fully as the code progresses toward version 5.0.

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CONTENTS (continued)

TABLES

ACRONYMS AND INITIALISMS

BIOMOVS	Biosphere Model Validation Study
CCA	Certification Compliance Application
CNWRA	Center for Nuclear Waste Regulatory Analyses
CSH	Calcium-Silicate-Hydrate
DCF	Dose Conversion Factor
DOE	U.S. Department of Energy
EDA-II	Enhanced Design Alternative-II
EPA	U.S. Environmental Protection Agency
EPR	External Peer Review
ERG	External Review Group
FEPs	Features, Events, and Processes
FP	Fission Products
GM	Geometric Mean
GSD	Geometric Standard Deviation
HMIP	Her Majesty's Inspectorate of Pollution
KTI	Key Technical Issue
LHS	Latin Hypercube Sampling
NRC	U.S. Nuclear Regulatory Commission
PA	Performance Assessment
PCO2	Partial Pressure of Carbon Dioxide
PDF	Probability Density Function
PSA	Probabilistic Safety Assessment
Ptn	Paintbrush Unit
QA	Quality Assurance
SCC	Stress Corrosion Cracking
SF	Spent Fuel
SKI	Swedish Nuclear Power Inspectorate
SZ	Saturated Zone
TEDE	Total Effective Dose Equivalent
TPA	Total-system Performance Assessment Code
TPI	Time Period of Interest
TSPA	Total System Performance Assessment
UK	United Kingdom
UZ	Unsaturated Zone
WIPP	Waste Isolation Pilot Plant
WP	Waste Package
YM	Yucca Mountain

TPA PARAMETERS

AlluviumMatrixPorosity_SAV	Alluvium Effective Porosity of Amargosa Valley Alluvium (unitless)
ARDSAV	Alluvium Matrix Retardation Factor in the Saturated Zone (unitless)
C_i	Concentration of Radionuclide, I, in the Waste Package Water (mol/m^3)
DiffusionRate_STTF	Effective Diffusion Coefficient in Saturated Tuff (m^2/yr)
F_{mult}	Flow Diversion Factor (unitless)
F_{ow}	Factor to Account for Divergence/Convergence of Water at the Surface of the Drift (unitless)
FracturesPerMeter_STFF(1/m)	Effective Spacing Between Transmissive Zones in the Tuff Aquifer (1/m)
FracturePorosity_STFF	Effective Fracture Porosity of the Saturated Tuff (unitless)
F_{wet}	Fraction of WPs that are Dripped on by Flowing Fractures (unitless)
I	Initial Infiltration Rate at Yucca Mountain (mm/yr)
ImmobilePorosityPenetrationFraction_STFF	Effective Fraction of Saturated Rock Matrix Accessible to Matrix Diffusion During the Time Scale for Transport From Source to Receptor (unitless)
K_d	Retardation Coefficient (m^3/kg)
K_s	Matrix Saturated Hydraulic Conductivity for the Topopah Spring-welded Layer (mm/yr)
K_{sat}	Matrix Saturated Hydraulic Conductivity for the Topopah Spring-welded Layer (mm/yr)
OO-Coflc	Coefficient for Localized Corrosion for the Outer Waste Package Barrier (m/yr)
q_{in}	Water Flow Rate into the Waste Package (m^3/yr)

TPA PARAMETERS (continued)

q_{out}	Water Flow Rate out of the Waste Package (m^3/yr)
V_{max}	Maximum volume of water that can be contained in the waste package before water escapes through holes in the waste package (m^3)
w_{ci}	Advective Mass Transfer out of the Waste Package (mol/yr)
WPDef%	Percent of Waste Packages that are Initially Defective (unitless)

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QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT: The computer codes ORIGEN 2.1, GENII-S, TPA Version 4.1h, and MCNP-4A were used for analyses described in this paper. All of these computer codes are controlled under the CNWRA quality assurance program. No CNWRA-generated original data is used in this report.

1 INTRODUCTION

The U.S. Nuclear Regulatory Commission (NRC), with assistance from the Center for Nuclear Waste Regulatory Analyses (CNWRA), developed a series of Total-system Performance Assessment (TPA) codes for use in quantitatively evaluating the U.S. Department of Energy (DOE) safety case for a proposed high-level waste repository at Yucca Mountain, Nevada. These TPA codes have already been used to demonstrate the NRC capability to conduct a performance assessment (Codell, et al., 1992), to evaluate preliminary Total System Performance Assessments conducted by DOE [e.g., Total System Performance Assessments–95 (TRW Environmental Safety Systems, Inc., 1995)], and to investigate the safety case supporting the DOE Viability Assessment (1998). Ultimately, a version of the TPA code will be used by the NRC to aid in determining if the quantitative basis of the safety case for Yucca Mountain presented in a potential DOE license application is sufficient for regulatory decisions.

1.1 Approach

Building confidence in a computer code requires, at a minimum, that the software developers implement adequate procedural controls, prepare suitable documentation, and conduct appropriate code testing and benchmarking. However, establishing the technical soundness of the code requires validation or verification of the underlying process models and their abstractions. For a multidisciplinary software development project as complex as Total-system Performance Assessment, establishing technical soundness may require the publication of peer-reviewed journal articles on the structure of, and results derived from, the TPA code as well as the scientific basis for the data and conceptual models used in the code and the conduct of coordinated technical and programmatic reviews by internal advisory committees, such as the Advisory Committee for Nuclear Waste, or external, independent peer review groups. Various peer-reviewed publications are cited in the TPA Version 3.2 User's Guide (Mohanty and McCartin, 1998) that provide the technical bases for selected model abstractions and input data. In addition, several papers have been submitted or will be submitted to peer-reviewed journals that describe the development, structure, and results of the NRC TPA approach [e.g., Eisenberg, et al., (1999); Lu and Mohanty (2001); Jarzemba and Sagar, (2000)]. However, developing the extensive body of peer-reviewed literature needed to support the TPA code is a time-consuming process that may be only partially completed prior to the review of a license application.

Conducting organized peer reviews by external experts for the purposes of establishing the technical or scientific merit of research and development programs is a well-established practice among federal agencies (U.S. General Accounting Office, 1999). The timing and execution of the peer review process are largely controlled by the organizing body. Therefore, organized peer reviews can be an efficient procedure for vetting a research and development program and abbreviated timeframes, typical of the high-level waste program, are more readily met. Moreover, by conducting the review in a group setting, the external reviewers are able to formulate more probing followup questions based on the synergism of group interactions. In addition, a greater volume of background reading material can be provided to the reviewers than might be possible for peer review of journal articles.

For agencies of the Federal Government, procedures for establishing and operating advisory committees and panels are prescribed in the Federal Advisory Committee Act of 1972. The Federal Advisory Committee Act requires that advisory committees conduct open meetings, that timely notice of such meetings be published in the Federal Register, that detailed meeting minutes be recorded, that records of all working papers and reports used by the committee be available to the public, and that each advisory committee meeting be attended by a designated officer of the Federal Government. Typically, organized peer reviews produce a committee consensus or a compilation of the individual reports of the reviewers.

Approximately 3 years ago, DOE established a Performance Assessment Peer Review Panel charged with providing an independent evaluation of the Total System Performance Assessment–Viability Assessment and suggestions for improving the Total System Performance Assessment approach to be used to support the license application. The DOE Performance Assessment Peer Review Panel, which operated for approximately 2½ years under Federal Advisory Committee Act guidelines, produced three interim reports and one final report that reflected the consensus view of the panel.

NRC instructed staff of the CNWRA to conduct an organized peer review of the TPA Version 3.2 Code and the overall NRC TSPA methodology. This review was not undertaken with the purpose of obtaining a consensus opinion from a panel and, therefore, was not subject to Federal Advisory Committee guidelines. Instead, the experts selected for the external review of the TPA Version 3.2 Code were asked to provide individual reports whose content would not be modified. The entire content of the reports received from members of the external review group is presented in Appendixes A–H of this report. While reference is made within this summary report to the external review group, it should not be construed that any of the observations or recommendations presented here are the product of a group or consensus opinion. The summary of key results contained in Chapter 3 is not intended to be a substitute for the complete individual reports provided in the appendixes. The reader is strongly urged to read each of the appendices, particularly if wishing to examine in detail the strengths and weaknesses of the TPA Version 3.2 Code.

The goal of the external review was to get input from the technical experts on the External Review Group Panel on whether the TPA Version 3.2 Code was sufficient to support NRC role as the regulator for the Yucca Mountain repository. In accordance with the provisions of the Nuclear Waste Policy Act of 1982, NRC has the responsibility to evaluate any license application for geological repositories constructed for the emplacement of high-level nuclear waste. The NRC review of the DOE TSPA is intended to be risk-informed, such that the items most important to the performance of the repository system will be subject to the greatest scrutiny during the NRC review process. The TPA code has been developed to integrate the detailed technical assessments for the different repository systems into a single code to provide insights into the most important aspects for repository performance. The TPA code is not intended to provide a comprehensive safety case for the Yucca Mountain repository itself; it is intended to be a tool that supports the NRC staff review of the DOE license application.

1.2 Summary Results

Each external peer reviewer report is contained as an appendix to this report. Other than converting to WordPerfect 8.0 format and renumbering the pages to fit the format of this summary document, the content and wording of these reports are unchanged. In general, the external peer reviewers were positive about the overall quality of the TPA Version 3.2 Code and concluded the code was suited for use in reviewing any DOE license application. Numerous suggestions were made by the external reviewers regarding improvements that should be made to the model abstractions and data used in future versions of the TPA code. In particular, one reviewer had serious concerns about the technical bases supporting the saturated zone flow and transport module. A predominant theme of the comments focused on the failure of the TPA Version 3.2 Code to include or explain the exclusion of coupled thermal-hydrological-mechanical-chemical processes. There was a general sense that TPA documentation was insufficient to explain the technical bases for the model abstractions, input data, parameter values, and probabilistic approaches embodied in the TPA Version 3.2 Code. Furthermore, the overall transparency of the code could be enhanced by preparing documents that explain how features, events, and processes were included or excluded.

1.3 Development of Responses

Developing responses to the external peer review comments involved numerous technical experts with diverse skills. In March 2000, an action plan was completed for responding to the external review of the TPA Code Version 3.2.[1] This plan cataloged each comment or recommendation, its location in the reviewer's report, and its status of resolution. Similar comments from multiple reviewers were combined and a tracking number was assigned to each individual or combined comment. This process resulted in identifying 234 comments requiring response. These comments were divided and submitted to the developers of the different modules that make up the TPA Version 3.2 Code.

This report provides the comprehensive response to the external review of the TPA Version 3.2. There are several general categories into which the responses to the comments of the external reviewers fall. Many comments are resolved by indicating that the recommended changes have been incorporated in the latest version of the TPA code, which has undergone one major revision since the external peer review was conducted (Version 4.0) as well as minor revisions (Version 4.1). Many of the changes made in these later versions addressed weaknesses identified by the external reviewers. Many other comments are resolved by indicating that the comment addressed is being considered for incorporation into the next major revision of the TPA code. Coding has begun to develop the TPA Version 5.0 Code, and suggestions for improvements to be incorporated into the code are being compiled and prioritized. Many suggestions for improvement result directly from comments made during the external review of the TPA Version 3.2 Code. The changes that become incorporated into the code will be determined by the significance of the proposed change (i.e., how much it affects performance) and the complexity associated with the incorporation of the change. Although there has not been a final decision on whether to incorporate individual changes, code developers and technical experts will look into these issues and decide whether these improvements to the

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[1]Firth, J. "Action Plan for Responding to External Review of Total-system Performance Assessment Version 3.2." Memorandum (March 6) to C.W. Reamer, Division of Waste Management, NRC. Washington, DC: NRC. 2000.

code could significantly affect the results of the code. It is likely that all risk-significant changes will be incorporated into Version 5.0 of the code. Other responses will refer to published work (either peer-reviewed literature or an NRC or DOE document) that demonstrates the issue identified by the reviewer does not have a significant effect on the results of the analyses. Alternatively, the responder may provide additional documentation to defend assumptions made in the modeling or parameter values selected for the analysis. Finally, many of the comments resulted from the external reviewer not being able to determine how the code works, based on the documentation provided. These comments were responded to by simply describing how the code performs the calculations in a clearer manner than documented in the user's guide for the TPA Version 3.2 Code. These comments will help to guide future revisions to the user's guide as they highlight areas where the documentation is not sufficiently transparent to allow a reviewer to fully understand how the TPA Version 3.2 Code works.

2 CONDUCTING THE EXTERNAL REVIEW OF THE TOTAL-SYSTEM PERFORMANCE ASSESSMENT VERSION 3.2 CODE

This section describes the process used to identify and select participants in the external review of the Total-system Performance Assessment (TPA) Version 3.2 Code, identifies materials provided to the reviewers in advance of the meeting, outlines the primary goals of the review and the questions to be addressed by the reviewers, and documents the meetings and overall schedule used in the review.

2.1 Selection of the Members of the External Review Group

The members of the external review group were selected using a peer nomination process. More than 120 letters were sent to members of the international performance assessment community, soliciting nominations for experts in eight general areas of technical expertise, including

- Geochemistry
- Hydrology
- Material Science and Corrosion Engineering
- Rock Mechanics and Mining Engineering
- Health Physics
- Volcanology
- Overall Performance Assessment
- Features, Events, and Processes Analysis

More than 50 responses were received. Based on the nominations received, clear experts were identified by peer acclamation in hydrology, geochemistry, and features, events, and processes analysis. Insufficient responses were received to provide a clear-cut preference in the remaining technical areas. Consequently, technical staff at the U.S. Nuclear Regulatory Commission (NRC) and Center for Nuclear Waste Regulatory Analyses (CNWRA) were asked to nominate reviewers to fill the remaining positions on the external review group. A final short list of reviewers was identified for the eight positions on the external review group.

The nominees selected were contacted regarding availability and willingness to participate in the external review of the TPA Version 3.2 Code. Several potential reviewers were not able to participate because of scheduling conflicts. The remaining nominees were asked to provide detailed information necessary to evaluate their ability to meet the CNWRA conflict-of-interest requirements. Restrictions were placed to eliminate those nominees working either currently or in the past as employees of the U.S. Department of Energy (DOE) or its contractors on the Yucca Mountain high-level waste disposal program. Several identified experts were eliminated from further consideration due to conflict-of-interest concerns.

Eight participants in the named technical areas were selected based on availability and freedom from conflict-of-interest (Table 2-1). Because of conflict-of-interest restrictions, five of the eight reviewers were from outside the United States. Because of the uniqueness of the

Table 2-1. Members of the External Review Group for the TPA Version 3.2 Code		
Reviewer	**Affiliation**	**Area of Expertise**
Dr. Barry Brady	University of Western Australia Perth, Australia	Rock Mechanics and Mining Engineering
Dr. Paul Delaney	U.S. Geological Survey Flagstaff, Arizona	Volcanology
Dr. Ghislain de Marsily	Laboratoire Géologie Appliquée Université Pierre and Marie Curie Paris, France	Hydrology
Dr. Robert Kelly	University of Virginia Charlottesville, Virginia	Material Science and Corrosion Engineering
Dr. Gérald Ouzounian	Agence Nationale Pour La Gestion Des Déchets Radioactifs (ANDRA) Châtenay-Malabry, France	Geochemistry
Dr. Brian Thompson	Independent Consultants Twickenham, United Kingdom	Overall Performance Assessment
Dr. Frits van Dorp	Nationale Genossenschaft für die Lagerung Radioaktiver Abfälle (NAGRA) Wettingen, Switzerland	Features, Events, and Processes Analysis
Dr. F. Ward Whicker	Colorado State University Ft. Collins, Colorado	Health Physics

proposed repository at Yucca Mountain, Nevada, technical expertise in the different components of the repository was considered more critical than familiarity with the DOE high-level waste disposal program.

2.2 Materials Provided to the External Review Group

For their initial independent evaluation of the TPA Version 3.2 code, the TPA Version 3.2 Code User's Guide (Mohanty and McCartin, 1998) and the NUREG–1668 (NRC, 1999) were provided to each member of the external review group.

In addition, references cited in the reports were provided to the reviewers upon request. Reference sections in the individual expert reports attached as Appendixes A–H identify the additional material that was reviewed. The materials for review were provided to the members of the external review group prior to the group meeting to allow them to familiarize themselves with the conceptual approach to TPA used by the NRC and the CNWRA. Approximately 7 weeks were available to review the material prior to meeting with NRC and CNWRA staffs in San Antonio, Texas. Final comments (Appendixes A–H) were provided by the reviewers about 3–4 weeks after that meeting.

2.3 Primary Goals of the Review

The overall goal of conducting the external review of the TPA Version 3.2 Code was to receive an independent critical evaluation of the NRC approach to performance assessment from recognized authorities in different fields of research. The review focused on the TPA Version 3.2 Code and associated documentation. It was stressed to the reviewers that the purpose of the TPA Code is to provide a review tool for NRC staff reviewing any DOE License application, and is not intended to make a comprehensive safety case itself. More specifically, the members of the external review group were provided with a list of primary goals to establish the scope of the review and help focus their review of the TPA Version 3.2 Code. In particular, the reviewers were asked to

- Examine the methods and assumptions of the NRC studies as implemented in the TPA Version 3.2 Code
- Recommend improvements that could be made in subsequent revisions, modifications, and updates to the TPA Code
- Evaluate implementation of conceptual models, including parameter choices
- Determine whether the NRC approach to TPA is suitable for achieving its objectives to review the DOE license application and associated performance assessments

In addition to these primary goals, the external review group was provided with specific questions to consider in evaluating the TPA Version 3.2 Code.

- Is the TPA Version 3.2 Code sufficiently complete?
    - Are the included features, events, and processes sufficient to provide credible results and meaningful insights? If the included features, events, and processes are not credible, can the nature and degree of conservatism be explained?
- Are the conceptual model abstractions and data defensible?
    - Are the conceptual model abstractions and data appropriate for the spatial and temporal scales being considered and for the selected performance measure?
    - Are the model abstractions and data supported by site information or other related information to ensure the credibility of the results? If they are not credible, can the nature and degree of conservatism be explained?
    - Is the documentation sufficient to provide an understanding of the approach?
    - Is the level of conservatism and simplicity of approach appropriate considering the role of the NRC?

- Are parameter values reasonable?

  — Are the parameters used in the TPA Version 3.2 Code appropriate to the abstractions?

  — Is the functioning of the code adversely affected by the parameters or the ability to obtain values for the parameters?

- What are the strengths and weaknesses of the TPA Version 3.2 Code as a tool in supporting the NRC licensing decision?

- What improvements to the code would panel members recommend, taking into consideration the intended application of the code to support the NRC licensing decision?

As necessary, the reviewers were also requested to provide questions and discussion points to be raised with the staff in advance of the 3-day meeting held on July 27–29, 1999, in San Antonio, Texas.

2.4 Meetings and Schedule

Seven of eight experts attended a meeting held at the CNWRA in San Antonio, Texas, on July 27–29, 1999. Because of scheduling conflicts, Dr. Paul Delaney visited the CNWRA 2 weeks earlier on July 13–14, 1999. During the meetings, the reviewers were provided with additional information on the regulatory framework for high-level waste disposal in the United States, the role of the TPA Version 3.2 Code in the licensing process, site characteristics at Yucca Mountain, conceptual models used in the NRC TPA Version 3.2 Code, the basis for model parameters and parameter uncertainty, TPA Version 3.2 Code results, sensitivity analyses with the TPA Version 3.2 Code, and the CNWRA quality assurance program. Reviewers were provided copies of all presentation materials and encouraged to ask questions during the presentations. Time was also allotted for discussion at the end of each day, and the afternoon of the final day was reserved for a summary discussion.

At the conclusion of the meeting, all members of the external review group were asked to independently prepare a brief report evaluating their general areas of expertise in the TPA Version 3.2 Code. As appropriate, the reviewers were also asked to review and comment on other parts of the overall TPA Version 3.2 Code. In each report, the reviewers were specifically asked to provide

- Descriptions of areas of the TPA Version 3.2 Code reviewed
- Weaknesses of the TPA Version 3.2 Code in these areas
- Strengths of the TPA Version 3.2 Code in these areas
- Recommendations for improving subsequent versions of the TPA Code in these areas

Although the reviewers were requested to provide independent review comments, they were encouraged to contact each other following the meeting as necessary to ensure that comments made on areas outside their areas of expertise were sound and technically correct.

3 RESPONSES TO THE COMMENTS OF THE EXTERNAL REVIEWERS

This chapter provides a response to all comments made by the external reviewers. It is noted that the summary of a reviewer's comment does not necessarily include the full context of the comments made by the external reviewers. To get the entire context of the comments, the reader is encouraged to read the reports provided by the reviewers of the Total-system Performance Assessment (TPA) Version 3.2 code, which are included as Appendixes A–H. Specifically, the report written by Brady is attached as Appendix A; the report written by Delaney is attached as Appendix B; the report written by de Marsily is attached as Appendix C; the report written by Kelly is attached as Appendix D; the report written by Ouzounian is attached as Appendix E; the report written by Thompson is attached as Appendix F; the report written by van Dorp is attached as Appendix G; and the report written by Whicker is attached as Appendix H.

The detailed technical presentations made by U.S. Nuclear Regulatory Commission (NRC) and Center for Nuclear Waste Regulatory Analyses (CNWRA) staffs during the formal meeting relieved the initial concerns of several external reviewers regarding the technical bases for the code. Additionally, many reviewers had concerns about the quality assurance program under which the code was developed prior to the formal meeting. These concerns were mostly eased by the formal and informal briefings on CNWRA configuration control procedures. These concerns indicate that the currently available background material supporting the TPA Version 3.2 code, given to the reviewers prior to the formal meeting, did not provide sufficient information about the technical underpinnings for the model abstractions, input data, and probabilistic approaches embodied in the code.

Many comments were made by the external reviewers that applied to the TPA Version 3.2 code and the overall performance assessment process, such as comments related to code documentation. These comments will be addressed first, followed by the comments identified for each of the specific technical areas.

The comments relevant to the specific technical areas are organized by integrated subissues, which is the format expected to be used to review the U.S. Department of Energy (DOE) license application. The organization of the integrated subissues correlates well with modules of the TPA Code, however, there are some differences. Table 3-1 contains a crosswalk between integrated subissues and modules of the code. Note that some code modules are related to more than one integrated subissue.

Each specific comment is identified by comment number, the reviewer's name, and where the comment can be found within the reports of the reviewers. For example, the notation (A–3) in the comment indicates the comment is located on page 3 of Dr. Brady's review report, which is attached as Appendix A.

Table 3-1. Crosswalk between Integrated Subissues and TPA Code Modules	
Integrated Subissue	**TPA Code Module**
Degradation of Engineered Barriers (ENG1)	EBSFAIL
Mechanical Disruption of Engineered Barriers (ENG2)	FAULTO, SEISMO
Quantity and Chemistry of Water Contacting the Waste Package and Waste Form (ENG3)	NFENV, EBSREL
Radionuclide Release Rates and Solubility Limits (ENG4)	EBSREL
Climate and Infiltration (UZ1)	UZFLOW
Flow Paths in the Unsaturated Zone (UZ2)	UZFT
Radionuclide Transport in the Unsaturated Zone (UZ3)	UZFT
Flow Paths in the Saturated Zone (SZ1)	SZFT
Radionuclide Transport in the Saturated Zone (SZ2)	SZFT
Volcanic Disruption of Waste Packages (Direct1)	VOLCANO
Airborne Transport of Radionuclides (Direct2)	ASHPLUMO
Dilution of Radionuclides in Water due to Well Pumping (Dose1)	DCAGW
Redistribution of Radionuclides in Soil (Dose2)	ASHRMOVO
Lifestyle of the Critical Group (Dose3)	DCAGW, DCAGS

3.1 Comments Relevant to the Entire Code

Comment 5: A weakness is the possible lack of versatility in analysis of repository layouts different from the standard drift-and-pillar planar design. (p. A–2) It is doubtful if the code is sufficiently flexible to handle possible radical changes in repository layout. One objective of further development on the TPA Code should be to ensure that generic repository designs other than drift-and-pillar layouts can be simulated. (p. A–3) Concerns about the effectiveness of shedding as a method of controlling WP exposure to percolating and refluxing groundwater could conceivably lead to changes in repository layout more radical than those expressed in the EDA-II design. (p. A–8) This reviewer was left with the impression that the design change (i.e., EDA-II) was not accommodated readily by the current TPA Code functionality. (p. A–10) [Brady]

It is acknowledged that the code is not flexible enough to handle radical changes in design. However, it is believed that the code is sufficiently flexible to handle expected changes to design. Development of a code that is completely flexible such that it could accommodate all possible layouts would be more expensive than is appropriate for the needs of the high-level waste program. Limited staff resources are better spent improving models for the expected repository design than developing models for other designs. The framework for the TPA Version 3.2 Code was consistent with the viability assessment repository design, but did not include features such as a drip shield or the revised spacing of emplacement drifts considered for the EDA-II repository design. Revision to the TPA Version 4.0 Code was necessary to evaluate the EDA-II repository design. It is expected that radical changes to design are less likely as the project matures.

Comment 6: Decoupling of many FEPs raises questions about the extent to which all the possible modes of repository response will be captured in the performance simulations. A qualification study on a repository analogue could provide strong support for an inference of an acceptable level of completeness of the formulation. (p. A–2) [Brady]

Appropriate coupling of features, events, and processes for inclusion in performance assessment is currently being evaluated. An attempt is made to represent key features, events, and processes with a sufficient degree of coupling, either represented in the TPA Code or through abstraction of detailed process-level model results. In many cases, the conceptual models and supporting data are highly uncertain and, therefore, a conservative approach is considered. NRC and CNWRA staff are concerned about the decoupling of features, events, and processes in performance assessment and have raised questions to DOE about considering the range of repository performance when evaluating features, events, and processes for screening. While analogs for pieces of the repository model may exist, the repository system has no relevant analog. Typically natural analog information is used to develop a basis for the detailed process-level conceptual models and data used in the TPA Code. If conceptual models are able to accurately model natural analog systems, it provides confidence that the degree of coupling in the models is sufficient. For example, one alternative for the dissolution of the source term uses a model for the dissolution of schoepite based on data collected from natural analogs. However, due to insufficient knowledge of the conditions of the natural analog, it may be difficult to justify the use of a less conservative model based on evidence from a natural analog system. However, natural analogs are used to provide insights into the processes modeled by the TPA Code as appropriate.

Comment 12: The documentation of the code would be improved considerably if the interaction or coupling between the FEPs was mapped as an influence diagram or a matrix, and the strength of each interaction was evaluated explicitly. (p. A–9) It would be useful to build an "influence diagram" in which all the FEPs taken into account both as internal and external are linked to all the relevant processes on which they may have an effect. An additional document then describes, for each link, the reason why this link is not considered important in the TPA, or on the contrary how it is incorporated in the process system. (p. C–8) [Brady/de Marsily]

Model abstraction chapters in the TPA user's manual conclude with a section on assumptions and conservatisms. These sections list the main features, events, and processes addressed by the models. The suggestion of developing a cross-matrix to show the couplings addressed by the TPA Code will be taken into account for a future revision of the user's manual. The reasons for couplings not accounted for will be explained better in the documentation for the code, either in the form of appendixes or as an independent document. NRC and CNWRA staff will consider elaborating a cross-matrix of features, events, and processes to highlight considered couplings in a future TPA Code. Couplings not accounted for will require additional explanation.

Comment 13: Flexibility in application is a feature that must be provided intrinsically in further development of the code. (p. A–10) [Brady]

Flexibility in application is a feature that will be included to the extent practicable. However, experience to date with the TPA Code suggests that the flexibility in application of the tool is not the limiting feature. Rather, creativity of the analyst is most important in determining how the code can be used. In addition, continual analyses with the code [such as documented in the NRC sensitivity analyses report (1999) provided to the External Review Group and the TPA Version 3.2 Code sensitivity analyses report] (NRC, 1999) identify weaknesses in the code that are improved in future code versions. It is common to have proposed code changes that do not technically influence the models or computation but are targeted at improving flexibility of application.

Comment 25: It is not clear which FEPs were excluded and based on what reasons. A more rigorous classification of the FEPs, of their roles and of the consistency of their introduction in the Process System or the Scenarios would be desirable. (p. C–3) Documentation of the origins of many of the modules, data, and side analyses needs to be more traceable. The methodologies used for the selection and rejection of different FEPs are not clearly outlined in the documentation. (p. D–8) The scenario development methodology must be explained and documented. Sensitivity studies may also be used to focus some of the scenarios. QA and traceability are important in order to record how decisions were made at each step, to include or not an event or process. For those scenarios which have not been analyzed, justification must be given. In order to allow NRC to independently review DOE's approach, NRC needs to have its own capability to generate a set of FEPs and scenarios. For each of the scenarios, definition of the range and boundaries of the given set of models and data is requested in order to prove that computation was not performed out of the valid domain. (p. E–5) [de Marsily/Kelly/Ouzounian]

The TPA Code is designed as a review tool to look at vulnerabilities in any DOE license application, not to make a comprehensive safety case itself. The TPA Code has been developed by an iterative process and the gradual identification of the elements relevant to performance. It is the responsibility of the DOE to produce a comprehensive collection of features, events, and processes applicable to the proposed geologic repository system at Yucca Mountain. In case relevant features, events, and processes are identified that are not currently addressed by the TPA Code, effort will be made to include those in the TPA models. Model abstraction chapters in the TPA user's guide conclude with a section on Assumptions and Conservatisms. This section lists the main features, events, and processes addressed by the models. In the future this section will be enhanced with an explanation of why some features, events, and processes have not been addressed. The TPA Code and the user's manual have been produced following internal quality assurance guidelines that require traceability of modules and data. Nonetheless, additional effort will be made to enhance traceability in future versions of the manual. The enforced quality assurance requirements guarantee that the TPA Code is fully traceable to our internal records. Scenario development in the TPA Code has been accomplished through an iterative process. Several potential and relevant disruptive scenarios such as volcanism, faulting, and seismic activity have been identified. If other scenarios and processes not currently modeled are noted as important, the TPA Code will be modified accordingly. Sensitivity studies (among other studies) have been used to revise the DOE approach of considering only two relevant scenarios: volcanic disruption and nominal. Staff disagree with the viewpoint that the only way to independently review the DOE approach to scenario analysis is to develop a comprehensive set of features, events, and processes and scenarios. Resources are better used by gaining familiarity with the scenario analysis process and reviewing DOE studies by NRC subject matter experts. Relevant testing has been completed to verify that computations are performed within valid domains. Sensitivity studies have been used to complement the testing effort. Elaboration of a separate document outlining the ranges of operation of the system submodels or TPA Code submodules would be beneficial, and its future production will be considered. See also the response to Comment 12 in this section in this section.

Comment 40: The level of QA for the TPA Code appears to be less than the level DOE prescribes for its contractors. Should NRC use a different level of QA than DOE? (p. C–9) [de Marsily]

The TPA Code was designed and built in accordance with a technical operating procedure designed to produce quality results with a significantly smaller staff than DOE. The CNWRA uses Appendix B of 10 CFR Part 50 and NQA1-1986 (American National Standards Institute/American Society of Mechanical Engineers, 1986) requirements for its quality manual and these flow to the controlling procedures. These standards include requirements to validate computer codes. Validation of the TPA Code is expected to be completed in fiscal year 2003. The DOE procedures are more prescriptive than the CNWRA's procedures, but the CNWRA procedures have been judged to be adequate to produce a quality code. The TPA Code is meant to assist the NRC in confirming certain DOE assumptions regarding the high-level waste repository, not to build a licensing case.

Comment 41: The test cases and comparisons for each of the modules of the TPA Code made during the course of code development should be better documented to provide evidence of the confidence that can be placed on the TPA Code. (p. C–9) [de Marsily]

A software validation test plan for the TPA Code is being developed. This document will outline the types of tests that will be performed to build confidence that the software accurately implements the conceptual and mathematical models. The validation of the TPA Code is expected to be completed and documented in fiscal year 2003.

Comment 42: The TPA Code should be verified against the DOE TSPA Code using a test case where the two codes could be given parameters and assumptions as close as possible to each other. (p. C–9) [de Marsily]

Because of substantial differences between the TPA Code and the DOE Total System Performance Assessment Code in modeling and parameterization, it is difficult to verify the TPA Code against the DOE Total System Performance Assessment Code. Nevertheless, an initiative was undertaken to model the DOE conceptualization and parameter values using the TPA Version 3.2 Code. Results from these analyses were presented at a DOE and NRC technical exchange. An example comparison for container life modeling can be found in

Pensado and Mohanty (2000). Because of serious limitations encountered during this effort, no additional attempts have been made to replicate the DOE conceptual models using the TPA Code. New efforts are currently underway to model the NRC conceptualization using the DOE Total System Performance Assessment software for selected components of the TPA Version 4.1 Code. In addition, outputs from the TPA Version 3.2 Code have been compared at the intermediate results level where such comparison is possible. For example, the validity of the DOE use of the Gaussian Variance Partitioning approach was assessed by performing stylized calculations using the TPA Version 4.1 Code.

Comment 43: The decision not to include couplings, heterogeneities, and complexities into the PA models needs to be reevaluated periodically. (p. C–9) [de Marsily]

The need for coupling between processes and modules was identified early in the development process for the TPA Code. Early development of the TPA Code attempted to incorporate the most signficant couplings in the repository system into the code. As development of the code has continued, additional couplings have been added to the TPA Code to improve the modeling of the system. Heterogeneity within the repository system is accounted for through the use of different subareas to model different regions of the repository and through the use of distributions for parameter values that may vary spatially. As more information becomes available on the heterogeneity of the natural system, the system is divided into a different number of subareas. The repository area is now divided into ten subareas instead of the seven subareas that were used in the TPA Version 3.2 Code. The level of heterogeneity, as well as the level of complexity in the TPA Code is re-evaluated during the development of each new version of the TPA Code. There is a delicate balance to be achieved between increasing coupling, heterogeneity, complexity, and maintaining a tool that is computationally efficient. It is expected that the TPA Version 5.0 code will have improvements in coupling of modules and processes.

Comment 45: Another method to be considered for the sensitivity studies is to fix one parameter at selected values and perform a full stochastic analysis for all other parameters. (p. C–10) [de Marsily]

This concept has been applied to verify approaches to select influential parameters. Example applications of this approach can be found in Lu and Mohanty (2001) and Mohanty and Wu (2001).

Comment 47: The lumping of the water from all four SZ streamtubes is inadequate since they represent different zones of the repository that may have different waste package failure rates, etc. (p. C–17) [de Marsily]

The regulations require dose to be calculated to the reasonably maximally exposed individual. The Reasonably Maximally Exposed Individual is a member of a rural-residential community defined to be located 18 km [11.2 mi] south of the repository. The TPA Code models the dose to the Reasonably Maximally Exposed Individual by assuming that 100 percent of the radionuclides that reach the Reasonably Maximally Exposed Individual location are captured by wells that pump a specified quantity of water each year. These radionuclides are diluted by this volume of water to determine the concentration of radionuclides in the water. The four streamtubes contribute to the total quantity of radionuclides that reach the Reasonably Maximally Exposed Individual each year, and, therefore, the TPA Code representation of variability in waste package failure times and transport properties in the different areas of the repository is sufficient to check compliance with the regulation.

Comment 49: Documentation that allows a full analysis of the entire structure of the code needs to be assembled. (p. D–2) The User's Guide is inadequate for a comprehensive review of the approach being taken by NRC to analyze the eventual DOE license application. It is recommended that a document that provides a traceable overview of all aspects of the TPA Code be developed and maintained. (p. D–4) [Kelly]

The methods used by NRC to use the TPA Code in a review of the DOE license application will be documented directly in the quantitative review strategy and the demonstration of the review strategy, which are both expected to be completed in fiscal year 2003. Note that the TPA Version 5.0 code or one of its subsequent revisions will be used to evaluate any DOE license application. The TPA User's Guide will provide a traceable overview of most aspects of the TPA Code, including a better description of the structure of the code. (Also see response to Comments 115, 123, and 129 in this section.)

Comment 62: The documentation system needs substantial improvement to allow newcomers to the code to efficiently develop a grasp of what factors are and are not being considered, the process by which the selections were made, and the influence of the selection of the various parameters. (p. D–9) [Kelly]

The purpose of the Assumptions and Conservatisms section for each module was intended to convey to the reader what is considered in the model and their potential impacts. For additional clarity, these assumptions will be expanded and revised and additional references to the most recent supporting documents will be added (also see Comments 115 and 123 in this section).

Comment 63: This documentation can be improved, especially by adding a logical flow-chart for each module, as given for some during the EPR meeting. (p. E–3) [Ouzounian]

An attempt was made to develop a flow diagram for the TPA Code, particularly for the executive driver of the code. Because the code is largely serial in nature, such flow diagrams were not considered essential to improving transparency and traceability of the code. Flow diagrams for several abstracted models exist in supporting documents, such as the container life and source term module presented in the EBSPAC User's Guide (Mohanty, et al., 1996). Similar flow diagrams will be developed for other abstracted models if warranted by the complexity and level of coupling of the processes.

Comment 64: The underlying work, models, data, and assumptions should be more traceable. The links between the phenomenological or process level and the performance assessment level should be described in a comprehensive and accessible way. (p. E–4) [Ouzounian]

Traceability is valued as an important component of the TPA Code, and the NRC has continually attempted to improve the documentation of the code to make connections between process-level work and the TPA Code more traceable. Although the NRC does not have the need or resources to build a comprehensive documentation pyramid similar to the DOE where analysis and model reports contain the detailed calculations and bases for parameter samples that are summarized into process model reports which are then combined into the top-level total system performance assessment documents, the traceability of the TPA Code will be improved in future versions of the user's guide.

Comment 65: Having teams in charge of describing the processes and mirror teams performing sensitivity analyses gives certainly all chances for an efficient work. (p. E–4) [Ouzounian]

This recommendation does not address either the substance of particular models or other approaches used in the Total-system Performance Assessment code, so no changes in the Total-system Performance Assessment code are needed to address this comment.

Comment 67: Each iteration between a new selection and calculated dose to man will lead to a new ranking of radionuclides and selection as to be reconsidered for each step. Thus, exercises performed with TPA Version 3.2 Code would have benefited from previous results. (p. E–5) [Ouzounian]

Early versions of the TPA Code tracked 43 radionuclides, which were selected based on inventory considerations and review of DOE work. As the development of the code progressed and experience with the code increased, developers were able to identify various radionuclides that did not contribute significantly to the results. Many radionuclides were removed from the base case to reduce the computational burden. Therefore, the current set of 20 radionuclides tracked for the groundwater pathway is indeed based on previous results with the code. Periodic analyses, such as the one described in Appendix I, are conducted to ensure that the set of radionuclides tracked is sufficient for the latest models in the TPA Code.

Comment 68: A specific methodology, starting from the total inventory of radionuclides to be disposed of, must be defined and described. It can lead to the same selection as the one used, but will be justified. (p. E–5) [Ouzounian]

Periodic analyses are conducted to ensure that the set of radionuclides modeled in the TPA Code are sufficient to represent the dose from the repository. The latest iteration of this process is described in Appendix I of this report.

Comment 76: On p. 2-10, the residential community is indicated to be < 20 km from the repository. Is it possible to be more specific about the location? (p. H–5) [Whicker]

The residential receptor was defined as an alternative for perspective only. The U.S. Environmental Protection Agency (EPA) has defined the Reasonably Maximally Exposed Individual as a member of the public expected to be located 18 km [11.2 mi] south of the repository. More information on the selection of the Reasonably Maximally Exposed Individual is provided in the Federal Register notice for 10 CFR Part 63. Because the location of the Reasonably Maximally Exposed Individual is now specified by 10 CFR Part 63, the option of using the residential community is no longer used.

Comment 90: The fourth column in Appendix A often gives two values. Do these represent the range, the 5th and 95th quantiles, or what? For lognormal distributions (e.g., p. A–48), why not give the GM and GSD? (p. H–7) [Whicker]

The TPA Version 3.2 Code uses a utility called SAMPLER to access either Monte Carlo Sampling or Latin Hypercube Sampling routines to calculate and manage parameter distributions. In TPA Version 3.2 Code, Latin Hypercube Sampling has been modified by (i) adding log-triangular, exponential, and finite exponential distributions; (ii) modifying the user-defined distribution; and (iii) replacing the beta distribution, but is otherwise used as described in NUREG/CR–3624 (Iman and Shortencarier, 1984).

Detailed descriptions of each distribution available in TPA Version 3.2 Code are included in Section 3.3.1 and Appendix D of the TPA Version 3.2 Code User's Guide. Typically, where two numbers are listed, they represent either the 0.1 and 99.9 percentile values (for distributions such as normal and lognormal) or the minimum and maximum values (for distributions such as uniform and log-uniform). It was decided to display these values instead of means and standard deviations because they both define the distribution equally well, and displaying the extreme values gives the reader a quick idea of the actual range of the parameter.

Comment 91: Also, many parameters in Appendix A appear to be treated as constants, yet many of these must be somewhat uncertain. Is it clear anywhere why these are treated as constants? (p. H–7) [Whicker]

As stated in the introduction to Appendix A of the TPA Code User's Guide, the base case data set evolves as technical staff use the TPA Code and analyze the results. Additionally, sensitivity analyses were performed (NRC, 1999) to determine which parameters were most important to repository performance. A parameter's importance is characterized by its influence on performance or on uncertainty in the performance measure. The sensitivity studies allow the staff to focus on what is likely the most important phenomena relative to performance and to point out deficiencies in the current state of knowledge. Parameters that have been shown to not have a significant effect on performance may be set to constant values to reduce computational burden and focus sensitivity studies on the most important parameters. The TPA Code retains a high level of flexibility in that most parameter values, even those listed as constants, can be treated as sampled parameters if new information or analyses make it necessary. The TPA Code's flexibility gives the NRC the capability to analyze a great number of repository configurations and scenarios that may require study. The introduction in the TPA Code User's Guide has been improved to include additional information on the purpose and intended use of the TPA Code. NRC agrees that information on the current status of parameter distribution development would be helpful to many users of the TPA Code in the future and will consider adding such information.

Comment 94: A "Knowledge Management" system to coordinate all data, models, simulations, etc., together with records of decisions, assumptions, and omissions that led to a particular PA result, should be implemented. If such a system is not already being set up by NRC, then the most important recommendation that results from the present review is that NRC management should have the courage to pause the apparently continual process of PA development and refinement in order to consolidate a well-defined release of TPA and all related assessment tools, techniques, and datasets. Then to spend substantial time and resources designing and implementing

this support system and all the resulting linked documentation in order to reveal the strength of their achievements to the scientific and technical world beyond the Yucca Mountain program. (p. F–1) The justification quantitatively for these model abstractions and the reference data is not clear as written and requires the new documents to provide traceable, transparent, and defensible support for each module. This should be done in combination with the aggregation of data and compatible accounting of uncertainty. (p. F–10) [Thompson]

A regulator does not need to develop a documentation system for their performance assessment tool as comprehensive as recommended; however, future revisions to the user's guide, as well as future iterative performance assessment reports based on use of the TPA Code, will endeavor to improve the traceability of the major decisions made in the performance assessment program. NRC and CNWRA staff expect that the potential license applicant (DOE) will produce documents that describe the Total System Performance Assessment process in a traceable and transparent fashion, similar to what one would expect in the knowledge management system described in the the comment.

Comment 95: Should the time period of interest be extended beyond about 100,000 years (say), then considerable further development is likely to be needed. (p. F–1) Substantially longer time periods of interest will require consideration of futures with two or more volcanic events and somewhat larger seismic magnitudes. The complexity of the sampling scheme explained during the ERG Meeting may then approach that of the WIPP CCA, Helton (1998). (p. F–10) [Thompson]

10 CFR 63.311 requires an evaluation of repository performance for 10,000 years. Extension of the time period of interest beyond 100,000 years would require considerable further development to account for features, events, and processes not considered for the 10,000-year calculation. 10 CFR 63.341 requires the DOE to perform calculations out to peak dose for the Environmental Impact Statement, so changes to the TPA Code to extend analyses to longer times are under consideration for incorporation into the TPA Version 5.0 Code.

Comment 97: The reasons for including the present combination of features, events, and processes in the TPA system model are not stated nor the procedure followed to decide what should be left out. Therefore, it is not possible to be sure that the representation is sufficiently comprehensive for purpose. (p. F–3) Nowhere is this process of conceptualisation and reduction described and justified, whether using FEP analysis or by some other method. There is no visualisation of the results of this process, for instance, using influence diagrams as in the regulatory assessments undertaken in Sweden, SITE '94, SKI (1996), and in the UK, Dry Run 3, Thorne (1993). (p. F–10) Formal elicitation and documentation of all steps from raw data and FEP catalogues, for instance, to the conceptual model of the integrated system used in TPA is needed. (p. F–10) How all potential relevant FEPs and, in particular, the KTI have been selected, including detailed reasons for this selection and for the omission of others, should be documented. This should include all potential interactions between FEPs (e.g., coupled processes) and the reasons why they are in- or excluded. How the included features, events, and processes and their interactions are treated in the different scenarios as well as in the different process level models and in the modules of the TPA Code should be documented. (p. G–3) In order to allow the NRC having an independent review of DOE's

approach, it is also needed to have its own capability to generate a set of FEPs and scenarios. For each of the scenarios, definition of the range and boundaries of the given set of models and data is requested in order to prove that computation was not performed out of the validity domain. (p. E–5) [Thompson/Van Dorp/Ouzounian]

The TPA Version 3.2 Code User's Guide is complete with regard to the listing of the features, events, and processes addressed by the models. The TPA Code has been developed through an iterative process, not necessarily starting from features, events, and processes catalogs. The approach taken by staff has been to gradually enhance the TPA model by expansion (i.e., include new elements considered relevant to the Yucca Mountain system) and revision (modify implemented models). Identification of important features, events, and processes for inclusion in the TPA Code depends on staff insights, which are augmented by review of the results of the DOE's studies.

Comment 100: There appears to be no overall mass or activity balance maintained throughout the entire system. (p. F–3) [Thompson]

Overall mass balance or activity balance that verifies that the code is working correctly has been conducted and documented in scientific notebooks. Figure 3-30 of NUREG–1746 (Mohanty, et al., 2001) provides a summary-level plot of cumulative activity releases at the engineered barrier subsystem, unsaturated zone outlet, and saturated zone outlet as a function of time, that qualitatively demonstrates the correctness of activity release. More quantitatively rigorous tests will be performed and documented in accordance with the software validation test plan currently under development. The validation of the TPA Code is anticipated to be completed in fiscal year 2003.

Comment 101: The three methods of abstraction outlined in Section 3.1 are all acceptable, in principle, but it is impossible to say from the present documentation if they have resulted in sufficiently precise approximations to observation and/or the results of calculations at a more detailed level. Evidence of quantitative verification/calibration is required, under conditions that lead to the higher dose realisations in TPA simulations, rather than for realisations based upon expected values of the independent variables. (p. F–3) [Thompson]

The TPA Version 3.2 code represented only a snapshot of the ongoing NRC performance assessment capability development effort. Quantitative analysis (e.g., cross-comparison of models and scenarios) for building confidence in the correctness of calculation can be found in several documents, such as NUREG–1746 (Mohanty, et al., 2001) and Mohanty and Rice (2000). For subsequent versions of the TPA Code, rigorous technical bases have been developed for abstracted models; though the effort is not uniform across all abstracted models. A software validation test plan is currently under development for the TPA Code. The validation of the TPA Code is expected to be completed and documented in fiscal year 2003. This validation will encompass the range of parameter values used in the TPA Code.

Comment 102: In order to independently reproduce the models (and their associated data) from fundamental source information, the entire chain of reasoning needs to be recorded, together with the uncertainties and biases accumulated at each stage and the evidence used, for instance, in expert elicitations. Such a record typically may be distributed over several supporting documents and a roadmap diagram, see Sumerling

(1992), provided in each section of Chapter 4 would then enable the reader to recover the abstraction process. (p. F–3) [Thompson]

The recommendation to include a reasoning roadmap diagram in each of the module description sections of Chapter 4 (NOTE: Chapter 4 was divided into separate sections for each module in the interim TPA Version 4.0 User's Guide) is being consided for inclusion in the User's Guide for the TPA Version 5.0 Code. Roadmaps may be included in the reports outside the TPA User's Guide that describe the model abstraction process from detailed process models, field studies, or expert elicitations.

Comment 103: Appealing to a bibliography indexed solely by authors' names is inadequate and does not satisfy fundamental requirements of traceability or transparency. (p. F–4) [Thompson]

The bibliography is indexed according to the Chicago Manual of Style. The references in the main text and in Appendix A of the TPA Code user's manual as referenced should be sufficiently traceable to allow a reader to find the referenced information.

Comment 104: High-risk reanalysis should be performed and documented to provide confidence in the modules of TPA and, hence, give a better idea of their domain of applicability. (p. F–4) [Thompson]

Several documents, such as NUREG–1746 (Mohanty, et al., 2001), Lu and Mohanty (2001), and Mohanty and Wu (2001), produced subsequent to the external review, describe the effort toward high-risk reanalysis, although the term is not used explicitly. Important barriers and processes and associated models and parameters have been identified through sensitivity and importance analyses. Based on this information, important subissues have been identified. This information has been further used by the key technical issues to conduct additional process level studies, which are then used to update abstracted models or parameter ranges for additional confidence. NRC and CNWRA staff plan on improving model support for the abstracted models used in the TPA Code.

Comment 105: The extensive and honest comments show that at least 230 of the approximately 830 items listed in Appendix A seem not to be justified by a clear, traceable record back to reliable sources. (p. F–4) Have the items 'assume;' as quoted in the references, been independently reviewed and justified or are they open to further challenge because they may not be traceable to relevant sources? (p. F–4) [Thompson]

Indeed, many sources for the parameter values cannot be currently cited and include descriptions like assumed, best estimate, conservatively assumed, assumed due to lack of information, and assumed due to limited information. This area should see improvement in future versions of the TPA Code, but it is one that may never be completely resolved, for several reasons. One reason is that the DOE repository design is not final, so although the TPA Code has been in development for nearly 10 years, many of the parameters, parameter values, or both are relatively new additions made in response to design changes. A second reason is that priority has been placed on parameters demonstrated to be important to repository performance. Less important parameters have received less attention in the update process. Nonetheless, NRC is working toward using the best available data and using a more traceable and transparent methodology to report the sources for the TPA Code parameter values.

Comment 106: The need to distinguish clearly where proponent's data and assumptions are adopted and if these have been done only after independent review? (p. F–4) [Thompson]

It is agreed that sources for all data and assumptions should be transparent and traceable. The NRC has and will continue to ensure to the extent practical that all data and assumptions provided by DOE are made known. The TPA Code was developed to permit NRC to study and gain understanding of the potential repository system. Where DOE data are used in the TPA Code, NRC staff considers their appropriateness for the Yucca Mountain repository system. If DOE submits a license application for the repository, all data and assumptions provided by DOE will be independently reviewed by NRC during the licensing review. Until such time, the TPA Code and its supporting data will continue to be iteratively improved and updated.

Comment 107: Data from design studies and site-specific investigations, including the ESF, should be highlighted, as opposed to information from other sites or of a general nature. (p. F–4) [Thompson]

Attempts have been made to ensure that data and assumptions generated from design studies and site-specific investigations are clearly indicated in Appendix A. The highlighting of such data will continue to be improved as development of the TPA Version 5.0 Code User's Guide continues.

Comment 108: When data or judgements are 'expected,' or are to be further 'evaluated,' the references to explicit work packages in NRC or DOE (YM) forward programmes should be given. (p. F–4) [Thompson]

We agree that it would be useful to provide information in Appendix A related to expected future work or studies. In a general sense, all parameters within the TPA Version 3.2 Code are being reviewed and refined. Because this is implicit, it would be useful for NRC to provide a brief reference to ongoing work related to a parameter, when that information is available. In this way, future TPA Version 3.2 Code users would know if a particular parameter was being actively studied and by whom. Currently, Appendix A includes a reference to the staff member responsible for developing the parameter range so an interested reader could contact that staff member directly to find out the current status of additional work to improve estimates of the parameter's range. NRC agrees that information on the current status of parameter distribution development would be useful to many users of the TPA Code and will consider adding such information during development of the User's Guide for the TPA Version 5.0 Code.

Comment 109: Many 'constants' could misrepresent the true level of uncertainty. Elicitation of Maximum Entropy PDF's over ranges bounded by physical fundamentals (say) would be much better. (p. F–4) [Thompson]

Parameter values are set to constants in the TPA input file for one of two reasons: (i) there is little uncertainty in the parameter value (items such as waste package dimensions or physical constants like the boiling point of water at the repository horizon) or (ii) reasonable ranges of the parameter value have little effect on the results of the calculation, and, therefore, the parameter value is set to a constant to reduce the computational burden on the code. Neither reason for setting the parameter values to constants misrepresents the true level of uncertainty in the code.

Comment 110: Unbounded Gaussian PDF's are unjustified surely as the truncation is open to endless discussion. (p. F–4) [Thompson]

The distribution selected to represent parameter values is the distribution that was judged to best represent the available data. For many parameter values, unbounded Gaussian probability distribution functions are used because they represent the data reasonably well and are more mathematically tractable than other distributions. As implemented in the TPA Code, the input file specifies the 0.1 percent and the 99.9 percent values of the distribution, but these do not limit the values that can be sampled. In theory, any value in the distribution could be sampled if enough realizations of the code were run.

Comment 112: Much is made of correlations, but in hardly anywhere are they to be found or elicited (especially if not multivariate Normal?). (p. F–5) [Thompson]

Correlation is introduced through the sampling techniques in the Latin hypercube sampling program. Parameters that are nonnormal can also be correlated. The TPA Version 4.0 User's Guide (prepared after the external review) provides documentation on parameter correlation in Appendix A as well as in the main text where the models that use correlated parameters are described.

Comment 113: Uncertainty is not well expressed by point estimators such as means, medians, etc., but rather by showing how the percentiles of dose, and other output of interest, vary over time and depend upon assumptions. Comparisons of design options (as in NUREG–1668) could be compromised by not showing (say) the 95 to 5 percentile range as well as sample estimates of the mean. (p. F–5) [Thompson]

One factor in favor of the emphasis on the mean dose is that the regulation, 10 CFR Part 63, is based on mean dose. In this regard, the mean results are more meaningful than the extreme values of the output distribution. Nevertheless, the 5^{th} to 95^{th} percentile range of results would enhance the presentation of the effects of parameter changes and alternative conceptual models, and the range will be included in future TPA sensitivity studies.

Comment 114: Displaying only indications of high doses does not give a balanced 'reasonable' account of estimated behaviour when a large proportion of realisations show values that are much lower than regulatory limits and may satisfy targets for acceptable or negligible levels of risk. (p. F–5) [Thompson]

Peak expected dose in the compliance period is the regulatory standard to be met. The use of Monte Carlo or Latin Hypercube Sampling technique to calculate peak expected dose generally involves giving equal weight to all realizations, including the most optimistic and pessimistic realizations. Because the NRC primary emphasis is on safety, the focus on high doses is aimed at revealing features and processes represented through models and parameters that are most significant to safety.

Comment 115: Uncertainty needs to be logically and defensibly determined at the level of basic information from site studies, design, and research in terms of scales appropriate to the quantities concerned. Then it needs to be translated into estimates for the various modelling levels of detail, used as the assessment proceeds, ending in the PDF's and bias evaluation for the aggregated quantities used in TPA models. This

reasoning, including questions posed to elicitation groups operating at a system or at a process level, was not readily apparent from information supplied. (p. F–5) [Thompson]

The process modelers provided the uncertainty representation of data (i.e., probability distribution and nominal data) based on site data, and multiscale studies. Many reports have been produced by the process modelers documenting the analyses and time-dependent values presented in Appendix B of the TPA Version 3.2 Code User's Guide. In future installments of the TPA Version 3.2 Code User's Guide, rationale will be provided either by referencing those documents or using abstraction from those documents to support the probability distributions used for the parameters described in Appendix A.

Comment 116: Importance sampling was clearly shown to have considerably greater efficiency than either random or LHS and should be considered seriously for the NRC programme in future developments of TPA. (p. F–6) Further examination of sampling methods and of statistical convergence is required. (p. F–11) [Thompson]

There were several earlier studies conducted by NRC and CNWRA staffs, not directly related to TPA, that explored forms of importance sampling including mean value, advanced mean value and adaptive importance sampling in which the results were compared to standard Monte Carlo and Latin Hypercube Sampling strategies (Wu, et al., 1993). The mathematical models were restricted to relatively small numbers of independent variables. The model results show the superiority of the importance sampling strategies by results converging with fewer samples, but proved troublesome for complex models with large numbers of independent variables such as the TPA Code.

More recently, NRC and CNWRA staffs have been including alternative sampling strategies to enhance sensitivity and uncertainty studies of TPA Code results. Staff used the Fourier Amplitude Sensitivity Technique (Cukier, et al., 1975) for selectively sampling the input parameters to extract sensitivity information in a non-random way, which covers the ranges of the input parameters. Staff are also exploring factorial design of experiment methods such as the Morris method (Morris, 1991) and those methods based on orthogonal matrices (Plackett and Burman, 1946).

NRC and CNWRA staffs continually try to update methods used for sensitivity and uncertainty analyses. Further evaluation of new sampling strategies will be made based on priorities for NRC and CNWRA resources.

Comment 117: Without confidence intervals on results, such as those in NUREG–1668, however, the conclusions from sensitivity analysis, and the comparison of different PA, cannot be entirely credible. (p. F–6) [Thompson]

Staff agree with this comment and will endeavor to include confidence limits in future TPA Code results. These confidence limits will be included by (i) running the TPA Code several times starting with different random seeds, (ii) approximating the confidence interval of fractiles of the distribution of results such as the median or 90th percentile directly from analytical expressions using distribution-free statistical methods, and (iii) approximating the confidence interval of the mean by the bootstrap method (Efron, 1982), where the mean results would be calculated by resampling from the output pool or results.

Comment 118: Sophisticated statistical methods appear broadly to support the general conclusions reached in this study, but they appear to this reviewer to rely upon non-intuitive assumptions of monotonicity and normality. They seem to have been overruled by engineering ceteris paribus methods when planning future DOE work. (p. F–7) [Thompson]

This comment refers to the fact that the TPA Code may not have a monotonic response to the independent variables (i.e., there could be more than one peak response for each independent variable). Regression methods applied to the Monte Carlo results may fail to show a multimodal response for some of the independent variables even if they exist because the regression equations tend to be low-order (first or second order only). Furthermore, these regression equations are applied over the whole range of the independent variables, so responses in certain parts of the space of the independent variables cannot be discriminated.

Staff recognize the shortcomings of regression methods for sensitivity analyses. However, the problem of multimodal response surfaces is not overlooked. The results of the Monte Carlo analyses are examined carefully to notice if there are particular ranges of parameters leading to unexpected or high peak doses. When high dose realizations are found, the staff tries to find reasons for the high values, and does not simply rely on the results of the regressions. Furthermore, the staff uses peak dose for each realization as the dependent variable because it is likely to show the most sensitivity. The regulatory criterion (10 CFR Part 63) however, is the peak of the dose averaged at each time step over all realizations. This mean dose is less likely to show a multimodal response to the independent variables. CNWRA staff have recently developed a sensitivity method based on the peak of the mean dose, and this method will likely be added to future performance assessment analyses (Mohanty and Wu, 2001).

Comment 119: Elicitation of PDF ranges and shapes may not achieve confident consensus. The implications of differing opinions about inputs to PA should be explored. (p. F–7) [Thompson]

Alternative conceptual models are considered in the NRC (1999). See response to Comment 125 in this section.

Comment 120: Overuse of bounding or conservative reasoning can be a serious concern if it leads to estimates for mean values that are so biased that they nullify the entire logic of a risk-informed simulation approach using Monte Carlo sampling to account for uncertainty. (p. F–7) [Thompson]

Overuse of bounding or conservative reasoning can be a serious concern if propagated through a performance assessment model. The performance assessment staff have a goal of maintaining as much realism in the TPA Code as possible. For instance, the amount of moisture that may flow into drifts is highly uncertain. Instead of setting seepage equal to the infiltration rate, highly uncertain parameter distributions are used to represent the processes. However, because a key goal of the NRC is to maintain public safety, some processes or distributions are represented conservatively when minimal information is available.

Comment 121: The assessment 'Toolkit' needs to be explained clearly and not only from the analyst point of view, but also from a software engineering standpoint. A full structured documentation system seems invisible as yet (from the material supplied) and should be stated well in advance of licensing reviews. (p. F–8) [Thompson]

Software engineering for the TPA Code has been largely documented in the software requirements description document and the software development plan document. These documents were maintained to fulfill quality assurance requirements and were not available to the reviewers. A software validation test plan is currently being developed. This plan will be applied to the TPA Version 5.0 Code. Additional stand-alone documents will be developed if funding is available. This work is planned to be performed during fiscal year 2002 and beyond.

Comment 122: The TPA manual and all related documents should show the document structure and give references to standards, etc., separately from general scientific references. Data flows could be illustrated graphically and could, in principle, be obtained from CASE tools. Configuration management is understood to apply to everything consistently, including program versions, simulation cases, data sets, control files, output files, and post processing results, all co-ordinated and recorded to avoid mismatches, etc. and, of course, all related documentation. (p. F–7) [Thompson]

A complete coordinated set of documentation is an admirable goal, and it is our intent to provide a consistent set of documents as much as possible. However, high performance CASE tools can be expensive and require a shift in operating procedures with associated training for all involved. In addition, consideration must be given to the resources required, because some of the test runs produce more than 6 GB of output data. The TPA Code uses the Software Configuration Control System, provided by the Solaris operating system, to control all source codes developed as part of the TPA system. The data files associated with test cases are submitted to the quality assurance staff who place the files in a permanent archive. Staff believe these actions are sufficient for this project.

Regarding data flow, Figure 3-1 in the TPA Version 3.2 Code User's Guide presents the best compromise of a flow diagram for the TPA Code. A complete calling tree was generated automatically by the SUN compiler, which resulted in too much information on one page to be usable. Also, Table 5-2 in the TPA Version 3.2 Code User's Guide presents a topically arranged list of data files used by the TPA Code. This information has been enhanced and appears in Table 19-2 in the TPA Version 4.0 User's Guide.

Comment 123: It is somewhat disturbing that no documentation was referenced for the following TPA Modules: UZFLOW, NFENV, EBSFAIL, EBSREL (are these in EBSPAC?), UZFT, SEISMO, VOLCANO, ASHPLUMO, ASHRMOVO (are these in ASHPLUME?), DCAGW, DCAGS. (p. F–8) [Thompson]

The development of abstracted models was documented either in journal papers or reports. Many of these documents were being developed at the time of the external review. Also, many abstracted models represent the current state of knowledge. Consequently, for those cases, the abstracted model represents the corresponding detailed models. For all stand-alone codes, there were corresponding user's guides that describe the models in detail. For example, EBSFAIL and EBSREL are described in the EBSPAC User's Guide. In the TPA Version 5.0

User's Guide, the references will be updated, and a clearer connection will be established between abstracted model support and detail process-level model support.

Comment 124: There is no clear reference to EXEC in the User Guide, and there appears to be no separate document showing how best to design and implement new modules for incorporation into TPA. It is not clear if EXEC permits loops in the call sequence of modules. (p. F–9) [Thompson]

The EXEC module is a high-level control module and, as such, is typically not made available to the consequence module developers. All execution controls are in EXEC and are separate from the consequence modules. It was intended that the consequence module developers would have limited need to know of the mechanics of how subareas or realizations are controlled. The only requirement is that the consequence module developers accept the array that contains the physical quantities that are input to their module, and return their output in a second array. This interface is described in the software change report. New TPA Code modules are added with the consent of the NRC and the Program Manager. Face-to-face meetings are required with the program manager and the development staff before work on a new module can be authorized via a software change report or similar instrument. The EXEC Code loops through realizations and subareas during the execution of the code. However, the order in which the modules are called are hard-wired into the code and cannot be changed to allow loops in the call sequence of modules.

Comment 125: No attempt seems to have been made to explore the sensitivity of the results to the shape and range of parameter PDF's. (p. F–10) Further sensitivity studies might usefully explore the influence of uncertainty over such PDF elicitation. (p. F–11) Has the influence of the choice of parameter distribution function on the result been evaluated? (p. G–7) [Thompson/van Dorp]

Evaluation of the sensitivity of the results to the shape and range of probability distribution functions is currently ongoing. Because of the large number of parameters sampled, efforts were focused on parameters identified as influential from previous sensitivity analyses.

Comment 126: The present implementation of TPA seems somewhat dated and the user interface requires too much knowledge about and interest in FORTRAN and in-file handling from the user, who should be allowed to concentrate upon the regulatory tasks without distraction of computing considerations. There is a confusion between 'Auxiliary Codes' and 'Auxiliary Files,' which are unrelated. There is no general purpose Post-Processing Module, as seems standard for other PA codes. (p. F–10) [Thompson]

The TPA Code was developed to satisfy the NRC requirements and interests starting in 1991. No requirement was provided for language independent I/O files or graphical user interfaces. Development of TPA pre and post-processors are currently ongoing. When these processors are fully developed, the user of the code will not have to use UNIX or FORTRAN commands to exercise the TPA Code and, thus, can concentrate more on regulatory tasks. While it is true that the auxiliary codes are not necessarily related to the auxiliary files, they both are auxiliary to the main TPA execution module and its input file (tpa.inp). The auxiliary codes are stand-alone codes that run at the request of and are controlled by the TPA executive. The auxiliary files are a library of reference data files that are seldom modified.

Comment 127: 'Conservatism' is claimed but not demonstrated for the assumptions underlying many models, data values, and distributions. No formal decision logic records seem to have been kept nor is the subsequent evaluation of cumulative bias undertaken as proposed under the HMIP programme, Thompson and Williams (1997) for instance. (p. F–10) Conservatism needs to be evaluated by a bias evaluation procedure at all stages of model development. If consistent levels of conservatism are not achieved, comparisons between performance assessments may be misleading, and the present data and results using TPA Version 3.2 Code should be evaluated to see if significant further development is really necessary to meet 10 CFR 63 requirements. (p. F–11) [Thompson]

The claims of conservatism have been substantiated with straightforward reasoning where possible and documented either in the main text or in the assumption section for each module. In those areas where straightforward reasoning is difficult, either the calculation has been propagated through the TPA Code to determine conservativness or detailed process-level analyses have been conducted outside the TPA Code to determine the conservative bound. For instance, a complete TPA calculation is conducted to determine whether high temperature or low temperature is conservative. A detailed thermo-hydrological coupled process calculation is then conducted using the MULTIFLO computer code to corroborate the TPA Code estimation of thermal regime. A greater effort will be made in future revisions to better document information produced to substantiate assertions of conservativeness. A bias evaluation procedure may be adopted (to the extent feasible) to evaluate the level of conservativeness propagated at various levels (e.g., model level or component level) in the TPA Code.

Comment 128: Model + data + uncertainty must be handled at each stage in a comprehensive and compatible manner. (p. F–10) [Thompson]

The performance assessment team relies extensively on the other KTIs for data interpretation, identification of relevant FEPs, development of key process-level modules, and related abstracted modules. The documentation for the TPA Code will provide direct reference to other NRC and CNWRA reports that describe in detail the processes that led to the construction of each consequence module. Particular attention will be paid to providing references that support the treatment and propagation of uncertainty.

Comment 129: Detailed documentation can show whether the developed code fulfills the requirements implied by the assessment context. The document does not contain sufficient information. Scenario development can be a tool to demonstrate, in a structured manner, sufficient completeness or comprehensiveness of an assessment. It can be used to identify interactions between different FEPs. (p. G–2) [van Dorp]

NRC will include a modest treatment of features, events, and processes and the scenario analysis procedure adopted when developing the TPA Code in future versions of the TPA Code User's Guide. NRC will not conduct the type of exhaustive scenario analysis required of the DOE, upon whose performance assessment results the licensing decision will actually be based. The features, events, and processes that NRC views as important for consideration in the performance assessment have been passed onto DOE. DOE included those features, events, and processes in its database. Because NRC has been reviewing the database for comprehensiveness, knowledge gained from the review is used in developing the TPA Code.

Comment 130: It is not clear what the position of this document is within a documentation system. Such a documentation system could show the past and future phases and the different tasks and results of a series of performance assessments. (p. G–2) [van Dorp]

Past iterations of the performance assessments have been summarized at a high level, and key findings and issues are documented in the TPA Version 4.0 Code User's Guide and the TPA Version 3.2 Code sensitivity analyses report. These documents also provide rationale for the current phase of the study, though in a highly condensed form. A regulator does not need to develop a knowledge system as comprehensive as is recommended; however, future revisions to the user's guide, as well as future iterative performance assessment reports based on use of the TPA Code, will endeavor to improve the traceability of the major decisions made in the performance assessment program. In particular, greater emphasis will be placed on describing how risk insight have changed as the TPA Code has evolved with clear ties drawn to the findings which led to the evolution of the code. NRC and CNWRA staffs will certainly expect the potential license applicant (DOE) to produce documents to support a transparent and traceable license application

Comment 131: The flow of information from field and laboratory observations, measurements, and experiments, through system understanding, the development of conceptual models, the development of process level models, to the development of the Total-system Performance Assessment code should be documented. This should include the source of the information, e.g. general, DOE, or NRC and CNWRA. (p. G–4) [van Dorp]

See the response to Comment 130 in this section.

Comment 132: Although scenario development techniques are being applied, they seem not to be used for demonstrating "comprehensiveness". (p. G–5) [van Dorp]

NRC has not completed and documented a systematic effort to determine comprehensiveness of scenario analysis by compiling, categorizing, and screening features, events, and processes. NRC, has, however, used the experience gained from the previous iterations of performance assessment and from the review of the DOE effort toward ensuring that the TPA Code represents all important features, events, and processes in the Yucca Mountain system. NRC does not believe the systematic development of a comprehensive list of features, events, and processes is necessary for future development of the TPA Code. NRC, however, has identified numerous features, events, and processes documented in the key technical issue-specific issue resolution status reports, and has communicated those to the DOE. DOE has now included these features, events, and processes in its database.

Comment 133: The Document concentrates, as the title suggests, on the description of the code. However, in a review, the evaluation and assessment of the actual system understanding and the conceptual models behind the codes are more important. (p. G–6) [van Dorp]

The user's guide documents what is included in the abstracted model and the assumptions made in developing the abstracted model. Many documents have been developed since the external review providing process-level support to these abstracted models. The list of references and the description in the user's guide will be updated for consistency with the process-level documents.

Comment 134: Imposing too many restrictions and/or simplifications, to assure short runtimes for inclusion into a probabilistic code, can reduce transparency and the code might, under certain conditions, not behave as expected. (p. G–6) [van Dorp]

NRC agrees with this comment in that a balance is needed between complexity and execution time. A tool that is extremely complex and represents processes in great detail but cannot be executed is of little value. There are a couple of components to the code development process that address this issue. First, at the process-level, staff typically conduct extensive evaluation and modeling external to the TPA Code to evaluate what is needed and what is important. Second, simplified abstractions of the effects of the processes are developed for incorporation into the TPA Code. For example, a thermohydrology calculation may take 10 hours of computation time to develop the temperature and moisture response for the near field. Fully coupling this calculation to the TPA Code would be computationally prohibitive. However, after the response is developed, it can be abstracted into the TPA Code via a look-up table or regression relationship. Process-level staff evaluate the output of the TPA Code to see if the abstraction of the process in the TPA Code adequately represents the process model output.

Comment 135: Uncertainty in parameters might dilute the calculated risk (as discussed at the External Review Meeting of 27–29 July 1999) [D. Hodgkinson in D. Savage (editor) The scientific and regulatory basis for the geological disposal of radioactive waste, Wiley and Sons Chichester 1995, Section 10.1.6 Risk dilution in PSA, page 364]. (p. G–6) [van Dorp]

NRC staff are aware of the phenomenon of risk dilution in performance assessment calculations. Interestingly, one of the reviewers (Thompson) (Page F–7, Section 3.6.1 of this peer review) comments that changing the shapes of the distributions (but maintaining the same mean values) can either lead to a decrease or an increase in risk, depending on the functional dependence of dose on the variable. He further states that " ... judgements during probability elicitations should not be swayed by concerns over so-called dilution effects on risk."

In an effort to gain confidence in the extent to which risk dilution is a problem, staff have performed some numerical experiments with probabilistic codes similar to TPA in which the input distributions for the independent variables were changed by making them broader, but with the same mean values. In this regard, it is important to recognize that NRC has adopted the peak-of-the-mean as the metric for compliance with the proposed regulations. In this approach, the values of dose at each instant in time are averaged for all stochastic realizations. The peak of the realization-averaged dose is then compared to the standard. An alternative metric, the mean-of-the-peaks, reports the average value of the peak doses calculated for each realization. NRC staff decided that the peak-of-the-mean metric better reflects risk to the target person or group exposed to effluents from the proposed repository. With either metric, results based on limited numerical experiments indicate that broader distributions lead to lower risk values (thus, apparently risk dilution). However, broader distributions decrease the mean-of-the-peaks dose to a significant extent, but decrease the peak-of-the-mean dose only slightly.

Staff will continue to pay attention to the possibility of risk dilution, although experiences with the current model results indicate that it is not a serious problem.

Comment 136: The transition from field and laboratory observations, measurements, experiments and general knowledge through conceptual models to computer code or modules should be demonstrated, otherwise, how is it assured that a consistent 'picture' or system understanding is the basis for the different assumptions? (p. G–6) [van Dorp]

The descriptions of the modules and the model abstraction each implements (Chapter 4 of the TPA Version 3.2 Code User's Guide) will be expanded to better describe the NRC and CNWRA interpretations of the physical repository system. Please see the response to Comments 115 and 123 in this section.

Comment 137: What will be the effects of uncertainty in knowledge of processes, in conceptual models, etc. on the application of the code? (p. G–7) [van Dorp]

Currently, some alternative conceptual models are represented in the code and their effect can be evaluated by turning one model off and turning another on (for example bathtub versus flow-through for water contacting waste form). It is recognized that many more conceptual models exist than those represented in the code. Process-level staff are encouraged to evaluate alternative conceptual models by changing parameter distributions, when possible. If risk significant, changes are then suggested for future code revisions. In general, the uncertainty resulting from alternative conceptual models is in many instances larger than parameter uncertainty. The insights obtained from the consideration and implementation of alternative conceptual models will allow staff to focus their review of DOE models to ensure that model uncertainty is adequately considered in their performance assessment.

Uncertainty in knowledge of processes is addressed by conducting analyses such as (i) the barrier component sensitivity analyses in which the functions of a barrier component or a group of barrier components are suppressed (neutralized) and (ii) distributional sensitivity analysis in which the distribution functions describing parameter uncertainties have been changed to deliberately bias the data.

Comment 138: The documentation should show which information has been used for the development of the models and codes and which for validation or confidence building and benchmarking [benchmarking can be both verification (check on correctness of the calculations and validation; check on 'fit for purpose')]. (p. G–4) Which information and data have been used for the development of the models and codes and which for validation or confidence building? Validation should be discussed mainly in relation with the conceptual models and verification in relation with the codes. Have codes been benchmarked against independent data? (p. G–7) [van Dorp]

A software validation test plan for the TPA Code is currently being developed. The plan will enumerate various tests to validate various components of the software. Model validation will be pursued for various key technical issues responsible for developing model support. A clear separation will be made between calibration and validation. However, model and software validations are planned to be conducted during the last phase of the TPA Code development. The CNWRA quality assurance procedure TOP–018 requires software validation for the TPA

Code. NUREG–1636 (Eisenberg, et al., 1999) provides an example staff may use for model validation.

Comment 139: Although the Document deals with a code, a major part is devoted to input data. In general, both the code or modules of the code and the input data are insufficiently justified. (p. G–7) [van Dorp]

This is a recognized deficiency with the TPA Version 3.2 Code User's Guide. Because the TPA code is continuously updated, much of this poor documentation is improved as new versions of the code and user's manual are released. NRC is committed to improving the TPA code documentation. The use of the TPA Code differs from the TSPA Code in that the latter must support the DOE safety case, and thus requires must more rigorous documentation and justification. NRC will produce documentation that justifies the models and data in the TPA code to the level required for its use as a review tool.

Comment 140: It might be useful to document the source of the data and information, (e.g., (1) generic literature, NRC and CNWRA, DOE; (2) site specific, generic; and (3) peer reviewed, other quality assurance, no quality assurance.) (p. G–7) [van Dorp]

Staff agree that sources for all data and assumptions should be transparent and traceable. All data and assumptions reported in Appendix A and throughout the TPA Code user's manual will be clearly indicated by ensuring that the sources for all data and assumptions, including those for site-specific studies, are clearly referenced.

Comment 153: The code should be able to evaluate the consequences of the maximum radionuclide release by groundwater beyond 10'000 years. (p. G–8) Many of the results depend strongly on the time of interest. Regulators and regulations in other countries require that consequences are calculated until the peak(s) have been reached. Experience shows that peaks often appear long after 50'000 years, in particular, in the more realistic scenarios and calculations. (p. G–18) [van Dorp]

The code can be executed for time periods of interest longer than 10,000 years. In addition, it is believed that important processes are represented such that calculations beyond 10,000 years are pertinent up to at least 50,000 years. As explained in the response to Comment 95 in this section, significant code revision would be needed to evaluate time periods of interest beyond 100,000 years.

Comment 155: It is important to have rigorous and documented criteria for the selection of radionuclides to be included in an assessment. (p. G–10) How has the list of 43 radionuclides been derived? It seems, according to 3-20, that selection was performed based on decay equations, and that environmental conditions (i.e., retention, retardation, migration) were not taken into account for the second and third iterations in the calculation process. (p. E–13) What support is available to the selection of radionuclides (justification for Tc99; why other radionuclides such as Nb, Se, or many other were not included in the list?) (p. E–15) Why fission products, such as Cs, Nb, Sn, Se are not considered at a large extent? (p. E–17) [van Dorp/Ouzounian]

Periodic analyses are conducted to ensure the set of radionuclides modeled in the TPA Code are sufficient to represent the dose from the repository. These analyses take into account the varying characteristics of the different radionuclides including half-life, solubility limits, retardation coefficients, biosphere transport characteristics, and decay characteristics. The latest iteration of this process is described in Appendix I of this report, which can be consulted to determine why specific radionuclides were not included in the analyses.

Comment 156: Why does the Cm-244 chain stop at Th-232? (p. G–11) [van Dorp]

Because of Th-232s extremely long half-life, the quantity of daughter products produced is extremely small; however, these daughter products have been shown to not contribute significantly to dose (see Appendix I) and, therefore, are not considered in the model.

Comment 157: Justification of why conceptualisations were chosen should be documented. (p. G–12) It is very important that reasons and evidence for the choice of the conceptual models are given. (p. G–13) [van Dorp]

Justifications for the choice of conceptual models where alternatives were available have been documented in the TPA Version 4.0 Code User's Guide, which was prepared subsequent to the period when the external review was conducted. The approach adopted involved emphasis on realism when reasonably sufficient data were available. When there was a high level of uncertainty in data and models, an appropriately conservative model was chosen for the nominal case. However, in many cases, it was not clear which model was more realistic or more conservative. In such cases, alternative conceptual model analyses were conducted through stylized TPA calculations, and the results were evaluated by the analyst.

Comment 164: The statement that doses from gaseous releases are negligible should be documented here or in a reference. (p. G–13) [van Dorp]

As part of the latest radionuclide screening exercise documented in Appendix I of this report, calculations were performed to determine the maximum possible dose from gaseous radionuclides released from the repository. Even a conservative calculation shows that the dose from gaseous releases of C-14, H-3, Ar-39, Kr-81, and Kr-85 would lead to a negligible dose to a receptor 18 km [11.2 mi] south of the repository. This small dose, combined with the conservative calculation, provides confidence that the dose from gaseous releases will be an insignificant fraction of the 15-mrem [0.15-mSv] standard specified in 40 CFR Part 197.

Comment 165: That chain decay can be neglected for transport in the invert should be demonstrated and documented. (p. G–13) [van Dorp]

Although neglecting chain decay introduces approximation that is nonconservative, the results are not expected to be excessively nonconservative because (i) radionuclides important to dose from groundwater releases have long half-lives (> 200,000 year), (ii) key radionuclides are abundantly available at the inlet end, (iii) the groundwater travel time is small because the invert is only 0.75 m [2.5 ft] thick, and (iv) the flow in the invert is through fractures (thus, small travel time) for most realizations. However, the assertion that the chain decay can be neglected will be substantiated with quantitative support in the future revisions to the TPA user's guide. Also, the TPA Version 5.0 Code has been influenced by the desire to increase realism in the TPA Code consistent with the performance goal to make NRC activities and decisions more effective, efficient, and realistic.

Comment 178: How is Quality Assurance documented? (p. G–16) [van Dorp]

Quality assurance is documented via the procedures outlined in TOP–018. This includes, but is not limited to, showing how the software meets the objectives presented in the Software Requirements Description. Furthermore, scientific notebooks used to document progress are retained as quality assurance records in a fire-resistant room at the CNWRA. Additionally, documentation is provided in Software Change Report forms and in the Design Verification Report. Finally, software is required to be validated. A software validation test plan for the TPA Code is currently under development, and validation is expected to be completed and documented in fiscal year 2003.

Comment 179: How is it assured that the interaction of the KTIs and the TPA does not cause potentially relevant features, events, and processes to be omitted or forgotten? (p. G–17) [van Dorp]

There is a continuous effort at enhancing the TPA Code. As of October 30, 2000, four major revisions to the code have been completed along with multiple minor revisions. Each major revision results in a new version of the code (e.g., TPA Code Versions 1.0, 2.0, 3.0, and 4.0). Minor revisions are tracked by increasing the version numbers by tenths (e.g., Versions 3.2, 4.1, and so on). Before each major revision, meetings are held to evaluate the current stage of the code, to identify missing elements or features, events, and processes; and to elaborate action plans for code revision and enhancement. The whole endeavor is managed by the total system performance assessment and integration group, however all technical staff are involved in the planning and implementation process. Minor code revisions are aimed at cleaning the code, improving the numerical methods, and revising data files. Computations with the TPA Code are used in numerous NRC reports and papers. This documented, iterative process gives staff confidence that the most important features, events, and processes are considered when developing the TPA Code. Additionally, DOE conducted a comprehensive features, events, processes identification process, which NRC staff are responsible for reviewing. If a significant feature, event, or process was identified that is not currently included in the TPA Code, the staff member could recommend incorporation of this feature, event, or process into the TPA Code as development of the code continues.

Comment 180: Description must be given about how scenarios have been generated and how they are adjusted to the new acquired knowledge or to the evolution of the disposal design. Another important step in scenario development is to explain how decision is made to take account of a disruptive event and with which level of detail. The scenario development methodology must be explained and documented. (p. E–5) [Ouzounian]

NRC does not intend to develop a scenario analysis document as this is not the role of the regulator; however, future revisions to the user's guide, as well as future iterative performance assessment reports based on use of the TPA Code, will endeavor to make reference to the database DOE is currently developing. NRC and CNWRA staffs have presented features, events, and processes they view to be important, which DOE has included in its database.

Comment 195: Variability in the rate at which radionuclides transit the UZ reach the water table may be an important factor if time required is significantly important compared to the time in the SZ. (p. E–10) [Ouzounian]

In the TPA Code, transport in the saturated zone generally is substantially longer than transport in the unsaturated zone. Groundwater transport times in the unsaturated zone are typically less than 100 years, compared to 500–1000 years in the saturated zone. Therefore, variability in the transport of radionuclides through the unsaturated zone will not significantly affect the results. Additionally, some of the variability in transport in the unsaturated zone is accounted for through the use of the different subareas, in which the thicknesses of the subareas vary for unsaturated zone transport. These different subareas have varying thicknesses of the different hydrostratigraphic rock units below the repository and, therefore, will result in varying results in the transport of radionuclides below the repository.

Comment 214: Why ASHPLUMO is not weighted by a 10-7 probability, as done for the VOLCANO event? (p. E–16) [Ouzounian]

The consequences of an igneous event are weighted by the 10^{-7} which is the probability used by the NRC to estimate the consequences of volcanism. Given that an extrusive volcano intersects the repository, the consequence is calculated assuming a volcanic event occurs and the results are weighted by the probability of the scenario as a post-processing step.

Comment 220: It would be interesting to measure the contribution to the TEDE peak of the main radionuclides in each of the cases. (p. E–17) [Ouzounian]

The contribution of main radionuclides to dose as a function of time has been computed using the TPA Version 3.2 Code and presented in NUREG–1746 (Mohanty, et al., 2001). Release rates of main radionuclides are dissolution-limited and are either not retarded or only slightly retarded in the natural system. Consequently, for all cases presented on Page E–17 of NUREG–1746, the contribution of radionuclides to peak total effects dose equivalent is not expected to differ significantly. However, calculations in NUREG–1746 will be extended further in future sensitivity and uncertainty analyses to determine if the radionuclides contributing to peak total effective dose equivalent remain invariant in spite of the numerous changes planned for the future TPA Code.

Comment 221: Radionuclides providing the majority of dose are probably release rate limited for the alternative conceptual model where infiltrating water is focused to one quarter of the WPs. Needs to be explained. (p. E–17) [Ouzounian]

For the base case, each waste package in the subarea was assumed to get an equal amount of infiltrating water. In the alternative conceptual model, Focused Flow, the same amount of water was instead focused or funneled to one-quarter of the waste packages, producing two effects.

- For the bathtub model, the failed waste packages would fill faster and, therefore, start to release their contents sooner. For the flow-through model, release happens immediately on failure, so flow-focusing is not a consideration.

- Ignoring the first effect, a radionuclide that has its release rate limited by solubility would be insensitive to the distribution of the water passing through the repository. All water contacting the fuel would reach this solubility limit, and, therefore, the flux of that radionuclide would be equal to its solubility times the water flow rate through the subarea. A radionuclide limited by the dissolution rate of the spent nuclear fuel matrix instead of solubility would show different behavior. The rate of release would depend on the amount of spent nuclear fuel exposed to flowing water (i.e., the one-quarter of the waste packages that have flow, because there can be no release from the waste packages without infiltrating water).

The statement on Page 3-17 of Volume 2 of the sensitivity studies report (NRC, 1999) is best supported by the 50,000-year results that show a peak dose of 283 μSv [28.3 mrem] for the base case and 78 μSv [7.8 mrem] for the focused flow case. The ratio of 3.63 is close to the expected ratio of 4.0 for the dissolution-limited release rate. For the 10,000-year case, this effect is offset by faster filling time of the waste packages in the alternative model, leading to a ratio of only 1.2.

Comment 222: At 10,000 year, the use of C-22 makes the waste package insensitive to Chloride and to OO-Coflc. However, new critical parameters appear like WPDef% and those related to pumping at 20 km and retardation (ARDSAV). But this has to be weighted by the fact that the TEDE peak is lower by a factor of 40 between the base case and the C-22 case (Table 3-2 in page 3-8). Thus, erasing effects from the major phenomena or processes contributing to the TEDE by the use of a more robust device will shift down the ranking. Transport related parameters become important at 50,000 year. (p. E–18) [Ouzounian]

Alloy 22 was considered in the performance assessment calculations because at the time of the development of the TPA Version 3.2 Code DOE was in the process of moving from Alloy 625 to Alloy 22 material for one of the overpacks. In the latest design, Alloy 22 has replaced Alloy 625. Therefore, the important parameters are determined only in the context of the Alloy 22 material. Use of importance analysis also addresses the concern raised by the reviewer.

Comment 223: For 10,000 year and alloy 625, the peak TEDE resulting from the volcanism scenario class is comparable to the nominal case, after being weighted by its probability. What is the significance and validity of such an approach? Saying that it's the same, is a good opportunity to lose confidence. Volcanism occurs or not. In the case it occurs, its consequences cannot be weighted by anything. There must be a class of consequences for the nominal case and classes of consequences for the volcanism scenario, depending when the event occurs. (p. E–18) [Ouzounian]

As recommended by the National Academy of Sciences (1995), the performance objective for the Yucca Mountain repository in 40 CFR Part 197 and 10 CFR Part 63 is a probability weighted dose. The consequences of unlikely events are weighted by their probability of occurrence to accurately reflect the risk posed to an individual from the repository at some time in the future. Because it is impossible to know with certainty whether or not an igneous event will disrupt the repository during the next 10,000 years, the probability of the event must be factored into the assessment of the suitability of the repository in some manner. Any manner of separating the nominal results from the results of disruptive events would have to be based on the probability of occurrence of the disruptive event, and the acceptable consequences of these disruptive events would have to be based on the risk of the event. The methodology prescribed in 10 CFR Part 63 simply makes this probability weighting more transparent. It is also noted that this methodology is consistent with the rationale of performing a performance assessment. While conducting a performance assessment, there is some probability that a parameter or a group of parameters will be sampled such that high results are obtained in a given realization. However, by performing many realizations, these unlikely realizations will be averaged with realizations with lower consequences to obtain a mean result that can be compared to the standards.

Comment 228: Redistribution of infiltrating flux: why are the differences in sensitivity attributed to solubility limited radionuclides dominating the peak TEDE for the TPI at 5 km and release-rate limited radionuclides controlling the peak TEDE for the TPI at 20 km? Is this justified by a change of process along the time (but this was not recorded previously in the documents)? Is it because high flow rates on the SF have been assumed for the 5-km case, and lower flow rates on the SF for the 20-km [12.4-mi] case? (p. E–19) [Ouzounian]

In the TPA Code, radionuclides are specified as unretarded in fractures. Solubility limited radionuclides that dominate the peak total effective dose equivalent for the time period of regulatory interest at 5 km [3.1 mi], are unretarded because of fracture flow up to that distance. However, to reach the reasonably maximally exposed individual, which is expected to be located 18 km [11.2 mi] from the repository, consistent with 10 CFR Part 63, radionuclides must travel through the alluvium. Solubility limited radionuclides are highly retarded in the alluvium, whereas radionuclides that are least retarded in alluvium are generally release-rate limited and are the dominant contributors to peak dose at 20 km [12.4 mi].

Comment 232: TPA works more like a simplified representation of the total system, than like a mechanisms- or phenomenology-based model. Thus, its limits can be overcome by implementing processes via a transfer function approach, which advantage will be to keep a clear and easy analytical tool, as it appears now. This approach assumes to have a 2-stage analysis, the first being at the phenomenological level (process level), in order to determine those parameters which will have to be analyzed in the second stage with the TPA Code. The other alternative is to fully couple phenomenological models to TPA, but analyses may become more difficult, and this can result in a loss of transparency. (p. E–19) [Ouzounian]

Different modules in the TPA Code have different levels of abstractions. For example, waste package corrosion and source term calculations are mechanistic. These models also represent the NRC phenomenological models for waste package corrosion and source term. The TPA Code also embodies highly abstracted models when process models either do not exist or are computationally time-consuming. In the latter case, phenomenological models are used outside the TPA Code and the results are used to develop the abstracted model for use in the future TPA Code. The process of developing abstracted models from phenomenological models is documented in separate reports. Although such documents do not exist for all abstracted models used in the TPA Code, efforts are made to clearly document the processes, at least for the complex and risk-significant models.

3.2 Comments Relevant to the Degradation of Engineered Barriers Integrated Subissue (ENG1)

Comment 33: The potential effect of rock debris or dust on the surface of the canister, or even rock blocks, if the drifts are partially backfilled with fallen rock, could influence the corrosion rate of the metal beneath it. (Raised as a question, tempered by declared lack of expertise.) (p. C–7) Another area of coupling that must be considered is that of rockfall-induced defects/stresses to corrosion via the possibility of SCC. In addition, the possibility of either rockfall-induced or backfill-induced capillarity should be considered. If areas of the waste package are in contact with either rockfall or backfill, those areas will be more susceptible to corrosion attack via crevice corrosion. (p. D–6) [de Marsily/Kelly]

Rock debris and dust on the container surfaces may have several effects including formation of a crevice on the waste packages, changes in the chemistry of the water that contacts the waste package surface, and the promotion of a stable water film by capillary action. For the Total System Performance Assessment–Viability Assessment waste package design, which used a carbon steel outer barrier, changes in the water chemistry by the deposition of dust or debris could be expected to result in changes in the carbon steel waste package outer barrier corrosion rate. Since the Total System Performance Assessment–Viability Assessment was distributed, the favored DOE waste package design calls for a corrosion resistant Alloy 22 outer barrier. Accordingly, tests have been conducted to measure the passive corrosion rate, localized corrosion, and stress corrosion cracking susceptibility of Alloy 22. The performance of the waste packages is modeled in the TPA Code using parameters from these tests. To date, these tests have shown that the passive corrosion rate of Alloy 22 is low and largely independent of solution composition. Because the localized corrosion susceptibility of Alloy 22 is modeled by comparing the repassivation potential for crevice corrosion (measured in laboratory tests) to the corrosion potential, the effects of crevices as a result of rock debris are inherently included in the model. Additional tests are being conducted to expand the capabilities of the model with respect to water composition. If necessary, the parameters used in the TPA Code will be modified to include the effects of trace elements, which may destabilize the passive film and alter the susceptibility to localized corrosion, and the effects of long-term changes in the passive film properties. The effect of drift collapse on infiltration rates is also currently being assessed and will be incorporated into future versions of the TPA Code, if necessary. The effect of rockfall-induced stresses are currently being evaluated to determine whether they are likely to affect the onset of stress corrosion cracking. If induced stresses are sufficient to lead to stress corrosion cracking and releases through cracks are significant, this failure mechanism will be added to a future version of the TPA Code, appropriately accounting for the probability that a rock of sufficient size would strike a waste package.

Comment 36: Cooler waste packages could serve as condensation surfaces and may be dripping with water. (p. C–8) [de Marsily]

Condensation on the waste package surfaces will depend on many parameters such as ventilation, thermal loading, waste package spacing, and drip shield design. For the Total System Performance Assessment-Viability Assessment waste package design with a carbon steel outer barrier, condensation on cooler waste packages would be expected to promote general corrosion and lead to perforation of some carbon steel outer barriers. For the current waste package design with an Alloy 22 outer barrier, formation of a condensed water film is still possible especially with the recently proposed low-temperature operating mode (CRWMS M&O, 2001). The presence or absence of liquid water does not, by itself, affect the corrosion of Alloy 22 significantly. The general corrosion rate for Alloy 22 is similar in the presence of liquid water or humid air. However, condensation could affect the chemistry on the surface of the waste package. The response of the waste package is modeled in the TPA Code using the passive corrosion rate and the susceptibility to localized corrosion (corrosion potential and repassivation potential). The evolution of the condensed water chemistry is important because this will likely determine the degradation mode of the waste package outer barrier.

In the new analysis by the DOE, condensation of water may lead to the formation of concentrated aqueous solutions in the presence of hygroscopic salts already deposited by evaporation of dripping water or transported by aerosols. The composition of the hygroscopic salts will determine the relative humidity at which a condensed water film will form on the waste package surface. Eventually, this extended regime of corrosion at low relative humidity can be incorporated in an updated version of the TPA Code.

Currently, in the TPA Version 4.1 Code, the time at which an aqueous or humid-air environment, which is needed for the onset of general corrosion, is established is not significant for dose calculations. This insensitivity is because of the lack of localized corrosion for Alloy 22 in the simulations and the average penetration time of the waste package due to general corrosion is about 40,000 years. A delay of up to 1,000 years from the establishment of humid-air conditions does not significantly affect the dose calculations. If it is determined that condensation could significantly affect the results of the TPA Code, the effects of condensation will be added to a future version of the TPA Code.

Comment 50: There is a pressing need for a more realistic abstraction of the development of the environment on the WP surface. (p. D–2) The corrosion of the waste package canisters will be directly coupled to the nature and evolution of the environment present around them. There is a pressing need for an improved estimate for the container-surface environment. (p. D–4) It does not appear that either MULTIFLOW or REFLUX3 can capture the concentration of solute that would appear in the flow of water to the waste package. (p. D–5) Experimental work would be required to determine the connections between the near-field environment, conditions on the waste package surface, and corrosion. (p. D–5) [Kelly]

At present the TPA Code only considers the chloride concentration in water contacting the waste packages. The basis for this simplified approach are the results of initial tests where the aggressive (i.e., promotes corrosion) or inhibitive (prevents corrosion) nature of the anionic species in J–13 water were determined. In these tests, chloride was determined to be an aggressive species and nitrate was determined to be an inhibitor for iron-nickel-chromium-molybdenum alloys. All other anionic species in J–13 water were determined to be neither aggressive nor inhibitive. By choosing only chloride the inhibitive effects of nitrate were ignored and therefore the approach adopted was conservative for determining the susceptibility of the waste package to localized corrosion.

A more realistic approach is preferable for several reasons.

(1) The inhibitive effects of nitrate could be included in the TPA Code. Work conducted at the CNWRA has shown that at a nitrate to chloride ratio of 0.2, localized corrosion of Alloy 22 is suppressed. Higher nitrate to chloride ratios are needed to suppress the localized corrosion of other alloys.

(2) Tests conducted to determine the effect of mixed salts on the deliquescence point will be used to assess when a water film can be formed on the waste package surface. The deliquescence point of chloride salts has a wide range. A combination of chloride and nitrate salts can have a lower deliquescence point than any of the pure salts.

(3) The boiling point of water is also strongly dependent on solution composition and ionic strength and can reach values as high as 150°C in a saturated solution of $CaCl_2$

(4) Aggressive species other than chloride are not considered. For example fluoride is known to be an aggressive species to titanium. Fluoride may also be important in the stress corrosion cracking of Alloy 22 in concentrated alkaline groundwater. Reduced sulfur species (e.g., thiosulfate) are also known to be aggressive to nickel and nickel chromium alloys.

Preliminary tests were conducted to study the evolution of chloride and pH in the simulated heater test. These tests and the results were reported in CNWRA reports 2000-06 Revision 1, 2001-003 and 2002-03. These tests have since been discontinued. Modeling simulations are being conducted to calculate the evolution of water chemistry as a function of time and temperature.

Comment 52: More work needs to be done in the abstraction of localized corrosion rates due to the sensitivity of the predictions of dose to the corrosion rate. (p. D–5) [Kelly]

A comparison of the corrosion penetration rate used in the TPA Version 3.2 Code to both literature and tests conducted at the CNWRA was provided in Cragnolino, et al., (1999). While the localized corrosion rate used in the TPA Code is comparable to the literature reports and test results, it is recognized that these measurements are conducted in relatively short-term tests with shallow localized corrosion penetration depths and may result in penetration rates that may be faster than would actually occur in a repository setting. As DOE continues to get more data from their long-term corrosion tests, the abstraction of localized corrosion rates will be updated to represent the appropriate data. In the TPA Version 5.0 Code, the localized corrosion model will be consistent with the abstraction of the salts formation model. It is uncertain at this stage if the penetration rate is a relevant parameter. If penetration by localized corrosion occurs in a single time step, then the penetration rate will be irrelevant, provided it is large enough. This will be decided via sensitivity analyses, provided the salts formation model indicates that localized corrosion is feasible.

Comment 53: It is important to keep the option to evaluate the production of peroxide via radiolysis to allow for the assessment of alternative designs. (p. D–6) [Kelly]

It is agreed that the ability to evaluate the possibility of peroxide formation is important. For example, the increase in corrosion potential as a consequence of peroxide formation may lead to the start of localized corrosion. Changes in waste package design and thermal loading may also alter the consequence of peroxide formation. The current version of the code (4.1) has a simplified model to account for the effect of γ-radiolysis by adding a term with an exponential time decay to simulate the contribution of the H_2O_2 concentration to the corrosion potential.

Comment 54: The code should be able to handle a change from the expected localized corrosion to a rapid, more uniform corrosion in the presence of elemental sulfur or reduced sulfur species. Data needed to address the corrosion rates must be developed in the proper environment. (p. D–6) [Kelly]

As indicated in the response to comment 50, the TPA only considers chloride and does not consider the effects of reduced sulfur species on the corrosion of Alloy 22. While the prevailing conditions at the proposed Yucca Mountain site may be slightly oxidizing, occluded regions may lead to local conditions that are reducing. Microbial activity may also produce reduced sulfur species. Tests are being conducted to determine the effect of reduced sulfur species (i.e., thiosulfate) to chloride concentration ratio on the localized corrosion resistance and uniform corrosion rate of Alloy 22. These tests will be completed in fiscal year 2003.

Comment 55: It seems that there is no direct connection between pit area density and the important parameter in EBSREL of q_{in}. The release rate is dependent on the total area of perforation, so a means to estimate this area based on the localized corrosion characteristics of the material is needed in the TPA. (p. D–6) [Kelly]

Modifications have been made in the TPA Version 4.0 Code to allow the code to make the F_{ow} and F_{mult} factors time dependent so that changes in drift geometry and increasing degradation of the waste package can be modeled. A simple and conservative model is used in the TPA Code to represent package failure and subsequent water contact. When a pit breaches a waste package, the package is assumed to have failed and can transmit water. The water contact parameters have the capability to be time-dependent in TPA Version 4.0 Code, therefore the amount of water transmitted through the waste package can have temporal dependence. The only release mode represented in the TPA Code is advection. The amount of failed surface area is conservatively assumed to not be a limitation to advective release.

Comment 56: The effects of welds on the corrosion behavior of the materials should be studied and given high priority. The possibility of dissimilar metal crevice corrosion between the construction materials should also be studied. For some corrosion resistant alloys, dissimilar crevice corrosion can be far worse than the deformable crevice corrosion. (pp. D–6 and D–7) [Kelly]

The effect of welding has been and will continue to be studied. The effects of other fabrication processes are also being investigated. Preliminary tests have shown that the localized corrosion susceptibility of welded material is not significantly greater than the as-received base alloy. Passive current density measurements have shown that the uniform corrosion rate of the welds are up to three times that of the base alloy. Even with the increased passive corrosion rate of the welds, the passive corrosion rate remains extremely low. Additional tests are ongoing to examine the effects of fabrication processes, such as induction annealing after the final closure weld.

The TPA Code uses localized corrosion susceptibility parameters obtained from the base alloy. Because the initial tests with welded material were not significantly different than those of the as-received base alloy, the use of parameters obtained from the base alloy are well supported. It is important to note, however, that the waste package design and fabrication processes are still being developed. Close attention will be paid to the development of the design and fabrications specifications. Testing will continue as needed to determine the effects of the fabrication processes. Changes to the TPA Code parameters used to characterize the uniform corrosion rate and localized corrosion susceptibility of the waste package, including the effects of fabrication and welding, will be determined based on tests of the effects of the fabrication methods specified by the DOE.

Comment 61: Some of the models rely on extremely limited data and/or experience (e.g., corrosion rates over millennia for modern alloys). As indicated above, there are aspects of some conceptual models that require more effort to make them more defensible. (p. D–9) [Kelly]

Parameters for the corrosion models used in the TPA Code are typically derived from laboratory tests. The repassivation potential, one of the parameters used to determine the localized corrosion susceptibility of the waste package outer barrier, is typically determined in short-term tests. However, long-term tests, which typically run for several years, are used to test the validity of the data generated in the short-term tests.

Although the results of long-term tests indicate that the localized corrosion resistance of Ni-Cr-Mo alloys does not decrease, the question about the extrapolation of passive corrosion rates for long periods is significant. Tests are currently ongoing to determine if there are changes in the properties or chemistry of the passive film. These changes may include preferential dissolution, growth of the oxide film, or spalling of the oxide. At present, there is no indication that changes in the passive dissolution rate occur during long periods. Changes to the parameters used to model the passive dissolution of the Alloy 22 outer barrier will be modified as necessary to account for changes in the passive film properties. In addition, NRC and CNWRA staff continue to perform fundamental modeling of passive corrosion to provide insight for further testing and improved understanding of the factors that may promote instability of the passive film in Ni-Cr-Mo alloys.

It is acknowledged that this extrapolation of passive corrosion rates for long periods is a critical and difficult problem, which has been the subject of an expert panel meeting on July 19–20, 2001, organized by the Nuclear Waste Technical Review Board. Results from this meeting will be published as a proceedings volume and will be taken into account to make the long-term extrapolation model more defensible, if warranted.

Comment 142: Example of coupling which does not appear to be accounted for in the TPA Code: increased ventilation will increase salt content of solution which might enter drift during or after ventilation => increased corrosion. (p. G–7) [van Dorp]

The passive dissolution rate of Alloy 22 has been shown to be largely independent of chloride concentration. The susceptibility of Alloy 22 to localized corrosion increases with chloride concentration. The parameters for determining the corrosion mode and penetration rate for Alloy 22 are already present in the TPA Code.

Modeling issues related to increased corrosion by the formation of salt deposits is addressed in the response to Comment 50 in this section.

Comment 147: Example of coupling which does not appear to be accounted for in the TPA Code: interaction between materials on corrosion potentials, (re)passivation potentials, and localized corrosion. (p. G–8) [van Dorp]

Interactions among some of the alloys used in the emplacement drifts have been studied. The galvanic interaction of A516 steel and Alloy 825 was examined to determine the effect on corrosion potential and the localized corrosion susceptibility. Interactions between carbon steel, used as ground support material, and titanium-palladium alloys (proposed materials for the drip shields) are now being investigated to determine the susceptibility of the titanium-palladium alloys to hydrogen embrittlement. Investigation of other material interactions may be necessary as the waste package and repository drift designs evolve. The determination of how the effects of these interactions will be included in a future TPA Code version will be made on a case-by-case basis.

Comment 152: Not clear whether effects of welds in waste packages on corrosion and mechanical stability. (p. G–8) [van Dorp]

The effect of welds on the corrosion of the waste packages is addressed in the response to Comment 56 in this section.

The effects of welds and fabrication processes on the mechanical stability of the waste packages will be investigated.

At present, there is no specific treatment of the effects of welds on mechanical failure of container materials in the TPA Code. If necessary, treatment can be implemented in a simplistic fashion by introducing a change in the values of K_{ic}, the fracture mechanics that account for any brittle failure. However, it should be justified that the applied stress and the resulting stress intensity factor can reach sufficiently high values to make changes in the code necessary prior to implementing this change. At present, it is not evident that this item is sufficiently risk-significant to warrant its incorporation into a future version of the TPA code.

Comment 161: Pages 4-48 and 49: Bullet points: other approaches might be possible, e.g., (1) determine a minimal thickness required for mechanical stability or integrity of the canister, (2) calculate corrosion rates, and (3) assume that a canister fails if the minimal thickness required for mechanical integrity is reached. (p. G–12) [van Dorp]

The minimum thickness for mechanical integrity is determined by the inner Type 316 nuclear grade stainless steel container. Because DOE does not take credit for the corrosion resistance of the inner stainless steel container, the effect of corrosion on the mechanical integrity of the container is not considered. The waste package is considered to be breached once corrosion has penetrated the Alloy 22 waste package outer barrier.

Comment 181: An upper bound on the chloride concentration has been derived assuming equilibrium with halite (NaCl). However, this upper bound appears quite speculative, and alternate conceptual models can give rise to very different results. (p. E–6) [Ouzounian]

This comment originally addressed the possibility that concrete, presumably from the concrete lining of the drifts, may significantly alter the water chemistry. In the most recent repository design, the influence of concrete on the water chemistry is substantially reduced.

The effect of other species on the degradation of the engineered barriers has been examined. A factorial matrix was conducted that examined the effect of numerous species on the localized corrosion resistance of Ni-Cr-Mo alloys. In some cases, more detailed tests have been performed. For example, the aggressive effects of fluoride ion and the inhibitive effects of sulfate and nitrate on the corrosion rate of titanium-palladium alloys proposed for the drip shield have been investigated. For the localized corrosion resistance of Alloy 22, the effects of chloride concentrations in excess of what can be expected for water in equilibrium with NaCl, as well as the effect of temperature in excess of the boiling point at atmospheric pressure, have been examined. Changes in the corrosion rates and the localized corrosion susceptibilities as a result of aggressive species, in addition to that which can be expected from NaCl or inhibitive species, could be accounted for in the TPA Code by changing the parameters used to model these various degradation modes. As mentioned in the response to Comment 50, an abstracted version of the salts formation model is being considered for incorporation into the TPA Version 5.0 Code.

Comment 191: The weight of radiolytic effects has not been considered in the document. Either a comment explaining that they are not relevant on the considered time scale, taking account of the width of the overpack, or, on the other hand, that those effects may be important and will have to be considered in further developments. (p. E–9) [Ouzounian]

The effect of radiolysis on the waste package is expected to result in the production of peroxide. This effect has been addressed in the response to Comment 53 in this section.

Comment 199: What is the signification, in the last paragraph, of a statistically sampled parameter to scale the chloride history? Is the range of measured chloride known? (p. E–13) [Ouzounian]

The range of chloride concentrations in the water dripping in the emplacement drifts is estimated by the DOE by modeling thermal-hydrological-chemical coupled process using as input J–13 well water or pore water. However, there are large uncertainties in the range of chloride concentrations that can be expected in the water in contact with the waste packages and concentrations can reach values close to the saturation of NaCl at temperatures close to the boiling point of these saturated solutions. Therefore, the sampled parameter is varied to reflect the spatial variability that can be found in the repository. In some evaporation experiments conducted by DOE, values of chloride concentration in the range 3–5 M have been measured. As discussed in response to Comment 50 in this section, an abstracted version of the salts formation model is being considered for incorporation into the TPA Version 5.0 Code.

Comment 201: For the bathtub model, the outlet height is statistically sampled. What is the signification of such a statistical sample? Is there any implicit assumption that we are faced to a uniform process, such as those given in 2-7, dry air oxidation or humid air corrosion? (p. E–13) [Ouzounian]

The assumption is that the outlet hole in the waste package can form at any point on the perimeter of the waste package surface. There is not sufficient basis to determine preferential locations where the hole may form within the waste package. Therefore, a uniform distribution between 0 and 1 is sampled to determine the height of the outlet hole, which is defined as a fraction of the waste package height. This limitation could influence the calculated consequences.

Comment 202: In the case of aqueous corrosion, because the flow model is driven by gravity, the model can be refined to take account of gravitational forces. At least two different behaviors can constrain the statistical distribution: drip on a given emplacement on the upper half area of the canister and local hole on this part, or flow of the droplets to the bottom of the canister and accelerated corrosion in the bottom. Besides, this type of behavior has been considered among the limitations for the corrosion model. (p. E–13) [Ouzounian]

The TPA Code has made provision for these two types of behavior based on the bathtub and flow-through models. The bathtub model is characterized by the level of the exit hole (h), which is specified via the spent nuclear fuel wetted fraction parameter where zero implies an outlet at the bottom and one an outlet at the top of the waste package.

Comment 216: For the base case, alloy 625 is used for the inner overpack and carbon steel for the outer overpack. In the conceptual model described in volume 1, reference is done to pitting, but with those 2 materials, is there any analysis of the risk for galvanic coupling, and faster consumption of the carbon steel overpack after it started to fail? (p. E–17) [Ouzounian]

This issue is outdated. The current DOE waste package design does not have a carbon steel outer barrier. The effects of material interactions are addressed in the response to Comment 56 in this section. However, for the Total System Performance Assessment-Viability Assessment version of the waste package, the potential for galvanic coupling was analyzed in detail at the process level, and the limitations in the protection offered by the carbon steel as a result of its consumption by the galvanic corrosion process potential was evaluated. Changes in design made it unnecessary to consider modifications of the code regarding these interactions.

3.3 Comments Relevant to the Mechanical Disruption of Engineered Barriers Integrated Subissue (ENG2)

Comment 2: A more comprehensive model described during the review will permit a more thorough assessment of seismic effects on WP rupture. (p. A–2) Seismic rupture of WP is not expected to represent a major source of radionuclide release. (p. A–11) [Brady]

There are two potential effects of seismicity on waste package performance presently being investigated. The first is the consequence of direct rock block impacts on the waste package arising from seismically induced rockfall. Detailed finite element analyses are being used to rigorously assess the damage caused to the waste package due to impacts near the waste package closure lid welds (see the response to Comment 152 in Section 3.2 of this report), directly above the pallet support, and at the midspan of the waste package. The results of these analyses will be used to improve the SEISMO module presently used in the TPA Version 4.1 Code to assess the effect of rockfall on the Yucca Mountain Monitored Geologic Repository performance. The second effect is the creation of plastic deformations and concomitant residual stresses in the immediate region of the contact zone between the waste package and its supporting pallet during seismic excitation, or both rock block impacts that are sufficient to cause stress corrosion cracking in the event it is determined that the near-field environment will promote this potential failure mechanism. Current models in the TPA Code indicate that seismic events led to very few waste package failures. However, these conclusions could change based on the results of the detailed analyses being conducted.

Comment 3: The unfilled drift model may not be conservative for FAULTO. However, the result may not be important as only a very small number of waste packages are at risk of rupture under a seismic fault slip. (p. A–2) [Brady]

The FAULTO module looks at the failure process of waste packages in the emplacement drifts in a simplistic way. Without a good understanding of the nature of events that will lead to rupture of waste packages and release of radionuclides subsequent to a fault slip, several alternative scenarios were developed. It was realized during the early phase of this scenario development process that a seismic fault slip will not contribute to the resulting dose in any significant way. Any backfill that is used in the repository is likely to be loosely compacted and will not completely fill the tunnels, and therefore, is unlikely to have a significant effect on the consequences of a faulting event. Other conservative assumptions in the FAULTO module, such as the very small threshold displacement for waste package failure, likely bound any uncertainties in the model due to the presence or absence of backfill.

Comment 4: Thermal stresses are not taken into account and may have an important bearing on mountain-scale seismic effects and fault slip, and on the repository scale hydrology, by reducing vertical permeability at the repository horizon. (p. A–2) An effect that may be of consequence in the evaluation of seismic factors is the possibility that thermal stresses may lead to conditions sufficient to cause slip on existing faults, which may be co-seismic, within the repository domain. (p. A–5) [Brady]

Changes in fracture aperture with depth interpreted from injection-test data from several dam sites indicate that an increase in compressive stress at the proposed repository depth would not cause an appreciable decrease in fracture aperture. On the other hand, an appreciable fracture-aperture increase can be expected from shear-induced fracture dilation, vertical tension in the pillars, and excavation-induced rock loosening in the roof and floor areas of the drifts. Such changes can potentially cause a redistribution of the percolation flux crossing the repository. Their effects are currently being evaluated for inclusion into the TPA Version 5.0 Code. Thermal-mechanical analyses indicate a potential for thermally induced fracture slip close to the drift openings and within the pillars. However, the calculated slip magnitudes, length, and rates indicate that such slip would be either nonseismic or the potential contribution to seismicity would be negligible.

Comment 7: A more convincing analysis of the consequences of seismic loading would take account of the history of motion during a seismic event of both the WP and the local rock. This would require a more comprehensive representation of the WP and the drift near-field rock in terms of both structural detail and time history of motion. (p. A–5) [Brady]

Based on recent information presented by DOE (DOE and NRC, 2002), the free surface ground motion reduction factor for the repository horizon will be somewhere in the range of 0.7 to 1.0. As a result, the TPA Code seismic hazard curve input has been updated to be consistent with the current DOE design philosophy. To ensure the effects of seismic hazards are properly bounded, the free surface ground motions, without any reduction factor, are being used. Furthermore, recent analyses performed by the CNWRA indicate that discrete rock blocks of a size sufficient to cause damage to the drip shield are likely to occur only in the middle nonlithophysal rock unit (which represents approximately 25 percent of the repository footprint). Static rockfall loads attributable to accumulated rock rubble will occur in both the middle nonlithophysal and lower lithophysal rock units, however. These static loads have been determined to be sufficient to fail nearly 90 percent of the drip shield (as it is currently designed) within 1,000 years after cessation of maintenance of the ground support system. An assessment of the stresses that may be incurred by the waste package as the result of direct seismic shaking using finite element process level models is currently underway. These process level models will use site specific ground motion time histories and the resulting abstractions will be derived in terms of the mean peak horizontal ground accelerations (if at all possible). If it is determined that this type of loading is risk significant and additional seismic ground motion parameters are required to develop the abstractions, the TPA Code will have to be augmented to include them (e.g., mean peak vertical and ground accelerations, and mean peak vertical horizontal velocities, and so on).

Comment 8: The relatively simple formulation of seismic effects may be sufficient as a first pass, but the more comprehensive analysis is required to assess seismic effects thoroughly. (p. A–5) [Brady]

See the responses to Comments 2, 7, and 143 in this section.

Comment 9: The possibility of mountain-scale, thermally induced seismic events points to the need for comprehensive seismic monitoring of the repository during construction, to establish seismic baseline parameters, and in the pre-closure phase, to characterize seismic response which may bear some relation to the temperature field. (p. A–5) [Brady]

These comments are relevant to the performance confirmation studies that DOE will conduct during repository construction. NRC and CNWRA staff will consider these comments when reviewing DOE plans for confirming performance.

Comment 10: While the current displacement threshold figure for rupture i.e., 25 mm seems conservative, at some stage some hard data derived from experimentation would be useful in determining how corrosion and other modes of damage affect WP resistance to rupture under various types of imposed deformation. (p. A–6) [Brady]

See the responses to Comments 143 and 234 in this section.

Comment 11: Because the objective is to conduct a bounding calculation on TEDE, the possibility of thermally induced fault slip and associated seismicity (even though the slip may indeed be aseismic) is worthy of further consideration. (p. A–7) [Brady]

The reactivation of faults due to thermal stresses has not been ruled out, but sufficient data and technical bases to support an abstraction have not been developed. Moreover, the correlation between thermally induced fault slip and seismicity is presently believed to be weak because the fault slip area will be highly localized and the slip rate will be relatively slow. The goal of the TPA Code is to conduct a realistic calculation of the total effective dose equivalent, not a bounding calculation.

Comment 96: There is no link, at present, between faulting, seismics, and volcanism, or indeed between these phenomena and the regional groundwater system. (p. F–3). Example of coupling which does not appear to be accounted for in the TPA Code: faulting, seismicity, igneous activity, and hydrogeological processes are treated as not correlated. (p. G–7) [Thompson/van Dorp]

It is recognized that there is no direct coupling among faulting, seismicity, and volcanism in the TPA Version 3.2 Code. In nature, volcanic eruptions are often accompanied by pre- and syn-eruption earthquakes. For basaltic eruptions, these earthquakes have small to moderate magnitudes, moment magnitudes of five or less (e.g., Yokoyama and de la Cruz-Reyna, 1990). Similarly, even though faults within the repository are not themselves seismogenic, faulting events would probably be associated with seismicity on seismogenic faults, such as the Solitario Canyon or Paintbrush faults.

There are parameters within the current TPA Version 4.1 Code designed to take into account various aspects of these potentially coupled tectonic processes. For example, in addition to specific fault sources, the probabilistic seismic hazard analyses performed for Yucca Mountain by the DOE (CRWMS M&O, 1998) includes random or background seismicity defined within what are referred to as areal sources. Background earthquakes with magnitudes of six and larger are possible within the areal sources. Earthquakes associated were volcanism was specifically considered by the DOE probabilistic seismic hazard analyses experts as one of the sources of seismicity within these areal sources. Thus, no additional terms for volcanic seismicity are necessary in the TPA Code. In fact, developing such a term in the code would result in a double counting of seismicity. By a similar argument, seismicity that may trigger faulting within the repository is accounted for by the probabilistic seismic hazard analyses results because the probabilistic seismic hazard analyses already include the potential for seismicity on all seismogenic faults at or near Yucca Mountain.

There is little need to couple saturated zone or unsaturated zone flow to faulting, seismicity, or volcanism. The permeabilities of the volcanic tuff fracture networks are already very high and consistent with values typically seen in brittle volcanics elsewhere in the world. Increases in percolation rates above the repository along potential future faults will not significantly increase subarea averages of percolation rates because of the small areal ratio of a fault to a subarea. If future versions of the TPA Code move away from the use of subareas to some finer spatial resolution of percolation reaching the repository, a linkage between new faults and locally increased percolation reaching the repository would be recommended. There is an easily implemented mechanism in the TPA Version 3.2 Code to evaluate the sensitivity of radionuclide transport below the repository to potential future faulting.

Seismic pumping that could potentially lead to upwelling of water in the unsaturated zone to the repository horizon has been extensively discussed in the scientific community. For Yucca Mountain, this is not considered likely by a strong majority of researchers. If this process is shown to have likely occurred at Yucca Mountain, then it would be recommended that seismic activity and quantity of water entering the drift be linked in future versions of the TPA Code. For saturated zone flow, seismic effects on water table elevation are observed in nature, but these effects are typically small and short-lived.

Volcanism, seismicity, and faulting would all potentially affect the hydrogeological system. However, there are technical arguments for not including these effects in the TPA Version 3.2 Code and for not including a link between the processes of volcanism, faulting, and seismicity. The dose from igneous activity is dominated by extrusive and not intrusive igneous activity (NRC, 2000b). Therefore, there may be faulting and seismicity associated with igneous activity but the impact is expected to be minimal. Likewise, the impact of igneous activity on the hydrological flow system is not expected to be risk-significant based on the low doses from intrusive igneous activity. Seismic effects could potentially have an impact on the seepage of water into emplacement drifts. The abstraction of the amount of seepage potentially reaching the waste packages is represented as being highly uncertain in the TPA Version 3.2 Code. It is likely that potential uncertainty from seismic effects is already included in the parameter distributions. The existence of faults was considered in developing the flow models. The development of new faults was considered in earlier versions of the TPA Code, but not the associated impact on the hydrological system. Because the probability of occurrence was evaluated to be rather small, the calculated impact to risk was insignificant. In the Total System Performance Assessment–Viability Assessment (DOE, 1998), DOE demonstrated that emplacement of a subsurface igneous intrusion away from the repository would have little effect on groundwater flow paths. Intrusion into the repository, with associated volcanic eruption, would directly release a significant amount of high-level waste. Secondary effects, such as seismicity or minor changes in groundwater flow paths, would have small releases relative to direct volcanic release. Adding abstracted correlations, while improving apparent realism, would not change understanding of risk significantly.

Comment 143: Example of coupling which does not appear to be accounted for in the TPA Code: correlation of corrosion and mechanical failure model. (p. G–7) Why has a combination of container thickness reduced by corrosion and rockfall not been considered in the seismic failure criterion? (p. G–13) Is time taken into account for ageing of the WP, for example, for corrosion and mechanical resistance decreases in the conceptual model? (Time of occurrence has been taken into account to determine the radionuclides release.) Has the thickness of the WP been taken as a constant over time for the I parameter (4-52)? There are many assumptions, with a very detailed development. Is this at the scale of the question? Are the relevant parameters taken into account? The example given above could be considered as a non conservatism assumption. (p. E–15) In FAULTO, same comment as for SEISMO. Intensity of consequences on release will depend on the quality of the WP (corrosion) at the time of occurrence of the faulting event. (p. E–16) [van Dorp/Ouzounian]

Current information indicates that the general corrosion rate of the waste package outer barrier material (Alloy 22) is small. As a result, any potential reduction in the structural integrity of the waste package arising from reduced material thickness is presently considered inconsequential. Moreover, there is no technical basis at the present time to justify any reduction in the ductility of Alloy 22 due to material aging during the 10,000-year licensing period. See the responses to Comment 2 and 7 in this section and Comments 52, 152, and 161 in Section 3.2 of this report for additional information.

Comment 144: Example of coupling which does not appear to be accounted for in the TPA Code: reactivation of faults by thermal stresses. (p. G–7) [van Dorp]

The TPA Version 3.2 code does not account for the coupled effects of these processes. The assumption that these processes are independent leads to underestimation of consequences of faulting. However, the FAULTO module has several conservative assumptions that lead to overestimation of consequences of faulting. For example, the absolute probability of faulting assumes up to 50 percent of faulting at the repository will occur on new or underappreciated faults. Most geological observations suggest that nearly all faulting will reactivate existing faults (i.e., those that are known and mapped). Waste package failure mechanisms assume that after a minimum threshold displacement [in this case 25 cm (9.8 in.)] is exceeded, the entire waste package fails. In addition, all waste packages intersected by the fault zone are considered failed, instantaneously and completely. This is a conservative assumption. The staff believe that underestimation of consequence of faulting due to uncoupled faulting, seismic, and volcanic hazards will be adequately compensated by these conservative assumptions and by the fact that the probability of faulting at the proposed repository is quite small. However, future versions of the TPA Code will be influenced by the desire to increase realism in the TPA Code where appropriate, and the goal of improving the usefulness of the TPA Code during a potential licensing review.

Comment 146: Example of coupling which does not appear to be accounted for in the TPA Code: correlation of seismicity and rockfall. (p. G–7) [van Dorp]

In the latest version of the TPA Code (Version 4.1), rockfall occurs whenever seismic excitation occurs, and the number of rock blocks that fall is determined by the magnitude of the seismic excitation.

Comment 162: The assumption that the seismic acceleration at the repository level is half that at ground surface seems, for non specialists, a rough assumption in view of the many other seemingly more refined assumptions. (p. G–13) [van Dorp]

The assumption of a 50-percent reduction in ground motion from the surface to the repository horizon is based on the magnitudes of body waves (predominant in the emplacement horizon) versus the surface waves (predominant at the surface). This assumption will be reevaluated once the Seismic Topical Report #3 (Preclosure Seismic Design Inputs for a Geologic Repository at Yucca Mountain) is received from DOE.

Comment 234: Faulting is not a significant WP failure mechanism. This result is given by the sensitivity analysis, but as for seismicity or volcanism, does it have to be matched to the physical properties of the waste package system? (p. E–19) [Ouzounian]

In the case of volcanism, the answer is yes because of the elevated temperature effects on the waste package material properties. The use of room temperature waste package material properties is acceptable when assessing the potential consequences of seismicity. In addition, the welds of the outer barrier closure lids cannot be solution annealed because of the limits on temperature for the spent nuclear fuel sealed within the waste package. DOE is proposing to laser peen the inner closure lid weld and induction anneal the outer closure lid weld. Increased corrosion rates and reduced material ductility are still considered to be a real concern in the immediate areas of these welds. Material testing and finite element analyses are presently being conducted to provide the technical bases for potential failures of the waste package by either accelerated corrosion rates or large plastic deformations caused by rock block impacts on the welded areas of the waste package closure lids.

3.4 Comments Relevant to the Quantity and Chemistry of Water Contacting Waste Package and Waste Forms Integrated Subissue (ENG3)

Comment 1: Further study is required to show that the lack of coupling is consistent with the intention to conduct bounding calculations in the sensitivity studies. (p. A–2) The consequences of specific assumptions (particularly in terms of de-coupling of processes) need to be tested. (p. A–11) The TPA Code does not address a number of potential couplings of the various processes active in the repository. The coupling between the thermal loading, the mechanical behavior, and finally the hydrology of the infiltration (e.g., role of potential additional fracturing) is not addressed. The rationale for not considering these couplings is not presented. The 'cold wall' effect could significantly change the flux of liquid water reaching some canisters. (p. C–3) Several modules need more extensive coupling of processes between them. (p. D–2) Coupling amongst modules is sometimes missing. In some cases, this coupling could be expected to have significant effects as the results are cascaded. (p. D–8) [Brady/de Marsily/Kelly]

A major assumption of both DOE Total System Performance Assessment–Site Recommendation and the NRC TPA Code is that processes may be decoupled, evaluated, and then recoupled without adversely affecting reliability of the results. Full justification of this assumption by the NRC is not feasible, however, efforts are being made to identify couplings that have an important impact on performance. These will be evaluated in the TPA Version 5.0 Code. The exact nature of these couplings will be determined by subgroups working on coupled thermal-hydrological-chemical Processes in the Rock above the Drift; Seepage; Salts/Precipitates on the drip shield and Waste Package; and Radionuclide Release Rates and Solubility Limits. Of course, if a process or module should be coupled and is not, sensitivity analyses alone will not identify the importance of the coupling. The need for coupling between processes and modules was recognized early in the development process for the TPA Code. With each iteration of code development, staff attempted to more effectively couple the processes and modules. Sometimes coupling is done explicitly, while other times it is done implicitly. For example, it was recognized that near-drift thermohydrochemical processes may affect seepage into the emplacement drifts. Therefore, code parameter F_{ow} was developed, which can account for the large-scale features that create focusing on divergence of deep percolation toward or away from the drift. The current value that has been derived for F_{ow} does not include effects of thermal-hydrological-chemical coupling. It was also recognized that modeling of thermal-hydrological-chemical processes can be extremely computationally intensive, therefore, it was not beneficial to overall results and analyses to explicitly couple thermohydrochemical calculations to the TPA Code. Additionally, a parameter was introduced that can be used to increase the concentration of chloride in waters contacting the waste packages, which could potentially be increased significantly by thermal-hydrological-chemical processes. There is a delicate balance between increasing coupling and maintaining a tool that is computationally efficient. The TPA Version 5.0 Code will have improvements in coupling of modules and processes. The importance of a given coupling can also sometimes be tested using the code capability for correlated parameters. Creativity on the part of the analyst can sometimes replace computational burden.

Comment 57: Considering only the fraction of SNF below the water line would seem to be non-conservative. Within the canister above the water line, the relative humidity would be expected to be that in equilibrium with a saturated solution of SNF dissolution products. The effects of constituents from the container materials might also need to be considered. (p. D–7) [Kelly]

The "bathtub" model can be considered an abstraction of many poorly constrained processes within the waste package, such as the fraction of fuel that comes into contact with liquid water, the protection of the fuel by intact cladding, and the presence of a water film on fuel not directly wetted by dripping or immersion. The parameter F_{wet} (fraction of fuel that is wetted) can be sampled between 0 and 1 to represent the whole spectrum of none of the spent fuels being wet to all spent fuel being wet. Consequently, the F_{wet} factor can be adjusted to represent all possible states of fuel wettness, including fuel that might be wetted by a water film adsorbed from the atmosphere alone. NRC has modeled outside the TPA Code the likely contribution of fuel wetted by water films caused only by high relative humidity (e.g., for the case of waste package failure that allows only humid air, but not liquid water, to enter). The significance of releases caused by this phenomenon has been low for the cases studied. Should wetting by water films be determined to be important, this phenomenon will be incorporated into a future version of the TPA Code.

Effort is underway to estimate chemical environment inside the waste package in the presence of corrosion products. The newly estimated chemical environment that could be influenced by the presence of corrosion products will be abstracted for use in the future versions of the TPA code.

Comment 58: As the corrosion of SNF is electrochemical in nature, the local cathodic reactions may lead to alkalinization of the solution within the waste package. The effects of this rise in pH on the dissolution rate and nature of the SNF should be considered. For example, equilibrium may be achieved for one component of the SNF that dominates the local pH. Incongruent dissolution of the other components may follow. (p. D–7) [Kelly]

Coupling the local chemistry changes to the dissolution model will make the model too complex for TPA; however, the abstracted model includes the effect of pH, based on DOE experiments and analyses. Therefore, the effect of local pH can be included if independent calculations of local pH variations are performed. These have been suggested to DOE as potential separate calculations. As data become available, the effect can be incorporated into the TPA Code if it is likely to have a significant effect on the performance of the repository.

Comment 66: A methodology through which chemical pathways of water are analyzed and described all along its hydrodynamic path from infiltration in Yucca Mountain to the alluvium should be developed [strong recommendation]. (p. E–4) [Ouzounian]

The Evolution of the Near-Field Event Environment (NRC, 2000a) also identified the importance of tracking the evolution of the percolating water composition as it reacts with different natural and engineered materials in Yucca Mountain. It is, in part, the difficulty of this task that has prompted both the DOE and the NRC to assume that processes may be decoupled, evaluated, and then recoupled without adversely affecting the reliability of performance assessment models. For the same reasons, it is unlikely that the TPA Version 5.0 Code will be able to continuously track all couplings affecting the chemistry of the percolating water. However, CNWRA subgroups are making efforts to account for changes to water composition that may affect performance in the TPA Version 5.0 Code.

Comment 69: Chemical composition of water is difficult to predict during the reflux cycle, and except a sludge recovered during laboratory experiments, no data is available (care must be taken about early results, which in such a context are difficult to understand); as the system is complicated, processes need to be analyzed separately before being considered as coupled. It seems that there is a lack of grounds for a chemical model during the reflux cycle. Specific experiments could be considered in order to better define the chemical composition of water, and its evolution, during reflux cycles. Moreover, specific experiments could help in assessing effects of irreversible chemical changes due to thermal period, mainly phase changes with correlative porosity and permeability changes. (p. E–6) [Ouzounian]

It is important to define the chemical composition of the water, and its evolution, during reflux cycles. It is difficult, however, to define these changes in water composition via laboratory experiments. To do so reliably would require a nearly exact replica of natural conditions, precise control over boundary conditions, and the extensive monitoring of thermal-hydrological-chemical parameters. The CNWRA subgroup on Coupled Thermal-Hydrological-Chemical Processes in the Rock above the Drift will evaluate the evolution of water chemistry by performing MULTIFLO simulations. It is anticipated that the Third Laboratory Scale Heater Test simulations being performed at the CNWRA and the results of the DOE drift-scale heater tests may help constrain these calculations by providing empirical insights into the nature of reflux processes that complement site characterization parameters provided by the DOE.

Comment 141: Example of coupling which does not appear to be accounted for in the TPA Code: correlation of dripping model (EBSREL) and corrosion model; reflux would cause dripping => increased corrosion although relative humidity is still low. (p. G–7) [van Dorp]

See response to Comment 51 in Section 3.7 of this report. For the TPA Version 4.0 Code, a subgroup was organized to reevaluate the dripping model used in the TPA Versions 3.2 and 4.0 Codes. It is likely the treatment of dripping will be modified further in the TPA Version 5.0 Code. It is currently anticipated that the effects of seepage processes on the quantity of water that contacts the waste packages and waste forms will be evaluated explicitly by integrating the results of the dripping module with the water chemistry and corrosion modules.

Comment 182: The initial near-field chemical composition is described based on the general knowledge and a few data. Reference is made to the data compiled by Perfect, et al. and screened by Turner (1998). However, those data were generated and given for the saturated zone, for another purpose than that of the near-field chemical composition in the unsaturated zone. Same remark is made about J-13 well water, often used as a reference water, even for the unsaturated zone. As water chemistry will constrain further behaviors of the system, a reliable knowledge is requested. (p. E–6) A great uncertainty is associated to the composition of water, as it is not known along the pathway from surface to the WP. Assumptions are made on some of the characteristics, about the chloride content as well as the carbonate system, and conservatism is also retained based on unfavorable pH values (above 9 for pitting) for the considered alloys. Reliability and confidence can be improved with a reasonable description of the chemical evolution of water all along its interactions with the successive materials. (p. E–7) [Ouzounian]

Saturated zone waters, including J–13 well water, may not appropriately reflect unsaturated zone water compositions. Analytical pore water compositions in the unsaturated zone are available (Yang, et al.,1996,1998), but appear unreliable due to a lack of internal thermodynamic consistency. However, NRC and CNWRA staffs (Browning, et al., 2000) recently imposed charge balance and thermodynamic constraints on these analytical data to restore their internal thermodynamic consistency. Sensitivity studies will be performed to determine if variable ambient water compositions are important to performance. If determined to be important, the revised pore water compositions presented in the previous reference will be used in the TPA Version 5.0 Code to describe ambient water compositions in the unsaturated zone.

Comment 183: Other processes described in NFENV are relevant, but have to be applied in the context of each time scale, as for the two periods, the two-phase and the liquid phase period. As example, some of the corrosion figures presented during the meeting dealt with a life-time of more than 10,000 years for the waste canister. This means that except for early failure, which also has to be considered, there will be no release before at least 10,000 years. A detailed analysis in order to define the main processes occurring at each space and time situation is suggested. (p. E–7) [Ouzounian]

As noted previously (e.g., see the response to Comment 1 in this section), several subgroups were organized at CNWRA to define the main processes occurring at each space and time situation and to recommend changes to the TPA Version 5.0 Code, where appropriate.

Comment 186: As previously noticed, the J–13 well water is from the saturated zone, with a chemical composition reached after several thousand years of interactions with the rock matrix. Even if in some cases equilibrium is achievable within a few days, some reactions will require more than the flow-time through the upper UZ, and overall equilibrium condition will require much more time. (p. E–8) J–13 well water chemistry is used for dissolution of SF. How relevant is it to consider this water, while just infiltrated rain is supposed to reach the waste package? (p. E–17) How much is it relevant to consider an increase in carbonate? What is its effect? What is the full set of data for this alternative? Is it relevant to consider a reduction in silicate, whereas J-13 silica content is quite low, close to equilibrium with chalcedony, and that if we consider a just infiltrated rain, it can reach a very fast equilibrium with amorphous silica, at higher dissolved silica values? (p. E–17) [Ouzounian]

J–13 well waters may not be appropriate as a proxy for unsaturated zone waters that have evolved chemically as a result of coupled thermal-hydrological-chemical processing. Please see the responses to Comments 182 and 1 in this section. CNWRA staff are working to improve TPA Code capability so that it will more closely monitor the complex chemical evolution of percolating waters along flow pathways.

Comment 194: However, even if the model is valid for representing dripping, it becomes highly speculative to interpret the information which it produces in terms of water influx into the waste package and of water outflow. Conservatism is retained with a 3-percent value for the plan area of waste package to determine the potential quantity of water getting into all WP. The very over-conservatism here assumes that all drops get into all waste packages. At the beginning of WP leakage, only a very small fraction of the area submitted to dripping will allow for water penetration into WP. Then corrosion will progressively open the exposed area, inducing a full exposure corresponding to the 3 percent of the plan area. The time scale between the first drop getting in contact with the spent fuel and full opening may also be an important factor in the case of pitting or in the case of a very long time scale between first opening and full opening. This aspect may be considered, on conjunction with corrosion models, and may give rise to a model representing a progressive exposure which result may be significant on the final dose result. (p. E–9) [Ouzounian]

The reliability of the TPA Versions 3.2 and 4.0 Codes treatment of dripping is currently being evaluated by the CNWRA Seepage subgroup. The dripping model in the TPA Version 4.0 Code was modified to allow the parameters that control the fraction of dripping water that will enter the waste package to vary as a function of time such that increases in these parameters could reflect further degradation of the waste package. Differences between the treatment of dripping in Versions 4.0 and 5.0 of the TPA Code may affect the number of waste packages that the water drips onto and the quantity of water that contacts the waste packages as a function of time or temperature. Subgroups tasked with reevaluating the treatment of drip shield and waste package corrosion processes will consider the importance of allowing progressive corrosion and waste form exposure in TPA Version 5.0 Code.

Comment 203: What is the signification of the silica concentration from J–13 Well (0.0011M) compared to the values given for equilibrium with quartz, chalcedony, or cristobalite? (p. E–14) [Ouzounian]

The silica concentrations in J–13 well water are roughly equilibrated with cristobalite-beta, a phase not observed at Yucca Mountain. The J–13 waters are oversaturated in quartz and cristobalite-alpha and undersaturated in amorphous silica. As suggested in response to Comment 182 in this section, sensitivity studies will be performed to provide information about how different initial water compositions affect performance. It should be noted, however, that both analytical (Yang, et al., 1996,1998) and reinterpreted (Browning, et al., 2000) pore water compositions have similar silica concentrations to J–13. Quartz is kinetically inhibited and does not readily precipitate at ambient temperatures, explaining its supersaturation. It is more difficult, however, to explain supersaturation with respect to cristobalite-alpha, a SiO_2 phase observed at Yucca Mountain that does precipitate at ambient temperatures.

Comment 205: What is the relationship between the pH value set at a constant value of 9 (highest value obtained from simulations), the pH increase in the vicinity of the repository at approximately 10 (4-27), and values given for J-13 between 6.8 and 8.3 (Table 4-1)? With such a set of values, final results may differ at least by 3 orders of magnitude. (p. E–14) [Ouzounian]

In the TPA Version 4.1 Code, pH values are not modified continuously in response to environmental changes through time. For example, MULTIFLO simulations used to generate the chloride versus time/temperature look-up tables assume a constant pH. The code does not accurately represent the processes controlling pH in complex natural environments. The CNWRA subgroups will reevaluate the treatment of pH in the code, and, if it is determined that variable pH is important to performance, modifications will be made in the TPA Version 5.0 Code to treat pH as a continuous function of time and temperature.

Comment 207: How is the multiplication factor for chloride concentration derived to take account of the difference between groundwater chemistry and brine resulting from evaporation from the WP surface? (p. E–14) [Ouzounian]

The multiplication factor for chloride was first used in the TPA Version 3.2 Code to assure a maximum chloride concentration that was consistent with the solubility of the salt NaCl. It is likely that the TPA Version 5.0 Code will either eliminate the multiplication factor altogether, or else modify it to be consistent with the results of revised MULTIFLO simulations.

Comment 225: Does the J-13 water have a stable chemical composition? Was the process of its chemical regulation understood? Is it at equilibrium with the rock matrix? (p. E–18) [Ouzounian]

The J–13 well waters are likely to have a fairly stable chemical composition equilibrated with the surrounding matrix materials. However, changes in the saturated zone water compositions, like J–13, are likely to be affected by climatic changes. It has proven difficult to measure the J–13 composition accurately or to reproduce it in the laboratory.

3.5 Comments Relevant to the Radionuclide Release Rates and Solubility Limits Integrated Subissue (ENG4)

Comment 34: A concern is whether the amount of early release of radionuclides from those fission products that accumulate at the fuel grain boundaries is well accounted for. (p. C–7) [de Marsily]

The accelerated release of fission products that accumulate at the fuel grain boundaries was considered in the TPA Version 3.2 Code. Page 4-66 of the TPA Version 3.2 Code User's Guide briefly mentioned this aspect. The fission products present in the grain boundaries, along with those present in the cladding/fuel gap and in the cladding, are conservatively assumed available for instantaneous release following the failure of the waste package and submersion of the fuel in the water. The fraction of radionuclides assumed present in the gap and the grain boundaries is based on data in Johnson and Tait (1997).

Comment 163: An increased release rate for the 'gap inventory' is not mentioned (p. G–13) [van Dorp]

The fission products present in the grain boundaries, along with those present in the cladding/fuel gap and in the cladding, are assumed available for instantaneous release following the failure of the waste package and submersion of the fuel in the water. The fraction of radionuclides assumed present in the gap and the grain boundaries is based on data in Johnson and Tait (1997).

Comment 184: Concentration of radionuclide is directly derived from the spent fuel dissolution rate, which depends on the quality of water. Below solubility of limiting mineral phases, concentration of radionuclide will depend on the residence time during which water interacts with the spent fuel. This means that both terms C_i and q_{out} are not really independent in the advective mass transfer out of the WP (w_{ci}). (p. E–7) [Ouzounian]

Two models were used in the analysis of the release of the radionuclides, bathtub and flow-through: (i) For the bathtub model, the water flow rate out of the waste package, q_{out}, is zero if the volume of water in the waste package has not exceeded the waste package volume below the assumed exit hole, V_{max}. The water flow rate out of the waste package is equal to the input flow rate, q_{in}, if the volume of water exceeds the waste package volume below the assumed exit hole. (ii) For the flow-through model, the flow out of the waste package is assumed to be equal to the water flow rate into the waste package at all times. For both models, the water flow rate into the waste package is independent of the concentration of radionuclides in water in the waste package, and therefore, the water flow rate out of the waste package is also independent of the concentration of radionuclides in water in the waste package. The model assumes that, except for radionuclides initially located in the gap and grain boundary, only radionuclides released by the dissolution of the spent fuel matrix is available to be dissolved in the water in the waste package. It is also assumed that all this material is instantaneously dissolved up to the solubility limit of that element. The concentration of radionuclides in water in the waste package is related to the water flow rate out of the waste package because it has an effect on the residence time, which affects the quantity of spent fuel that dissolves while the water is in the waste package. Based on these simplifying assumptions, both C_i and q_{out} can be treated as simple functions of time for the analysis.

Comment 185: The very important role of secondary minerals is neglected in this approach; as illustrated with further works in the laboratory as well as on the field, it could account for orders of magnitude. (p. E–7) Conservatism of the approach is acknowledged, but its level is certainly to a far from realism. Even with this very high level of conservatism, a lack of description reflects a lack of understanding, a lack of confidence about the environmental context, and, hence, the right data to consider. (p. E–8) [Ouzounian]

The NRC base model has taken into account the secondary minerals. The dissolution rate was determined from corroborated data from flow-through tests, immersion tests, and drip tests, all with J–13 well water. All tests with J–13 well water included secondary minerals, although the thickness of the secondary minerals that form varies. Insufficient experimental data are available to quantify the potential importance of secondary phases to incorporate radionuclides. In the Total System Performance Assessment–Site Recommendation, the DOE decided not to take credit for secondary mineral formation because of uncertainties in how to characterize the process.

Comment 187: As 3 orders of magnitude remain between model 1, which is recognized to be very conservative, and the schoepite solubility model, efforts to reduce uncertainty margin can be valuable and help increase confidence by improving the overall knowledge and, thus, reducing the overall uncertainty. (p. E–8) [Ouzounian]

Efforts to reduce uncertainty in the spent nuclear fuel dissolution rate would be useful, but would have to rely on DOE studies that may or may not be forthcoming. Due to the large differences between the alternative models and the lack of data available to support less consecutive models, the TPA Code currently uses the most conservative model as the base model and has the option of using the other models to determine the amount of improvement in performance that could be attained if sufficient supporting data were collected. If DOE collects sufficient data to support an alternative model for spent nuclear fuel dissolution, the TPA Code has the flexibility to be able to use these data to evaluate the DOE model.

Comment 188: Thermodynamic based approach, as the schoepite model, does not depend on surface area of the exposed fuel, so another succession of assumptions on the geometry of grains in the SF is avoided. However, mineral phases involved in SF need to be well characterized as dissolution rate of the irradiated SF is higher by about 100 X than for fresh fuel. (p. E–8) [Ouzounian]

Only a few studies are available that characterized the mineral phases involved in spent nuclear fuel dissolution. The DOE tests that TPA solubility models are based on include irradiated spent nuclear fuel. Insufficient information is available to permit the use of a thermodynamic approach, like in the schoepite model.

Comment 189: Which are the secondary phases which can occur upon SF leaching, what is their stability, and what is their ability to trap FP or other radionuclides? (p. E–8) [Ouzounian]

Tests conducted at Argonne National Laboratory (1998) on spent UO_2 fuel reacted with groundwater and water vapor resulted in the formation of secondary phases including metaschoepite, dehydrated schoepite, soddyite, uranophane, Na-boltwoodite, and Cs-Ba-Mo-uranate. These phases are more stable than UO_2 in an oxidizing environment such as Yucca Mountain. Schoepite and similar uranyl oxyhydroxides are transitory phases in the paragenesis of uraninite alteration in nature, as well as in experimental studies. However, in some natural settings, schoepite can persist for many thousands of years. The Argonne National Laboratory experiments suggest that neptunium can be incorporated into dehydrated schoepite and may, therefore, be a long-term mechanism for neptunium retention from the standpoint of regulatory concern. The durability of dehydrated schoepite in conditions expected during the life of the repository at Yucca Mountain remains an important and poorly understood issue.

Comment 190: A level of inventory of grain boundaries and gaps up to 6 percent has been considered for the prompt release. According to different experiences, this value seems reasonable. It must be noticed that the fraction for the different radionuclides in grain boundaries and gaps may differ. However, a sensitivity analysis would show that even a factor of 2 on this value will not modify the final result. Nevertheless, it is important to describe a methodology about how values have been derived, how values have been selected for the model, and make sure the traceability. (p. E–8) [Ouzounian]
The fraction of radionuclides assumed present in the gap and the grain boundaries is based on data in Johnson and Tait (1997). Estimates of the fraction of radionuclides present in the gap and the grain boundaries are based on direct measurements of spent nuclear fuel. For nuclides that the gap inventory is assumed to be proportional to the release of fission gas release (Cs-137, Cs-135, I-129, and Cl-36), these measurements are from pressurized water reactor fuel. For other nuclides, the estimates are based directly on radiochemical measurements of primarily CANDU fuel. The gap fraction of the radionuclides include radionuclides assumed present in the fuel/cladding gap, the fuel grain boundaries, within the fuel cladding, and within any metal components of the spent nuclear fuel assemblies.

Comment 200: The conceptual model for radionuclide release seems to be a leaching process of the spent fuel, and then precipitation of limiting phases. Why isn't it clearly stated, instead of having an adjustment to ensure consistency? In case of adjustment, can we be clear about which of the end-members was good, or wrong? (p. E–13) [Ouzounian]

The concentration of radionuclides in the water can be limited by either the dissolution rate of the spent nuclear fuel or the solubility limit of the radionuclide in the water in the waste package. If the concentration of a radionuclide released from the spent nuclear fuel waste form exceeds its solubility limit, it is assumed to precipitate, and its concentration is set to its solubility limit. Otherwise, the entire release is assumed to be dissolved uniformly in the water in the waste package. Future revisions of the user's guide will describe the radionuclide release model more clearly.

Comment 208: Assumptions given to represent UO_2 solubility seem reasonable. Nevertheless, the validity of these assumptions have been checked against more sophisticated and complete geochemical codes. This needs to be mentioned in order to support the simplified models. (p. E–15) [Ouzounian]

Assumptions on the spent nuclear fuel dissolution rate have been checked against more sophisticated and complete geochemical codes and against experimental data. Several generations of EQ3 modeling were conducted to examine reasonableness of these distributions, and the results generally indicated that the dissolution rates used in the TPA Version 3.2 Code are conservative (i.e., more rapid dissolution rates than EQ3 calculations would indicate). These comparisons are documented in the quality assurance records associated with the TPA Code. The schoepite solubility model is rigorous for the solution of mass action relations for solubility and speciation as a function of temperature using sampled/fixed pH and total carbonate. Therefore, it is as good as EQ3 would provide, given the pH and carbonate values.

Comment 209: The surface area available for leaching is conservatively held constant. Leaching can lead to a higher fragmentation of the SF. In this case, the conservatively constant needs to be demonstrated, or at least justified. (p. E–15) [Ouzounian]

Only a small fraction of the spent nuclear fuel particle radius was penetrated with solution as the dissolution progresses. This increased surface area was taken into account. Sensitivity analyses will be performed to determine if a variable surface area for leaching will significantly affect dose.

Comment 210: Remarks on ionizing radiation are right, and the point really needs to be clarified because it can lead to orders of magnitude differences. In the same way as for thermal effects, synchronism of the different effects over time periods will be useful to analyze. If the ionizing radiation only occur before WP have been corroded, consequences will not be the same as in the case it occurs over a very long time period. (p. E–15) [Ouzounian]

Real and relatively fresh spent nuclear fuels with burnups ranging from 30 to 70 MWd/MTU were used in the flow-through tests for the dissolution rate of spent nuclear fuel (CRWMS M&O, 2000a). Therefore, the dissolution rates used in the analysis have taken into account this radiation effect. It should be noted that the ionization products could be washed away or significantly diluted in the flow-through tests because of the high flow rate. Real and relatively fresh spent nuclear fuel were also used in the unsaturated test (CRWMS M&O, 2000a). In the unsaturated test, because only small amounts of water were in contact with the spent nuclear fuel, ionization products should have had sufficient time to accumulate in the small amount of water that was nearly stagnant on the spent nuclear fuel surface. However, the experimental results did not show a significant correlation of the dissolution rates of the fuel to the burnup of the fuel.

Comment 211: About the discussion on assumptions, when writing 'if solubility controls the release, the fraction of fuel contacted is unimportant,' isn't it the intrinsic dissolution rate (4-63, ref. Gray and Wilson) rather than solubility? (p. E–15) [Ouzounian]

The radionuclide concentration calculated from the dissolution rate is compared with the concentration limit imposed by solubility constraints. If the former is larger than the latter, the latter value is used to determine the release, in which case the fraction of fuel contacted is unimportant.

Comment 215: What about instant release of iodine once water gets into contact with the SF? (p. E–17) [Ouzounian]

Iodine is instantly released from the spent nuclear fuel once the spent nuclear fuel is contacted by water, but release from the waste package occurs only if there is advective flux out of the container (bathtub versus flow-through models of releases from the waste package). Based on data from Johnson and Tait (1997), 6 percent of the iodine present in the fuel is assumed to be located in the fuel/cladding gap and the grain boundaries of the fuel and, therefore, is available for instantaneous release.

Comment 217: In the flow-through alternative, does the F_{mult} value simulate solubility limited contaminant release by limiting direct solubility of spent fuel (intrinsic as defined in volume I), or is there a solubilization step followed by reprecipitation of a more stable phase, in which case, depending on the phases, some contaminants can be released. (p. E–17) [Ouzounian]

F_{mult} is only a factor that limits the fraction of water that will enter the waste package and contribute to the release and transport of radionuclides. F_{mult} does not affect the dissolution of the fuel in any other way.

Comment 218: Natural analog: does the process consist in a congruent dissolution of U from the SF, or is there a non congruent dissolution, or a 2 steps process (with dissolution and then reprecipitation of secondary more stable minerals and release of some of the fission products)? (p. E–17) [Ouzounian]

The analog model assumes congruent dissolution of uraninite, an analog for spent nuclear fuel, and reprecipitation of uranophane, a secondary uranium mineral. The dissolution rate is calculated from (i) an estimate of the amount of oxidized uranium remaining at the Nopal I uranium deposit in Peña Blanca, Mexico; (ii) a maximum limit on groundwater flow rate through the Nopal I deposit; (iii) a minimum time period for oxidative alteration of uraninite; and (iv) the concentration of uranium in solution exiting the system determined by the solubility of uranophane (Murphy and Codell, 1999).

Comment 219: Immediate WP failure: all assumptions in WP failure are that failure occurs by the top of the canister. But as mentioned from volume I, there is also a possibility to have droplets flowing to the bottom of the canister and reacting (corroding) the lowest point. In such a case, if there is a short cut between top and bottom, release occurs immediately, by leaching, but probably with small amount of radionuclides

released. Isn't there an instant release for some radionuclides, once the WP fails? (p. E–17) [Ouzounian]

The model described in the comment refers to the bathtub model, which is the base case model for the waste package failure mode in the TPA Code. However, there is also a flow-through model in the TPA Code, which assumes a failure in the bottom of the waste package. There is instantaneous release of radionuclides located in the gap and grain boundaries (as discussed in response to Comment 190 in this section for the flow-through model). TPA Version 4.0 Code allows the user to specify the waste package failure mode (bathtub or flow-through) for different sources of waste package failure (e.g., corrosion, faulting, and seismicity).

Comment 224: Matrix dissolution is derived from dissolution rate experiments, in pure carbonate solutions. What is the signification of this approach, is it conservative, by how much, and of what is it representative? (p. E–18) [Ouzounian]

Formation of aqueous uranyl carbonate complexes enhances the dissolution of spent nuclear fuel, thus, at a given pH, experiments in pure carbonate solutions are conservative, assuming that carbonate is more effective than other anions at scavenging/complexing uranium. Dissolution experiments in carbonate solutions represent dissolution in carbonate-bearing groundwater typical of the Yucca Mountain system. The pure carbonate solution experiments provide a realistic model for the Yucca Mountain system, yet are conservative when compared to the carbonate solutions of the typical groundwater.

Comment 226: Are analog studies or drip tests representative of the spent fuel dissolution? To what extent, what are the limitations? (p. E–18) [Ouzounian]

Analog studies give information on potential alteration pathways for spent nuclear fuel for long periods of time. These studies can provide order of magnitude estimates of spent nuclear fuel dissolution rates. The use of analog studies assumes the properties of uraninite are close to that of spent nucelar fuel. The estimation of spent nuclear fuel dissolution rates based on analog work at the Peña Blanca site makes assumptions about the Nopal I uranium reserve, time of oxidation, and groundwater flow rate that have high uncertainties. These uncertainties in the characteristics of the Peña Blanca system provide limitations in the usefulness of the analog studies. The drip tests are one way of representing spent nuclear fuel dissolution in a system where water drips onto the spent nuclear fuel. It is not known whether water will actually drip onto spent nuclear fuel inside failed waste packages. The geometry and flow conditions in a real system will likely not be the same as in the simple laboratory drip tests.

Comment 227: Dissolution rates did result in peak TEDEs similar to those calculated for J-13 water, for dissolution rates 100 times less than the default value. What are the conclusions of this? Are the dissolution tests representative of the involved processes, are the main parameters known, is the J-13 water the good representative? (p. E–18) [Ouzounian]

The database used in the TPA Version 3.2 Code was obtained with tests in J–13 well water. Although DOE agreed to consider several in-package chemistries, the DOE conservative approach with pure carbonate solution may not be affected. On the other hand, the NRC dissolution model samples the dissolution rates obtained from immersion tests and drip tests, involving a range of chemistry (e.g., pH).

Comment 229: What is the stability of the secondary precipitating CHS compared to that of the primary CHS, which dissolves? (p. E–19) [Ouzounian]

The dissolution of spent nuclear fuel in an oxidizing environment such as Yucca Mountain will be controlled by an oxidative dissolution mechanism. It is conservative to assume that radionuclides in the spent nuclear fuel matrix will be released instantaneously as the matrix dissolves.

Comment 231: How do you justify the assumption that a release rate for each individual radionuclide to be equal to the oxidation rate of SF? (p. E–19) [Ouzounian]

There is not a sufficient technical basis to support an assumption that fission products and actinides will be created within the matrix of the uranium fuel. The TPA Code models a fraction of the fission products that migrate to the grain boundaries of the fuel or the cladding-fuel gap. These fission products are available for immediate release on failure of the waste package. This fraction is based on measured data, as discussed in response to Comment 189 in this section. Other than this fraction, there is no process that would release a significant amount of the radionuclides contained in the fuel structure until the fuel oxidizes and starts to degrade highly soluble radionuclides (e.g., technetium and iodine) are conservatively assumed to not be incorporated in secondary minerals, so these radionuclides are assumed to be available for release as soon as the spent nuclear fuel containing these radionuclides oxidizes. Additionally, in the base case model, credit is conservatively not taken for the incorporation of radionuclides in the secondary minerals. The release of less soluble radionuclides (neptunium, plutonium, and americium) adopts the solubility-controlled dissolution.

3.6 Comments Relevant to the Climate and Infiltration Integrated Subissue (UZ1)

Comment 23: Spatially variable infiltration rates with possibly higher values should be considered by incorporating neglected phenomena in the infiltration model. Neglected phenomena include (i) relationship of shorter periods of the Milankovitch theory representing tilt and precession to climate change, (ii) a different pattern of precipitation could produce higher Average Annual Infiltration, (iii) runoff can increase localized infiltration rates, and (iv) vegetation may increase the permeability of soil cover. (p. C–6) [de Marsily]

Responses are provided by number.

(i) Periods of climate change shorter than the Milankovitch cycle can be easily considered by modifying the precipitation multiplier function in the *climat02.dat* file. Additionally, the uncertainty of the annual precipitation value for the infiltration tabulator for Yucca Mountain preprocessor was included in the TPA Version 4.1 Code. Incorporation of uncertainty leads to greater values of shallow infiltration. However, the basis for uncertainty in the precipitation value (the technical basis for the choice of parameters to describe the precipitation distribution) is limited. Work is continuing to improve the technical basis for these uncertainty parameters.

(ii) The distribution pattern of precipitation changing with climate is being addressed by process modeling using BREATH (Stothoff, 1995) with precipitation and temperature data from different analog sites [monsoonal, lower bound glacial transition (no El Niño or Pacific Decadel oscillations), and upper bound glacial transition].

(iii) The effect of runoff is being analyzed in the Split Wash watershed model with the eventual goal to modify the TPA approach to account for runon. Runoff is implicit in the one-dimensional model, unlike runon (which is currently ignored).

(iv) Vegetation in future climates leading to increased values of Ksat: has not been formally analyzed; however, the expected change in soil texture due to climate evolution will lead to a decrease in Ksat of the soil. This decrease may be offset by the increase in Ksat caused by vegetation, biota, and shrink/swell cracking. DOE currently assumes that the present-day climate will last only 600 more years, followed by a monsoonal climate (warmer and wetter) for 1,400 years. A glacial transition (cooler and wetter) is assumed to prevail for the remainder of the 10,000-year period. This approach is relatively conservative to climate change because the paleorecord shows that many more than 10,000 years are needed for glacial climate stages to evolve and reach their maximum.

Comment 158: Runoff might tend to reduce infiltration if the water leaves the considered area. However, local runoff might concentrate the water in small depressions where it then might infiltrate into a fracture; evapotranspiration might, in such a case, be less than expected. (p. G–12) [van Dorp]

Runoff and runon are important and are being addressed with process-based modeling [see the response to Comment 23 (iii) in this section]. Evapotranspiration is qualitatively addressed in the one-dimensional model. Field observations support the notion that Evapotranspiration from fissures/fractures is lower than from the overlying soils (the soil in cracks often appears wet when the adjacent soil is dry). However, roots are commonly observed in the fractures/fissures, particularly perennial plant roots, which indicate that water extraction occurs within cracks/fractures. In the model, the water extraction function for extracting water from the soil and bedrock varies exponentially with depth down to the bottom of the rooting depth. This qualitatively supports the reduction in Evapotranspiration from bedrock fissures, but there has been no research that directly supports this for the Yucca Mountain case with fractured bedrock in the root zone.

3.7 Comments Relevant to the Flow Paths in the Unsaturated Zone Integrated Subissue (UZ2)

Comment 22: Once fracture flow has started at a given stratum, all fractures below it could also have fracture flow. (p. C–5) This can be addressed through changes to parameters. The net effect to the overall results will not be large. (p. C–3) [de Marsily]

Current field observations and numerical modeling do not support the concept of cross strata fracture flow in all units. Process-based modeling by DOE and CNWRA support the attenuation of fracture flow in nonwelded units. However, there is work underway by staff to evaluate the extent of this attenuation in heterogeneous porous media under transient conditions that could possibly exist at the site. This work is ongoing. It should also be noted that many of the fractures are stratabound, with terminations particularly common at the upper contacts of the nonwelded tuffs.

Comment 24: It is very difficult to justify the assumptions made and the values of the parameters used for the models of the thermal pulse. It will be very difficult for NRC to justify these choices. (p. C–3) [de Marsily]

These parameters have been investigated in a recent report by the CNWRA (Hughson, 2000). This report recommended parameter ranges that more closely represent the Enhanced Design Alternative II design. The general method for thermal hydrology in the TPA Versions 3.2 and 4.0 Codes is rather simplistic but could be justified if it gave results similar to a combination of process models and laboratory experiments. This combination has been investigated and the results were presented in Hughson, et al. (2000). The thermal flow abstraction code will likely be slightly modified and the parameter ranges will be adjusted to represent these results. The MULTIFLO code may be used to get liquid fluxes above the drifts and to distribute these fluxes (via a focusing factor based on fracture spacing) to Phillip's length-scale model (Hughson, 2000; Hughson, et al., 2000).

Comment 31: Thermal loading of the repository will induce dilation of the rock and create new fractures that could affect the infiltration rate. (p. C–6) [de Marsily]

Calculations conducted by CNWRA staff indicate that the thermal pulse will not affect rock at the surface and, therefore, will not affect the infiltration rate (Ofoegbu, 2000).

Comment 32: Derive conservative estimates for the results of thermal calculations using simplified models or develop more complex three-dimensional models. (p. C–7) [de Marsily]

Thermal calculations are now done for the TPA Code using a three-dimensional conduction model. Due to edge-cooling effects, some areas of the repository are cooler than others. Fully three-dimensional thermohydrologic models of the Yucca Mountain scale are computationally intensive. Staff have implemented two-dimensional models within the three-dimensional repository area. DOE has also implemented a multiscale thermohydrologic modeling approach in Buscheck (2001). CNWRA staff are currently working on developing more complex three-dimensional models to assess the accuracy of two-dimensional modeling.

Comment 35: Couplings between the thermal loading and the resulting effects is not considered. (p. C–8) [de Marsily]

CNWRA has looked at changes in fracture permeability resulting from coupled thermal-hydrological-chemical effects. These changes appear to be relatively small. CNWRA has also performed analyses investigating thermal-mechanical coupling and identified a potential for increased flow toward repository drifts resulting from thermal-mechanical effects on fracture hydrologic properties. CNWRA staff continue to develop thermal-hydrological-mechanical models to account for significant couplings. In its current configuration, the TPA Code allows the user to treat seepage parameters as time-varying, thus allowing consideration of time-varying drift geometry (e.g., caused by rockfall) and near-drift changes in hydrologic properties. What remains to be done is for ongoing studies of such thermal-hydrological-mechanical effects to be related to potential changes in seepage rates so that a time-series of seepage parameters can be developed and incorporated into TPA analyses.

Comment 38: Fault movements may induce increased infiltration on top of the breached waste packages. (p. C–8) [de Marsily]

Fault movements could affect infiltration into a drift. There could be two aspects if one looked at faults cutting the PTn and at faults cutting the drift crown. For the first aspect, process-based modeling described in Ofoegbu, et al. (2001) looked at the effect of flow patterns where faults cut the PTn. For the second aspect, Hughson and Dodge (2000) looked at the effect of increasing roughness of the drift crown on the seepage rate. Neither of these aspects has been incorporated into the empirical TPA Code flow factors for seepage. However, due to the low probability of faulting in the repository system, changes in water flow due to faulting would likely have little effect on performance. DOE is currently completing two key unsaturated zone tests: long-term monitoring of the isolated ECRB and variable infiltration tests at Alcove 8-Niche 3. Results of these tests of ambient seepage and induced seepage will ultimately be incorporated into the TPA Code.

Comment 51: The coupling of dripping to fracture flow should be considered. At present, the 'F' factors in the dripping abstraction are better than ignoring the effects, but are not defensible in any scientific way. The dripping abstraction is a good place holder, but it represents an area where substantial effort needs to be applied. (p. D–5) [Kelly]

The CNWRA will evaluate the F_{ow} and F_{wet} factors based on heterogeneous three-dimensional seepage simulations using MULTIFLO in a manner similar to the approach taken by Tsang and Wilson (2000). A subgroup has been formed to investigate potential improvements to the dripping model in the TPA Version 4.1 Code. This subgroup consists of experts in hydrology, geochemistry, corrosion science, and performance assessment. As for the F_{mult} factor, a process model based on reasonable assumptions about the permeability of corrosion products on the waste packages may be defensible.

Comment 60: The reflux effects need increased attention. The current abstraction must be compared to experimental results that need to be generated. (p. D–8) [Kelly]

The treatment of reflux water in the TPA Code is not yet fully satisfactory; however, experimental results have been generated to assist in improving the abstracted model. The MULTIFLO code may be used to get liquid fluxes above the drifts and to distribute then (via a focusing factor based on fracture spacing) to Phillip's length-scale model (Hughson, 2000; Hughson, et al., 2000).

Comment 145: Example of coupling which does not appear to be accounted for in the TPA Code: correlation of water fluxes with thermal, chemical, and mechanical processes. (p. G–7) [van Dorp]

The TPA Version 3.2 Code incorporates the effect of thermal processes on hydrology (thermohydrology); however, the code does not currently incorporate the the potential effects of thermohydromechanical or thermal-hydrological-chemical (thermohydrochemical) processes. Analyses by the CNWRA staff suggest that the impact of thermal-hydrological-chemical processes may be small. Refer to Comment 4 in Section 3.3 of this report for discussion of thermohydromechanical effects on flux (Ofoegbu, 2001; Ofoegbu, et al., 2001).

Comment 151: Not clear whether effects of collapsed drifts on the infiltration into the drifts and into the waste packages are included in the TPA Code. (p. G–8) [van Dorp]

The effects are not included, but may be important. Inclusion of these effects could be accomplished with MULTIFLO for heterogeneous parameter fields as per the response to Comment 51 in this section. Perhaps just as important is the effect of surface irregularities on the drift wall, which may also be evaluated using MULTIFLO simulations. For example, Tsang and Wilson (2000) performed such an evaluation for rock bolts. Additional work to incorporate this effect is being considered for incorporation into the TPA Version 5.0 Code.

Comment 159: Several geological units are discussed. To judge whether the assumptions for deeper infiltration are justified, one needs more information about these geological units than is given in the geological description of the site. (p. G–12) [van Dorp]

Hydrogeologic descriptions of stratigraphic units above the repository will be added for completeness of the TPA Version 5.0 Code documentation. Additional justification may also be needed to support the basis for the assumptions about deep percolation in the TPA Code. However, DOE performed more detailed three-dimensional modeling of flow in the unsaturated zone above the repository, and these results indicate there is little lateral flow of water above the repository (DOE, 2000). This modeling supports the assumption made in the TPA Version 3.2 Code that the water flow that reaches the repository horizon is equivalent to the shallow infiltration.

Comment 160: What would be the effect of backfill? This conceptual model differs considerably from the conceptual model(s) in Section 4.2.3.1; has it been shown that these differences do not cause inconsistencies? (p. G–12) [van Dorp]

Backfill is no longer being considered in the DOE reference design. However, backfill may mitigate the consequences of rockfall and volcanism, will increase the waste package and drip shield temperatures (which, in turn, will reduce the yield stresses of the various engineered barrier subsystem materials by varying degrees), and will affect water flow through the drifts. In addition, if the drip shield is included as part of the engineered barrier subsystem with backfill, the increased dead load supported by the drip shield may cause potential resonance effects during seismic excitation. In other words, the natural frequencies of the drip shield will be reduced as a result of the extra weight it must support if backfill is present. Because seismic excitation is a low frequency signal on the drip shield, it may resonate in a fashion that could potentially damage the waste packages.

Comment 169: Porosity and travel times: although the determination of porosity seems to be straightforward, the determination of the relevant flow porosity is very uncertain and may depend on the water velocity. Therefore, the calculation of travel times is subject to large uncertainties. (p. G–14) [van Dorp]

Large uncertainties exist in groundwater travel times due to incomplete knowledge of relevant flow porosity. For this reason, the effective flow porosity is a sampled parameter in the TPA

Code base case for both the tuff and alluvial flow systems. In the current TPA Version 4.0 Code base case, the effective porosity of saturated tuff (FracturePorosity_STFF) is sampled from a log-uniform distribution between values of 0.001 and 0.01. The technical basis for this range is Farrell, et al. (2000). The assumed log-uniform distribution favors selection of effective porosity values from the low end of the range, which results in shorter travel times. Staff believe this range reasonably bounds the parameter uncertainty, and the degree of uncertainty will not likely be reduced by the collection of additional data. There is also considerable uncertainty in the effective flow porosity of saturated alluvium (AlluviumMatrixPorosity_SAV). In the current TPA Version 4.0 Code base case, values for this parameter are sampled from a uniform distribution between values of 0.1 and 0.15. Ongoing and planned hydraulic and tracer tests in the saturated alluvium south of Yucca Mountain should provide a basis for improving this estimated range of effective porosity. Until additional data are available, however, it is assumed the currently used range is conservatively low, but within a reasonable range of expected alluvial sediment porosities.

Comment 192: One of the basic assumptions is that dripping occurs when I>Ks. Validity of this assumption depends on the homogeneity of the system, without rough patches at the wall of the drift, on surface interaction between materials and water, possible capillary forces, and others. (p. E–9) [Ouzounian]

It is a weak assumption that dripping will occur simply because percolation flux exceeds matrix saturation. The technical bases for the seepage abstraction and the stochastic ranges for seepage parameters have been significantly strengthened by documentation of observations and associated analyses in Hughson, et al. (2000). Discussion of this abstraction has also been updated in the TPA Version 4.0 Code User's Manual.

Comment 193: Questions remain about the model: does opening of the drift divert fluxes preferentially to the drift? On the other hand, isn't there any diversion along the walls of the drift? (p. E–9) [Ouzounian]

The opening of the drift diverts flux away from the drift, not toward it, and the amount depends on fracture capillarity and permeability. There is diversion along the drift wall now included in the F_{mult} parameter. An approach being considered for the TPA Version 5.0 Code would be to model the capillary diversion using a three-dimensional heterogeneous model, and assume that seepage breaking the capillary barrier would drip from surface asperities. The area of the waste package could be used to determine whether a seep dripped onto the package. Water landing on a waste package would then have to get inside, which is described by the F_{mult} parameter. F_{mult} could be modeled by using an unsaturated flow model through corrosion products. In this suggested approach, diversion along the wall would not be considered. The F_{ow} parameter would be capillary diversion in the boundary region of the drift wall rock, the area of waste package area of drift would discriminate between seepage contacting waste package and seepage falling harmlessly on the invert, and F_{mult} would characterize flow into the package based on flow onto the package.

Comment 204: Calculations show that a liquid phase is always present, and complete dryout does not occur following emplacement of WP. Is this result due to the scale of representation which is homogenized in the disk-shaped uniform heat-source? With MULTIFLO, or any other model/code, has a profile for the presence of water been drawn in the case of a single drift? Such a profile, as a function of time, would offer a better

resolution to understand the crucial point of the presence of water in contact with the WP. In the same way, with the disk-shaped uniform representation, pH increase and chloride increase are homogenized over the entire repository. A detailed profile at the scale of the drift would be helpful to discriminate local effects from large-scale effects, and to determine at which time scale homogenization can be considered. At the drift scale, the process described by MULTIFLO (4-26) of suction followed by vaporization and then condensation with a correlative salinity increase close to the heat source and a dilution at the condensation zone could also be described. But once adjusted on the above suggested profiles, due to the mass balances between high salinity waters and low salinity condensate would lead to the original water (except diffusion and mixing which can slightly modify the scheme). Quality of water getting into contact to the WPs depends on the involved time scales for the respective processes (heat generation, resaturation). Such an analysis could lead to avoid large overestimates of the consequences. (p. E–14) [Ouzounian]

The predictions of dripping in the drifts are based on thermohydrologic modeling using MULTIFLO with the drift represented explicitly. Chemistry was not included in these calculations, but will be coupled with thermohydrologic models to provide input for future versions of the TPA Code. Separate models are being developed to evaluate the impact of in-drift processes on water chemistry. Results include distributions of saturation and flux in the near-field environment as a function of time (Hughson, 2000).

Comment 206: About the reflux models, it is said that water that penetrates the dry-out zone would be available to contact the WPs, possibly accelerating the corrosion of WP materials and facilitating transport of radionuclides released from the failed WPs. But according to Figure 4-9, after 1,000 years temperature decreases below the boiling point. However, the lifetime of the WP overpack is designed to stand more than 1,000 years, even in the base case with 620 or 825. Synchronism between invoked processes needs to be explained. Moreover, the time the water begins to drip into the drift has to be considered, taking account of the near-field groundwater infiltration (REFLUX in 4-30). (p. E–14) [Ouzounian]

Any water that reached the drifts during the above-boiling period (<1,000 years) would have to contend with the dripshield and the waste package outer layer. So, the major effect of reflux in the current models would be to delay the initiation of corrosion processes until moisture returns to the near-field environment. In all likelihood the only release at this stage would be from waste packages with early failures from manufacturing defects. The NRC base case model has several packages that are initially failed as a result of these manufacturing defects. Therefore, reflux could influence radionuclide transport. The important thing is to determine the range of conditions during the thermal period, both probable and possible, and provide these environmental conditions to the degradation models. A process currently being evaluated for future code development is the impact of thermohydrology on the evolution of salts in the near-field environment.

3.8 Comments Relevant to the Radionuclide Transport in the Unsaturated Zone Integrated Subissue (UZ3)

Comment 74: It appears that retardation of radionuclides in fractures is not taken into account. While this is conservative, it would seem that at least some fine materials would be present in most of the fractures and that substantial retardation would occur there. (p. H–5) [Whicker]

Credit for sorption onto fracture walls and materials within fractures is not included in the TPA Version 3.2 Code. In the saturated zone, however, matrix diffusion processes are included and contribute to the retardation of radionuclides traveling within fractures. Although many fracture linings and fracture filling minerals have been identified during site characterization, distribution of these minerals within fractures is mostly unknown. Additionally, it is not known which fracture lining minerals are associated with active fractures (i.e., fractures likely to contribute to flow). Also, fractures that have been filled with mineral deposits or fine material are not expected to contribute significantly to flow and transport. Retardation of radionuclides is considered to be much more limited in fractures than in the matrix because sorption is assumed to be primarily controlled by the effective surface area, which is much greater in the rock matrix. Because of the significant uncertainty in the effectiveness of fracture sorption and because DOE has not taken any credit for fracture sorption, given the current level of characterization at Yucca Mountain, this process has not been included in the TPA Version 3.2 Code and is not anticipated to be included in Version 5.0 of the TPA Code. However, the code does have the capability to account for this process, if necessary.

Comment 88: I would strongly second the notion on p. 9-1 that colloid transport should be added to TPA Version 3.2. (p. H–7) [Whicker]

A capability to model colloid transport in the TPA Code would be beneficial. An approach, based on a similar methodology to that used by DOE in its Total System Performance Assessment code, is being evaluated for inclusion in the TPA Version 5.0 Code. In addition, an effort is ongoing to develop an analytical modeling approach that may be useful in conducting sensitivity analyses of colloid transport.

Comment 89: In Appendix A, p. A–47, a matrix K_d for Cm of 0 is assumed. I would expect Cm to have a K_d similar to that of Am. This would also seem inconsistent with the matrix retardation factor for Cm of 1.8e4 on p. A–80. (p. H–7) [Whicker]

The current TPA Version 4.0 Code User's Guide indicates (i) a value of zero is designated for the K_d of curium in the unsaturated zone matrix. The justification given is that no data exist to justify a value other than the conservative value of zero (i.e., no retardation); (ii) a value of 7.5×10^4 is given for the K_d of curium in the alluvium matrix (equivalent to the lower bound of the americium value); and (iii) a value of 1.8×10^4 is used for the K_d of curium in the saturated zone tuff matrix (equal to the value used for americium). It is unlikely that the use of curium K_d of zero has had a significant impact on results because of slow matrix flow and the exclusion of matrix diffusion in the unsaturated zone. However, a reasonable value for the K_d of curium other than zero will be obtained for inclusion in the TPA Version 5.0 Code.

Comment 148: Example of coupling which does not appear to be accounted for in the TPA Code: correlation of K_ds in the different environments (engineered barrier system, unsaturated zone, saturated fractured zone, saturated alluvium, biosphere) because of the chemical properties of elements in chemically different environments. (p. G–8) [van Dorp]

Correlation of K_ds between environments is not required if K_ds for each environment are explicitly considered in the TPA Code. Because each part of the system has assigned K_ds pertinent to that environment, and the K_ds are sampled from a distribution that represents uncertainties in that environment, then the K_ds are, in effect, correlated. One would expect changes based on the differences in environmental conditions.

The adequacy of the response above can be argued, depending on whether one thinks mineral characteristics or water chemistries play the largest role in determining sorption parameters. Noncoupling (as in TPA Code) may be better for mineralogically based variations inherent between rock types, especially for ion exchangers. Variations in groundwater are more subtle and, although they may be adequately reflected in the current model through distributions, coupling or correlation may be required if the groundwater evolves as a unit somewhat independent of stratigraphy (see responses to Comments 212 and 66 in Section 3.10 of this report). If the plume from Yucca Mountain evolves on its own and if water chemistry plays the most important role in sorption parameters, then K_ds would need to be properly transported to the next flow unit to be consistent with the evolving water chemistry.

A model is being considered for developing the TPA Version 5.0 Code to use response surfaces to correlate the K_d of radionuclides to the chemistry of the environment. If incorporated, this model would at least partially address the concern for a limited number of radionuclides.

Comment 150: Not clear whether transport of colloids are formed when radionuclides are released from the waste or during radionuclide transport in the engineered barrier system, through the unsaturated zone and through the saturated zone included in the TPA Code. (p. G–8) [van Dorp]

Transport of colloids in the unsaturated zone and saturated zone is being evaluated for inclusion in the TPA Version 5.0 Code. An approach, based on a similar methodology to that used by DOE in its Total System Performance Assessment code, was recommended for inclusion in earlier TPA Code. In addition, an effort is ongoing to develop an analytical modeling approach that may be useful in conducting sensitivity analyses of colloid transport. See the response to Comment 88 in this section.

Comment 166: Has the fracture flow model been benchmarked against other fracture flow models (with and without matrix diffusion)? (p. G–13) [van Dorp]

Formulation of the fracture flow transport model is documented in the NEFTRAN user's manual. Benchmarking against the analytical solutions employed is provided in that document. The analytical solution for the matrix diffusion conceptual model assumes a first-order, rate-limited mass transfer between interacting fracture and matrix continua, with advection in fractures only.

Comment 167: Another potential model for unsaturated zone transport is fractures with infill might exist, radionuclides could sorb on the infill material. Radionuclides could move by diffusion between the solute flowing through the fracture and the more or less stagnant flow in the matrix ("matrix diffusion") (see also section on NEFTRAN II). The flow through the fractures might be so fast that matrix diffusion would be negligible. (p. G–13) [van Dorp]

The comment suggests consideration for including matrix diffusion in the unsaturated zone in addition to consideration for including sorption on fracture fill materials. The sorption of radionuclides on fracture fill material is reasonable, but too little characterization exists regarding the fill materials and their distribution to adequately consider the process in the TPA Code. Matrix diffusion has been neglected in the unsaturated zone as a conservative measure because of the uncertainty in values for parameters needed to model the process.

It is likely that filled fractures do not significantly contribute to flow (unless these fractures are filled because they are the flow conduits). This assumption should apply to fractures filled with gouge or other fine material (unless the fill wicks flow into fractures) to concentrate flow in that fracture. Nevertheless, excluding sorption onto this material would be conservative. Current lack of necessary characterization would prevent adequate inclusion of these types of fractures. See also the response to Comment 74 in this section.

Comment 168: If no retardation is assumed in the fracture flow systems, colloids would not enhance the radionuclide transport. (p. G–14) [van Dorp]

The comment is correct with respect to the TPA Version 4.0 Code treatment of unsaturated zone transport, which includes neither matrix diffusion nor fracture sorption. Although no sorption is assumed within fractures in the fractured tuff saturated zone, retardation occurs by matrix diffusion and subsequent sorption onto the rock matrix. Because colloids may be less likely to undergo matrix diffusion due to size limitations, they may be transported through fractures faster than diffusing aqueous species, enhancing transport. Inclusion of colloids in the TPA Code would also have an important effect on release from the engineered barrier subsystem of radionuclides (e.g., plutonium) that tend to be associated with colloids. In summary, the inclusion of colloids would enhance release and saturated zone transport of some radionuclides. Should matrix diffusion be included for the unsaturated zone in future TPA Code revisions, then unsaturated zone colloid transport could become significant. The addition of a colloid model is being considered for inclusion to Version 5.0 of the TPA Code.

Comment 171: Paragraph beginning with NEFTRAN II: if matrix diffusion is taken into account, the choice of parameters needs to be carefully discussed and justified based on the/a conceptual model of the aquifer or stream tube. Has the model been validated or benchmarked for matrix diffusion? (p. G–14) [van Dorp]

As currently implemented in the TPA Code, matrix diffusion is not considered for contaminant transport in the unsaturated zone, although the capability exists with only slight modification. If matrix diffusion in the unsaturated zone is implemented in a future revision to the TPA Code, appropriate analyses will be conducted to determine appropriate parameter values. As discussed for Comment 166 in this section, benchmarking of NEFTRAN against analytical solutions is documented in the NEFTRAN (Olague, et al., 1991) user's manual. Matrix diffusion is considered for radionuclide transport in saturated fractured tuff. In the revised user's manual for the TPA Version 4.0 Code, the discussion of saturated zone transport has been revised, and a detailed rationale for selection of matrix diffusion parameter values has been added.

Comment 230: The balance between transport into the fractures and into the matrix needs further comments, as it is not really clear to me. (p. E–19) [Ouzounian]

In the UZFT module of the TPA Version 3.2 Code, a particular hydrostratigraphic unit can have either fracture flow or matrix flow, but both are not explicitly considered. In the new user's manual for the TPA Version 4.0 Code, discussion of the determination of fracture versus matrix flow has been revised and is described in a straightforward manner.

3.9 Comments Relevant to the Flow Paths in the Saturated Zone Integrated Subissue (SZ1)

Comment 21: The conceptual model of the saturated zone hydrology at Yucca Mountain is at present so uncertain, with so many alternatives and unknown transport properties, that it is not at this stage possible to derive a representative model to be included in the TPA Code, even with a range of uncertainties for its parameters. The conceptual models in the TPA Code are based at present on a series of unproved assumptions, not supported by the available data, and, therefore, underestimate the uncertainty. The only viable alternative at this stage and with the present level of data seems to me to be the use of a much more conservative saturated zone model. (p. C–3) The major issues are (i) role of the paleozoic carbonate, (ii) horizontal anisotropy of the fractured volcanics, (iii) connectivity of the fracture network, (iv) relation between the volcanics and the alluvium, and (v) exact geometry of the alluvium in the area. (p. C–4) [de Marsily]

The complexity of the geology and the hydrogeology along with uncertainty in groundwater flow and transport properties makes developing conceptual models (and abstracting the results of these models into the TPA Code) for the site difficult. The five major issues identified by the reviewer are being studied in an attempt to improve the representation of these uncertainties in the TPA Code. Activities are currently being undertaken by CNWRA to address various aspects of these issues. In an effort to reduce model and data uncertainties, CNWRA has been actively collecting and evaluating geologic and hydrologic data from the site. In addition, CNWRA is integrating (or will be integrating) these data with data from the Nye County drilling and testing program, DOE site characterization studies, and State of Nevada site characterization studies. Models developed from these integrated studies, as well as supporting data, will be used to improve model abstractions to the TPA Code and to better account for uncertainty. In the opinions of the developers of the TPA Code, there are sufficient data and a good enough understanding of the hydrogeologic framework to warrant the development of a reasonable saturated zone model.

Comment 26: It is not defensible to assume isotropy and determine that way the flow lines and flow tubes. (p. C–4) [de Marsily]

The assumption of isotropic behavior in the volcanic aquifers may not be entirely valid, and as a result, the flow tubes determined from this assumption may not be conservative. Recently published analyses of pump test data from the C-Holes Complex by CNWRA staff (Winterle and LaFemina, 1999) indicated a predominantly north-south anisotropy in the horizontal components hydraulic conductivity that ranges between 5:1 and 17:1. This anisotropy is expected to result in a more southerly flow. The quantitative impacts of this anisotropy on the performance of the site is going to be investigated in the near future using numerical models of the site, which are currently being developed. The results of this modeling effort will be used to improve the flow tube model in performance assessment.

Comment 27: The fraction of the pathway, which is situated in the volcanics, cannot be treated as a continuous equivalent porous medium, particularly if abstraction wells may be drilled directly in the volcanics. (p. C–4) [de Marsily]

This is a valid concern whenever flow and transport in fractured rock are modeled. However, field evidence at Yucca Mountain appears to suggest the contrary. Multiple-well pump tests and tracer tests performed in volcanic aquifer units at the C-Holes Complex and many other single-well tests at other locations indicate that, on the scale of tens of meters, the volcanic units may be treated as continuous equivalent porous media (e.g., dual porosity media). Models based on this approach appeared to provide a reasonable fit to the field observed data. Based on these results, it is plausible to model the flow and transport on a scale of tens of kilometers in the volcanics as a continuous equivalent porous medium. With regard to groundwater withdrawal wells drilled in volcanic or other fractured rocks, the effects of discrete fracture paths on the fraction of plume captured are not explicitly considered, but can be implicitly considered in the selected value or sampled distribution of aquifer thickness. This concern should be noted in a future update of the TPA User's Guide.

Comment 30: Replace the present models of the TPA Version 3.2 Code for saturated zone flow and transport with the following model: assume the entire flux of water and of radionuclides which seeps into each one of the infiltration subareas of the repository can be transported with little or no retardation into one single community well, without any additional dilution. (p. C–5) [de Marsily]

It is possible to consider this scenario with the TPA Version 3.2 Code by simply changing input parameter values. However, this model is excessively conservative and will not be used as the base case model in TPA Code.

Comment 37: Coupling between climate change and saturated flow, which could increase the hydraulic gradient and increase the saturated thickness, is ignored. (p. C–8) [de Marsily]

The assumption that climate change does not affect saturated zone flow will be reevaluated in the near future. It is reasonable to expect increased recharge in a wetter climate such as the predicted future pluvial period. This recharge should result in spatially varying recharge that should increase the elevation of the water table in the vicinity of Yucca Mountain. This increased water table elevation should reduce the thickness of the unsaturated zone beneath Yucca Mountain, thereby reducing the transport distance between the repository and the saturated zone. Spatially varying recharge may also impact groundwater flow and transport pathways. The impacts of climate change on groundwater flow paths in the saturated zone will be assessed in models for the site currently being developed by CNWRA. Results from these models will be abstracted into the TPA Code, where appropriate.

Comment 98: The effect of climate change upon the regional groundwater system is ignored but not justified. (p. F–3) Example of coupling which does not appear to be accounted for in the TPA Code: effect of climate on water table, exfiltration of water and biosphere. (p. G–7) [Thompson/van Dorp]

The assumption that climate change does not affect the regional groundwater flow system will be reevaluated in the near future. See the response to Comment 37 in this section.

Comment 170: Have fracture flow models been considered for the flow path before the alluvium? (p. G–14) [van Dorp]

Saturated groundwater flow in the vicinity of Yucca Mountain is known to occur in volcanic tuff units prior to transitioning into valley-fill deposits. Studies in the Yucca Mountain region have shown that flow in some of these volcanic units occurs primarily through fracture networks. Based on this information, NRC and CNWRA have considered the use of fracture flow models to simulate groundwater flow through these units. However, results from the C-Holes pump test performed in the volcanic tuff units near Yucca Mountain suggest that on the scale of the numerical models currently being used to simulate groundwater in the vicinity of Yucca Mountain (hundreds of meters to kilometers), these tuff units can be effectively modeled as a anisotropic single continuum. The anisotropy observed in the C-Holes test is assumed to result from preferred flow directions which result from fracturing. NRC and CNWRA staff are currently focusing on constraining the ratio of anisotropy in the hydraulic conductivity tensor indicated by the C-Holes pump test. This information will be incorporated in NRC and CNWRA single continuum models developed to simulate groundwater flow in the tuff units in the vicinity of Yucca Mountain.

Comment 196: Resolution of transport processes is matched to the use of results from SZFT. This choice is very important and must be explained, maybe with more details in the paragraph about assumptions and conservatism, in order to avoid any over-dimensioned request in the process analysis and in the data precision. (p. E–10) [Ouzounian]

It appears that the reviewer's concern relates to the application of the one-dimensional groundwater flow and transport model in the TPA Version 3.2 Code. In particular, the reviewer seems to be requesting additional documentation to support the abstraction of the model from multidimensional process models for the site. This need for greater clarification appears to be prompted by the statements in (i) the second to last paragraph on p. 4-85 of the TPA Version 3.2 Code User's Guide, " ... the approach adopted in DCAGW (section 4.8) for determining the radionuclide concentration of water consumed at the receptor location allows the SZFT model to neglect many of the high-resolution spatial and temporal variations in transport processes," and (ii) the first paragraph on p. 4-88 of the TPA Version 3.2 Code User's Manual which notes " ... because the estimated magnitude of water well pumping for irrigation at the receptor location is sufficient to capture most radionuclides emanating from the repository (Fedors and Wittmeyer, 1998), a relatively simple one-dimensional model can be used to convey radionuclides directly from the repository to the receptor location." More elaborate discussions on assumptions and conservatism used will be provided in subsequent versions of the TPA Code User's Manual.

3.10 Comments Relevant to the Radionuclide Transport in the Saturated Zone Integrated Subissue (SZ2)

Comment 29: The thickness over which matrix diffusion can occur, either as the half distance between two fractures, or by an *a priori* defined length, assuming the porosity to be 'closed' at larger distances. Such a limitation of matrix diffusion should be included in the TPA, if the matrix diffusion option is used. (p. C–5) [de Marsily]

The NEFTRAN transport code invoked by the SZFT module uses a first-order, rate transfer coefficient to approximate the rate of mass exchange between fractures and matrix due to matrix diffusion. Recognizing the reviewer's concern that large matrix blocks may not be fully penetrated during the time scale for transport through saturated tuffs, the TPA Version 4.0 Code includes a modification so that the rate transfer coefficient, which was previously specified in the input file, is now calculated using a formulation that includes three new input parameters: an effective diffusion coefficient (DiffusionRate_STTF), the effective spacing between flowing fractures [FracturesPerMeter_STTF (1/m)], and a factor to account for limited penetration of matrix blocks (ImmobilePorosityPenetrationFraction_STTF). The formulation and basis for parameter values are described in Chapter 10 and Appendix A of the TPA Version 4.0 Code User's Guide (Mohanty, et al., 2000).

Comment 75: It is indicated on p. 2-9 that lateral dispersion from streamtubes is neglected. I would like to see more rationale for this assumption because at first glance, this seems counter-intuitive. (p. H–5) [Whicker]

Lateral or vertical dispersion of a contaminant plume would reduce radionuclide concentrations within a contaminant plume. Thus, neglect of this dilution mechanism is conservative. Lateral dispersion coefficients are typically one or more orders of magnitude less than longitudinal dispersion coefficients. Additionally, the relative effects of lateral dispersion on plume dilution tend to decrease with distance when transport distances exceed a few correlation lengths of heterogeneity of hydraulic conductivity. Hence, neglecting lateral dispersion does not likely result in overlooking an important dilution mechanism.

Comment 197: A very interesting abstraction approach has been presented for deriving K_d values. This approach, which seems to correctly represent sorption processes, has been derived for actinides, but limited or no information was reported about FP. (p. E–10) [Ouzounian]

Actinide sorption is strongly influenced by solution chemistry (e.g., pH). Values and distributions used for actinide K_ds are best estimates derived from a surface complexation approach that incorporates the observed variations in groundwater chemistry at Yucca Mountain. This approach is especially useful because variations in groundwater chemistry are not explicitly incorporated into the TPA Code. The sampled K_ds for some actinides (uranium, thorium, neptunium, and plutonium) may also be correlated for a given TPA Code run. Although 43 radionuclides are considered in the TPA Code for direct release scenarios, only 16 radionuclides are considered in the groundwater pathway. Of these 16, only 6 fission products, (iodine, cesium, niobium, selenium, technetium, and cesium) sorbs through an ion-exchange mechanism. As such, the values for cesium K_ds are more dependent on mineralogy (ion-exchangeable phases). Values for cesium K_ds are estimated using experimental data reported in the literature (usually DOE experiments on tuff analogs from Yucca Mountain) for mineralogies similar to those included in the TPA Code model. Values for niobium and selenium (which may exist as the selenate anion) K_ds are also derived from experimental data based on batch sorption experiments as reported in the literature. Technetium, which speciates as the pertechnetate anion in oxidized groundwaters, is also assigned K_ds based on previously reported data. Because pertechnetate is often excluded from sorption processes because of its charge, technetium is given a K_d value of 0 in the unsaturated zone and the alluvium, which is supported by recent results of experiments conducted by DOE and CNWRA. Iodine is assumed to be nonretarding {K_d = 0 mL/g [0 gal/lb]}. Sorption process models have only been calibrated for actinides to date, and are not available for the fission products yet. Additional technical bases will be documented for the current K_ds for fission products while developing calibrated models to develop smart K_ds for additional radioelements, which are currently being considered for the TPA Version 5.0 Code.

Comment 198: Some data generated specifically for the purpose of validation of the model would be helpful in gaining confidence. All data are not possible to generate, but availability of a few will enhance reliability in all. Are data available for the alluvium as well as for the tuff? As distance increases from the disposal level, concentration in radionuclides decreases. Nevertheless, even alluvium is allowed to retain some species by sorption, and it will need a certain level of characterization in order to derive reliable K_d values. (p. E–10) [Ouzounian]

For the process level models (surface complexation models) used to develop K_d distributions for americium, neptunium, plutonium, thorium, and uranium, some confidence has been gained based on the capability of the models to predict results of laboratory experiments for a range in chemistry (pH, PCO_2). However, the surface complexation models explicitly account for chemistry variations (such as pH and PCO_2) that are not explicitly included in the TPA Version 3.2 Code. Although the probability distribution functions for K_d are calculated using the current observed ranges in water chemistry for the saturated zone in the vicinity of Yucca Mountain, a single realization of the code does not account for changes in solution chemistry, mineral chemistry within formations, or surface area, and results from the TPA Version 3.2 Code can not actually be validated through experimentation. A best effort might be to confirm the shape or type of distribution used to vary the K_d for sampling (e.g., lognormal versus log-uniform). This confirmation has been done in some recent DOE work.

A proposed modification for the TPA Version 5.0 Code provides for the sorption coefficient response surfaces to provide a more explicit link to geochemical effects on transport parameters. The response surface will be prepared using surface complexation models to calculate sorption for a range in key geochemical parameters. These surfaces will then be used to provide sorption coefficients for a given set of geochemical conditions.

Because of a limited amount of characterization and a lack of useful samples, little data has been collected to determine alluvium K_d values. DOE conducted some preliminary experiments using alluvium materials (well cuttings) and continues to develop more data. DOE focused on three radionuclides (neptunium, technetium, and iodine) in its experiments. Current data indicates that technetium and iodine are not effectively sorbed by alluvium, while neptunium sorption is similar to that observed for crushed tuff.

Comment 212: Transport of radionuclides is said complicated by, among others, spatial variability in the geochemical properties of the fracture surfaces and rock matrix. But reading this chapter, it appears that the system is made of 2 formations, the tuff and the alluvium. Except if those formations have variable properties regarding the chemical regulation of the water (but is there any reason for that?), the process must be homogeneous in each of those 2 formations. That means that even if variability is measured, it only reflects dilution effects, except for the very short times of contact between water and rock. A certain level of equilibrium must be reached (10km at 4m/yr = 2,500 yrs). If it is characterized and the process described, then spatial variability will no more be significant, all the more conservative approaches have been reasonably taken into account for differences between fractures and matrix. On the other hand, during the first stages of field studies, measuring and characterizing the chemical variability will help in understanding the processes. (p. E–15) [Ouzounian]

The saturated volcanic tuffs and alluvial sediments are abstracted in the TPA Version 3.2 Code (tuffs and sediments are organized based on flow and not retardation or chemical aspects) and do not reflect the many different units and heterogeneities within the strata. Each unit has distinctive mineralogical and chemical properties, and alluvial sediments reflect large- and small-scale variations expected in the complex regime of interfingered alluvial fans and ephemeral stream deposits. Fractures, which may penetrate several units, also have various fill and wall lining minerals. The fracture features are known, but are not well characterized spatially. Therefore, it would be expected that these variable properties would influence the chemistry of groundwater. Though the bulk alluvium and tuff mineralogies are similar, measurable variations in groundwater occur that are attributable to more than just dilution effects.

A summary of information from the Nye County Early Warning Drilling Program related to mineralogy, water chemistry, and sorption experiments is included in Bertetti, et al. (2001), which will be used to improve saturated zone transport modeling. Water chemistry data are already used to develop sorption parameter distributions through the use of surface complexation modeling (see response to Comment 198 in this section.)

It is acknowledged that the water chemistries of the saturated tuff and alluvium are closely related, probably because of the similarities in mineralogy and groundwater sources. Likewise, it would also be expected that, depending on travel time, groundwater would reach some level of equilibrium (or steady state) and, as such, would not undergo further significant changes in chemistry. Exceptions are that fracture mineralogies indicate chemical conditions different from the tuff matrix, thus creating a distinctly different water chemistry during fracture flow, and that changes in dissolved CO_2 may have a significant impact on actinide sorption properties even though bulk chemistry is not significantly affected.

The comment suggests that a plume emanating from Yucca Mountain would eventually reach some level of chemical equilibrium, and that successful reaction-path modeling of the plume for an appropriate time frame would allow calculations of the water chemistry. The result would be that small spatial variations in chemistry would no longer be a factor (i.e., contribute to uncertainty). Presumably, the chemical parameters derived from this process would then be used to guide sorption parameters.

An implied assumption seems to be that dilution and mixing of the plume from Yucca Mountain would be insignificant over the flow path, so that the chemical evolution of the plume would remain somewhat independent of effects from groundwater mixing. This approach seems reasonable, but is limited by the relative lack of information regarding the saturated flow path. Without better constraints on the flow path, it is difficult to include appropriate mineral assemblages for use in the water evolution modeling effort. An alternative approach, which would explicitly account for water chemistry variations based on site characterization, would accomplish the same goal and be somewhat independent of the flow path (assuming adequate chemical characterization). The alternative would also be useful if the plume chemistry is indeed modified by existing groundwater through dilution and mixing (so that the plume bulk chemistry is indistinguishable). In short, given the current uncertainties in saturated zone characterization and flow path direction, the modeling effort is not likely to reduce uncertainty.

3.11 Comments Relevant to the Volcanic Disruption of Waste Packages Integrated Subissue (Direct1)

Comment 17: The possibility of a combined seismic and volcanic event may be judged rather high as one might be thought capable of triggering the other. I see this as very unlikely, especially in view of the great depth from which magma must ascend before it is capable of eruption. (p. B–3) [Delaney]

Historically, observed basaltic volcanic eruptions are always associated with seismicity. Earthquakes of M4–5 are common, with hundreds of M2–3 occurring throughout the eruption. Compared to the effects of direct eruption through the repository, seismically induced rockfall onto remaining waste packages presents a relatively negligible risk (NRC, 2000b). Thus, seismicity associated with an eruption is not abstracted or modeled in performance calculations due to its relatively low significance.

Comment 18: I doubt that continued development of probabilistic models will be so beneficial as focused study of geologic analogs of the expected Yucca Mountain magmatic system. (p. B–3) [Delaney]

Agreed. The probability subissue is resolved as closed pending, and efforts are now geared toward magma-repository interation dynamics

Comment 39: Volcanic disruption on canisters not included in the explosion are not considered. Open drifts might be used as conduits for gases and/or magma, since they are not backfilled. (p. C–8) [de Marsily]

Volcanic disruption on canisters is the subject of ongoing investigations in fiscal year 2001–2002. Numerical and analog experimental models are being evaluated to better determine magma flow conditions on initial intersection with the drifts and more steady-state flow as the eruption progresses. The process of magma flow in drifts will significantly affect the volcanic release source term. The results of these investigations are documented in CNWRA deliverables that have been submitted to scientific journals for publication (Woods, et al., 2001; Bokhove and Woods, 2000). The TPA Version 4.0 Code included a modification that allows the user to directly input the number of waste packages affected by intrusive or extrusive volcanism so that the user has the ability to change the number of waste packages affected if process-level calculations show that a significantly different number of waste packages would be affected by igneous processes than would be expected from the base model in the TPA code.

Comment 59: Although the accuracy of the temperatures in the magma is unknown, and the interplay between the stresses during an eruption and the creep rates are unknown, some study of the possibilities is warranted. (p. D–7) [Kelly]

DOE concluded (CRWMS M&O, 2000b) that all waste packages will fail when incorporated into an erupting conduit. DOE also has committed to evaluate further the effects of magma flow on waste package performance, with results presented in June 2001. The significant expansion of Alloy 22 and reductions in ultimate tensile strength and yield strength from 25 °C to approximately 800 °C support the conclusion that a waste package exposed to magma flow for days to weeks will fail and allow the contained high-level waste to be entrained in the magma flow.

Comment 233: Short duration events result in a more concentrated ash deposit at 5 km. Longer-lived and larger eruptions dilute the dispersed inventory over a large area. Is it correct to take account of a fixed same amount of inventory released for both cases? (p. E–19) [Ouzounian]

Yes. There is no demonstrable linkage between conduit diameter and duration of the eruption. Small volume, high mass-flow rate eruptions may be capable of producing conduits of size comparable to larger volume, lower mass-flow rate eruptions. In addition, there is little correlation between the instantaneous mass-flow rate and conduit widening events. Doubik and Hill (1999) conclude the interplay between transient variations in magma flow rate, accumulation of degassed magma on conduit walls, and interactions with shallow {i.e., >500 m [1,640.5 ft]} groundwater controlled conduit widening during different stages of the 1975 Tolbachik eruption, Russia. Conduit diameter should remain independent of eruption power/duration.

3.12 Comments Relevant to the Airborne Transport of Radionuclides Integrated Subissue (Direct2)

Comment 14: Although the basis for and the implementation of the empirical ash-dispersal model proposed by Suzuki (1983) was extremely well defended by CNWRA staff, it is imperative that the underlying physical processes be better understood through focused field and theoretical studies. (p. B–1) Although better models may be obtained, at great cost to computer time, I expect the improvement would have a marginal effect, at best, on the total population of outcomes. (p. B–1) [Delaney]

A better understanding of the physical processes underlying the ASHPLUME model is one of many ongoing tasks in the Igneous Activity Key Technical Issue. For example, Woods (1988, 1993, 1995) thermo-fluid dynamic models for column rise are evaluated in NRC (2000b). Validated models based on thermodynamics and physics of eruptions, however, currently do not exist. Although empirical, the Suzuki (1983) model abstracts the eruption process at a level of accuracy sufficient for stochastic-process modeling.

Comment 15: Increased confidence in the parameterization will probably be crucial to the eventual acceptance of the results by both scientists and the general public. (p. B–1) [Delaney]

Agreed. A better understanding of the physical processes underlying the ASHPLUME model is one of many ongoing tasks in the Igneous Activity Key Technical Issue. For example, Woods (1988, 1993, 1995) thermo-fluid dynamic models for column rise are evaluated in NRC (2000b). Comparison of the results of these detailed models to the ASHPLUME results provides confidence that the parameterization in the ASHPLUME model is reasonable. Validated models based on thermodynamics and physics of eruptions, however, currently do not exist. Although empirical, the Suzuki (1983) model abstracts the eruption process at a level of accuracy sufficient for stochastic-process modeling.

Comment 20: If data (e.g., wind direction and speed, along with atmospheric structure to the expected heights of the ash clouds) were available, it may be found worthwhile to properly integrate the ash-fragment paths temporally and spatially through changing wind conditions. (p. B–3) [Delaney]

Near-vent dispersal of particles is dominated by advective-diffusive properties of the tephra cloud. Particle-tracking models (Lagrangian) are effective for dilute, very fine grained {<15 μm [0.00059 in.]} clouds relatively far from the vent, where atmospheric effects dominate the cold, dilute volcanic cloud. Although generalized atmospheric models and data likely exist for the Yucca Mountain region, projecting these models and data for a 10,000-year period would be challenging and highly uncertain. Work in this area probably would not lead to any significant insights on risk or confidence in the ASHPLUME model.

3.13 Comments Relevant to the Dilution of Radionuclides in Groundwater Due to Well Pumping Integrated Subissue (Dose1)

Comment 28: The potential layering in the alluvium must be determined, its exact geometry, and the manner in which the flux leaving the volcanics is distributed over the vertical when it enters the alluvium must be known before defensible dilution calculations can be made. (pp. C–4 and C–5) [de Marsily]

The reviewer's concerns that the structure of the alluvium is an important aspect of the performance of the site and should be taken into account in dilution calculations are valid. In addition, the reviewer correctly notes that the nature of the flow from the tuff to the alluvium will be affected by the structure of the alluvium. In particular, the distribution of radionuclide arrival times (and consequently dispersion) will be impacted by the structure of the alluvium. Because of lack of this information, a conservative approach was adopted in the TPA Version 3.2 Code, in which all radionuclides arriving at the compliance boundary are assumed to be captured by the pumping well, and a range of alluvial pathway lengths and hydraulic and chemical properties are used. Nye County is currently drilling and testing in the alluvium. It is hoped that these activities, along with future CNWRA field activities in the alluvium, will provide information on the structure of the alluvium that can be used to improve estimates of radionuclide arrival times at the compliance boundary, thus leading to improved estimates of dilution. It is also hoped that these data can be used to evaluate alternate conceptual models of dilution at pumping wells.

Comment 46: In alluvial deposits, there is very strong heterogeneity both vertically and horizontally. The analytical calculations to estimate the capture zone, depth, and width of a well depend really very strongly on the homogeneity assumption. (p. C–17) [de Marsily]

The reviewer is correct that the capture zone that results from well pumping will be influenced by heterogeneity (both vertically and horizontally) and possibly anisotropy. The analyses performed by Fedors and Wittmeyer (1998), which involved the use of a homogeneous model, should be seen as a first attempt to develop a conceptual approach for examining dilution. Currently, there are few data for characterizing the heterogeneity in the alluvium. When such data become available, more realistic numerical models capable of incorporating this data and performing groundwater flow and transport simulations with pumping conditions will be implemented. Dilution estimates from these models will then be used to improve dilution modeling in the TPA Code. CNWRA developed a numerical framework for performing these calculations, which is being considered for incorporation into the TPA Version 5.0 Code. However, 10 CFR Part 63 has specified the volume of water to be used for dilution due to well pumping, so performing additional analyses to determine the capture zone may not be necessary.

Comment 48: It is not defensible to use an equivalent continuous medium approach in a fractured aquifer to calculate dilution. (p. C–17) [de Marsily]

Wells within 5 km [3.1 mi] of the repository are expected to receive water from the fractured tuff volcanic units. Pump and transport tests were conducted in these volcanic units at the C-Holes Complex. Models of the pump test results indicate that at the scale of the test (tens of meters), these units behave as an equivalent continuous medium. Analyses of the breakthrough curves for transport tests performed in these units also support the fact that the porous medium can be treated as an equivalent continuum (Reimus and Turin, 1997). Available field evidence indicates that it is defensible to use an equivalent continuous medium approach to calculate dilutions. See also the response to Comment 27 in Section 3.9 of this report.

Comment 85: I would challenge, perhaps naively, that the entire radionuclide plume from the repository would be captured by wells (paragraph 5, p. 4-95). Is this a reasonable assumption? (p. H–6) [Whicker]

This is a conservative assumption for the case of a large pumping well that supplies the water needs of the entire community in which the reasonably maximally exposed individual lives. While it is true that one can envision scenarios in which complete plume capture does not occur, the capture of all radionuclides represents a reasonably conservative case from a dose perspective. Calculations described in NUREG–1538 (NRC, 2001) suggest that a well or a series of wells pumping the 3,000 acre-feet per year water demand for the reasonably maximally exposed individual, would easily capture all radionuclides released from the proposed repository.

Comment 172: Dilution of the radionuclide concentration as well as the fraction of the total radioactivity in the groundwater extracted by the wells depends strongly on the definition of the critical group, which is given by the proposed 10 CFR Part 63. Has a

sensitivity analysis been carried out, although given 10 CFR Part 63, this would not be required? (p. G–14) [van Dorp]

Dilution of the groundwater has been specified in the recently released EPA standards (40 CFR Part 197) and NRC does not have the flexibility to change it (i.e., NRC is directed by the U.S. Congress to implement EPA standards). However, NRC staff believe that the definition of the reasonably maximally exposed individual in 10 CFR Part 63 is protective. Although it is possible that individuals could live closer to the repository and still extract groundwater for domestic purposes, the rural-residential reasonably maximally exposed individual expected to be located at 18 km [11.2 mi] south of the repository still would be likely to incur the greatest exposures from the repository. Individuals located closer to the repository would be unlikely to pump the larger quantity of water needed for gardening or farming activities because of the significant cost of finding and withdrawing the groundwater from significantly greater depths. Therefore, these individuals would be exposed to fewer exposure pathways than a group that performed gardening or farming activities and, potentially smaller doses.

Comment 176: Why so much weight on what is permitted by local authorities? These rules might change, people might not obey the rules, and, anyhow, releases would take place when the rules will have been forgotten. (p. G–15) [van Dorp]

The current approach is to use the rules outlined in 10 CFR Part 63. This approach requires that the living style of the receptor group be consistent with that of people who currently reside in the Amargosa Valley, Nevada, and states that DOE should not project changes in society or the biosphere other than climate change. The well pumping rate of the rural-residential community is specified in 40 CFR Part 197 and 10 CFR Part 63 to be 3,000 acre-feet per year. This representative value was derived based on the water needs of a community with two average size alfalfa farms and is not dependent on what is permitted by local authorities.

3.14 Comments Relevant to the Redistribution of Radionuclides in Soil Integrated Subissue (Dose2)

Comment 16: My primary concern with the present TPA Code is its failure to estimate dosages due to fluvial dispersal from the vicinity of a volcanic vent to the critical population. (p. B–1) The fine-grained components of these deposits (i.e., thicker deposits near the vents) would, inevitably, be washed during rainstorms into the drainages, where debris flows and flash floods would carry it to the Amargosa Valley. Some assessment needs to be undertaken of doses caused by fluvial transport to the critical group of radioactive volcanic debris. (p. B–4) [Delaney]

Remobilization by wind and water is a focused topic for detailed investigations and model abstraction during fiscal year 2001. A model for the redistribution of radionuclides in volcanic ash due to fluvial and aeolian processes is being developed and considered for incorporation into the TPA Version 5.0 Code.

Comment 72: I gained the impression at the review that build up of radionuclides in the soil after years of irrigation with contaminated ground water was not accounted for in the TEDE computations. This could be particularly troublesome for radionuclides that are in relatively soluble form in deep groundwater but which become much less so in the

oxidizing surface soil environment. This potential decrease in solubility, of course, could reduce plant uptake, but the external gamma field could certainly increase over time as a result of radionuclide buildup in surface soil. In a similar vein, it would be important to account for return, year after year, of radionuclides in vegetation and animal wastes to the soil surface. I am not certain whether GENII-S keeps track of these sorts of phenomena. (p. H–4 and H–5) [Whicker]

GENII (Napier, et al., 1988) is able to account for the buildup of radionuclides in soil. By incorporating the GENII code into the TPA Version 4.0 Code, this ability has been added to the TPA Code. The current model uses a buildup time of 15 years, assuming that the concentration of radionuclides in the water being deposited is constant throughout this time. Buildup has little effect (<10-percent increase) on the dose conversion factors for most radionuclides because it only affects the direct exposure pathway, inhalation pathway, and uptake by plant roots. The concentration of radionuclides in plants is dominated by direct water deposition on the foliage for many radionuclides.

Comment 84: It would help to describe the type of resuspension model, since many exist. (p. H–6) [Whicker]

The resuspension model referred to is the resuspension factor model used in the GENII code to model resuspension of material on the ground onto plant surfaces. The model simply multiplies the areal concentration of radionuclides on the ground (Ci/m^2) by a resuspension factor (1/m) to determine the concentration of radionuclides in the air (in Ci/m^3).

Comment 87: Table 4-7, p. 4-123, lists a K_d of 550 for Pu 241. I have never seen such a low value for Pu in a natural environment. Is this a typo? Referring to Table 5-1, p. 5-7, the quantity and units for the EPA limit (last column heading) should be given. (p. H–7) [Whicker]

The K_d value for Pu-241 is correctly listed as 550 cm^3/g [15,000 in^3/lb]. It is taken from Sheppard and Thibault (1990) as the mean value for the K_d for plutonium in sandy soil. The EPA limit in Table 5-1 is a fractional release limit and, therefore, has no units. This fractional release limit is not present in the EPA standard for Yucca Mountain (40 CFR Part 197), and this column has been removed from the table.

Comment 149: Example of coupling which does not appear to be accounted for in the TPA Code: igneous release: correlation of the assumption that ash might be transported in different directions (not only towards the critical group as is assumed at present) and that the waste might not be homogeneously distributed in the ash (giving thinner layers with higher concentrations). (p. G–8) [van Dorp]

The ability to sample the wind direction is available in the TPA Version 3.2 Code, but is not currently being used. To at least partially compensate that the code does not account for the redistribution of the ash following an eruption, the code currently sets the wind direction blowing toward the critical group. Evaluation continues in fiscal year 2001 on the effects of remobilization of high-level waste-contaminated tephra by wind and water. A more realistic model would allow the tephra plume to blow away from the critical group at some times. However, most of these eruptions would deposit tephra on surfaces that drain into Fortymile Wash. This remobilized tephra would flow to the critical group location at some unknown rate, but accumulations could potentially exceed the mass of tephra originally deposited from the eruption. Although high-level waste may not be incorporated uniformly in the eruption, there is no basis to assume nonuniform incorporation processes. In addition, plowing and disturbance of the soil at the critical group location will effectively homogenize the high-level waste distribution in the tephra deposit. Nonuniform deposition would not likely change the results significantly because dose from the igneous scenario is dominated by inhalation. The dose from the inhalation pathway is controlled by the concentration of radionuclides in the resuspendable layer of the soil. Assuming that the location of the concentrated layer was random within the thickness of the deposit, any increase in dose achieved by having a higher concentration of radionuclides on the top of the deposit would be offset by the reduction in dose from those realizations in which the concentrated layer was buried beneath relatively clean material.

Comment 173: What period is assumed for accumulation of radionuclides in soil by irrigation? One of the aims of irrigation, besides providing sufficient water for crop growth, is to enable long-term irrigation without the accumulation of salts in the root zone in a sustainable agricultural system. (p. G–15) [van Dorp]

The accumulation of radionuclides in soil is assumed to last for 15 years before the plot of land is abandoned or used for purposes other than raising crops. A sensitivity analysis has been conducted by the DOE (CRWMS M&O, 2000c) that shows for the major contributors to dose (Tc-99, I-129, and Np-237), the dose conversion factors are relatively insensitive to the period of irrigation between 15 and 100 years.

3.15 Comments Relevant to the Lifestyle of the Critical Group Integrated Subissue (Dose3)

Comment 44: Consumption of two liters/day may not be reasonable for an arid climate. (p. C–10) [de Marsily]

The EPA standard defines the reasonably maximally exposed individual as an individual who drinks 2 L/day [0.53 gal/day] of water [40 CFR 197.21 (c)]. NRC uses the drinking water consumption rate {2 L/d [0.53 gal/day]} as a reasonably conservative value for risk assessments. Additionally, information from the DOE survey of local residents in Amargosa Valley suggests that average tap water consumption is 2 L/d [0.53 gal/day] and the 95th percentile is about 4 L/d [1.06 gal/day] CRWMS M&O (2000c). Therefore, the assumed value is considered reasonable for estimating dose to the reasonably maximally exposed individual. The TPA Version 3.2 Code has the capability to sample the value so NRC can conduct confirmatory calculations with any range used by the DOE.

Comment 70: It seems that NRC and DOE should agree on reference biospheres and human exposure scenarios up-front, so that cross-comparisons of performance assessment results can be directly compared at the appropriate time. However, I believe strongly that the conduct of the PAs by NRC and DOE should be quite independent from one another. (p. H–3) [Whicker]

NRC staff agrees with the concern and has attempted to achieve consistency in reference biospheres and human exposure scenarios by specifying the reference biosphere and receptor group in 10 CFR Part 63. These regulations specify the behaviors and characteristics of the receptor group and place constraints on reference biosphere assumptions. The NRC regulations result in much less speculation about the receptor group and reference biosphere.

Comment 71: Develop an appendix to the TPA Version 3.2 Code document which a) provides a structural (box & arrow) diagram of the GENII-S Code which shows all compartments and pathways treated; b) provides the entire set of equations (differential and analytic); c) provides a table describing all equation parameters (names, symbols, units, and single or distributional values assumed for the TPA Version 3.2 application); and d) describes how the GENII-S Code works (e.g., algorithms used to solve differential equation sets, time steps used, how it performs uncertainty/sensitivity analyses, etc.). (p. H–4) [Whicker]

NRC revised the structural diagram of the GENII-S code to include all compartments and pathways used in the TPA Code. The revised documentation will be included in the user's manual for the TPA Version 5.0 Code. Documentation of the GENII-S code equations is provided in the GENII user's manual (Napier, et al., 1988). Given the large number of equations used by the code, NRC believes production of additional (redundant) documentation of the equations is unnecessary.

Comment 73: Two things which would have added to the value of the report, 'CNWRA (1997). Information and Analyses to Support Selection of Critical Groups and Reference Biospheres for Yucca Mountain Exposure Scenarios. CNWRA 97-009,' are a listing of the equations used in GENII-S (and relevant to Fig. 3-2) and uncertainty expressions for the radionuclide-specific parameters in Table 2-5. (p. H–5) [Whicker]

The equations in GENII-S are documented in the user's manual that is cited in LaPlante and Poor (1997). Uncertainty expressions for the concentration ratios and transfer coefficients were not included in the table because one composite uncertainty factor was applied to all the values for plant uptake and another composite uncertainty factor was applied to the animal uptake values. These scale factors and their bases are discussed LaPlante and Poor (1997). Additionally, the user's guide for the TPA Version 4.0 Code includes a clarification that uncertainty in the transfer factors is accounted for through the use of a scale factor.

Comment 77: I question why the values were not treated as stochastic variables. There may be a reasonable rationale for this, but I believe that the overall TPA Version 3.2 Code output uncertainty may be less that it would be if the considerable uncertainty in the DCF values were accounted for. (p. H–7) On p. 2-11, it is implied that the mean values of the DCFs are used in the overall TPA Version 3.2 Code. Does this mean that they are used as single value parameters rather than being treated as distributions? If this is the case, then I think it would be more defendable, since the TPA Version 3.2 Code is billed as probabilistic, to treat the DCF values as distributions subject to Monte Carlo sampling. The report, CNWRA 97-009, summarized stochastic runs to show the uncertainties in the DCFs (e.g., Tables 3-1 and 3-2). The flow diagram on p. 3-3 certainly has the dose conversion steps in the correct sequence, but I'm bothered some if this step is no more than a single-value multiplication at the last step, which I think would lead to an overall underestimate of the uncertainty in the TPA Version 3.2 Code output. (p. H–3 and H–4) [Whicker]

Stochastic dose conversion factor calculations have been included for the groundwater pathway dose conversion factors in the TPA Version 4.1 Code. Inclusion was accomplished by executing a CNWRA adapted version of GENII (called GENTPA) as a module that can be executed for each TPA Code realization using sampled parameter inputs. A similar modification may be made for the calculation of dose conversion factors for the igneous activity exposure scenario (for pathways other than inhalation, which has a customized model). The change, however, is not a high priority due to the low relative importance of these pathways to the igneous activity dose.

Comment 78: Because of reliance on the GENII-S Code, I believe it would add credibility to the ultimate PA conducted by NRC and CNWRA to show some sort of results comparison for a given scenario between GENII-S and other 'mainstream' codes such as RESRAD, DnD, ECOSYS, etc., and even more importantly, blind comparisons with real data such as has been done in the BIOMOVS project using data sets from Chernobyl fallout. (p. H–4) I believe it would help if the GENII-S Code output could be compared with real data from various scenarios and with other commonly used codes. If this has already been done, then something could be said about the outcomes of such efforts. (p. H–8) [Whicker]

A code comparison of GENII and CAP–88 that concluded both codes results fall within the 95-percent acceptance region for the test protocol has been conducted by Maheras, et al. (1994). While this study focused on airborne release modeling, the exposure scenarios studied are relevant to the TPA dose modeling (e.g., soil contamination leading to ingestion, inhalation, and external exposures). The Pacific Northwest National Laboratories website at (http://www.pnl.gov/eshs/software/genii.html) also indicates the GENII package of codes was developed using a quality assurance plan based on the American National Standards Institute standard NQA–1 as implemented in the Quality Assurance Manual. All steps of the code development were documented and tested, and hand calculations have verified the codes implementation of major transport and exposure pathways for a subset of the radionuclide library. External peer reviews were performed for the internal dosimetry portions of the code, and for the entire code package, during the development phase. Recommendations of the review committees were then incorporated into the final product. GENII was included in the Validation of Model Predictions project—an acronym for the Coordinated Research Program on Validation of Models for the Transfer of Radionuclides in Terrestrial, Urban and Aquatic Environments), an international effort to compare environmental radionuclide transport models with measured environmental data. Results for a test scenario (based on environmental measurements following the Chernobyl accident) indicated that dose estimates from GENII were comparable to, although slightly higher than, those of other participating models, which is consistent with its primary function as a prospective analysis tool. The models included in the code have been validated to various degrees by additional studies, however, these models have not been compared directly to output from the code. In addition to these efforts, CNWRA verified the code is running as intended and plans to conduct additional validation testing in fiscal year 2003 pursuant to CNWRA quality assurance procedures. These efforts are considered sufficient for support of the model in the TPA Version 4.0 Code. DOE will also have to provide NRC with the necessary information to justify verification and validation of the code if it is used in a license application.

Comment 79: On p. 2-10, last bullet, does "direct contact" mean external gamma exposure from radionuclides in the soil? This term could have other connotations. (p. H–6) [Whicker]

The term direct contact refers to external gamma exposure from radionuclides in the soil. The statement about direct contact has been marked for clarification in the User's Guide for the TPA Version 5.0 Code.

Comment 80: On p. 2-10, the pathways for the farming community receptor group are listed, but the list does not seem complete. For example, what about soil ingestion by farm animals and people? (p. H–6) [Whicker]

The pathways diagram will be updated in the forthcoming TPA Version 5.0 Code User's Guide to include all major pathways. Human soil ingestion is considered in the GENII-S code; animal soil ingestion is not mentioned in the code documentation and is, therefore, assumed to be excluded. This exclusion is nonconservative; however, other conservative assumptions that impact the animal concentration (e.g., most feed is from forage and forage crops have all roots in contaminated upper soil layer) may offset the effect to some degree.

Comment 81: On p. 2-11, it is indicated that the residential receptor group is exposed only through drinking of contaminated well water and direct exposure from radionuclides in ash following igneous activity. It seems that this may not be conservative or realistic, because such people might purchase food products from farms in Amargosa Valley, or they may well have small vegetable gardens that are irrigated with contaminated well water. (p. H–6) [Whicker]

Both NRC and EPA defined the reasonably maximally exposed individual as a rural-resident community located 18 km [11.2 mi] south of Yucca Mountain as the most highly exposed group based on current conditions, to limit speculation about potential future behaviors. Using current conditions for the reasonably maximally exposed individual definition is a matter of NRC policy consistent with the recommendations provided to the NRC and EPA by the National Academy of Science committee on Yucca Mountain regulations. Nonetheless, to add perspective to the concern that doses might be significantly higher for the residential group with added pathways, consider the following results of the TPA Version 4.1 Code calculations. If the residential receptor dose were to include the same suite of exposure pathways as the 18 km [11.2 mi] group (e.g., crop and animal consumption), the highest expected annual dose (at 10,000 years) would likely only increase by a factor of approximately two. This is because the dose is dominated by Np-237 and the drinking water contribution to the dose for this radionuclide at the 18-km [11.2-mi] farming location is about 54 percent (therefore, adding the other pathways to the residential scenario would increase the dose by approximately two times). This estimate is expected to be an upper bound on the increase in groundwater pathway dose to the residential receptor due to addition of the suggested pathways. It is likely an actual resident would have fewer exposure pathways than the farmer, and, thus, the dose is more likely to be between the current drinking water only scenario and two times that value. Given that this residential group is much more speculative than the rural-resident community located 18 km [11.2 mi] south of Yucca Mountain (i.e., no current residents live that close to Yucca Mountain) and the magnitude of the change in dose is not great, the rural-resident community is considered reasonable choice for calculating doses. More information on the selection of the reasonably maximally exposed individual is provided in the Federal Register notice for 10 CFR Part 63.

Comment 82: Furthermore, has anyone considered the buildup of solid deposits on swamp coolers or humidifiers? (p. H–6) Another pathway that should be considered is a swamp cooler using contaminated water. (p. C–10) [Whicker/de Marsily]

NRC urged DOE at technical exchanges to include analyses of all reasonable exposure pathways including local use of swamp coolers. CNWRA conducted additional calculations to determine whether swamp coolers need to be included in the TPA Code. Initial results of the contribution of the dose from swamp coolers indicate that for the radionuclides that dominate dose (I-129, Tc-99, and Np-237), the contribution to the total dose to the receptor is minimal (less than 0.5 percent). For other radionuclides that have a more significant contribution from direct exposure (such as Nb-94), the total dose conversion factor could increase by 60 percent or more if the contribution of swamp coolers was considered. The contribution from the swamp cooler pathway is being considered with other improvements to the TPA Version 5.0 Code.

Comment 83: Given the extremely large variations with soil type and water chemistry, I am surprised that some of this sort of site-specific work (develop plant/soil concentration ratios) has not been carried out. At the very least, I would expect that one could narrow the range of reasonable assumptions based on soil characteristics in Amargosa Valley. (p. H–6) I do not think there is sufficient justification for the radionuclide-specific parameters (plant/soil concentration ratios and feed transfer coefficients to animal products). These parameters can vary a lot, depending on soil characteristics and chemical forms of the radionuclides. To do better in this regard, it would require site-specific experiments, which would be fairly expensive, or at least a more in-depth analysis of soil properties and expected chemical forms. On the other hand, if the current code comes up with doses and risks that are many orders of magnitude below current limits, then this kind of improvement may not be warranted. (p. H–8) [Whicker]

As the reviewer of a potential license application, NRC has used available information for parameters and TPA modeling code to conduct sensitivity analyses to determine what parameters may be important. In this role, NRC provides insights to help focus its review of the DOE work, but NRC does not conduct the research that will support the license application (that is the job of DOE). An initial problem with collecting data for radionuclide-specific parameters is that performance assessment analyses include many radionuclides, and most research is performed on individual or only a few radionuclides. During past literature searches, CNWRA was unable to find a better data set of transfer factors for all radionuclides. Conducting additional research was beyond the scope of the NRC prelicense application review activities. However, it was appropriate to raise the concern to DOE. At a prior technical exchanges with the DOE, NRC has identified the soil to plant factors as important biosphere parameters that are highly variable. Subsequent sensitivity analyses using the enhanced biosphere modeling capabilities of the TPA Version 4.0 Code show the plant transfer coefficients are important parameters in the total system performance calculation which indicates attention to bases and documentation by DOE is warranted. In recent prelicensing interactions, NRC noted the lack of site-specific data and asked DOE to use more site-specific or site-relevant data on transfer factors or to provide improved justification for why data are not available for the few important radionuclides DOE identified as important in its Total System Performance Assessment.

Comment 86: The first bullet on p. 4-96 indicates that food consumption rates are based on national averages. The Desert Research Institute in Las Vegas did a very large survey for areas near the Nevada Test Site in the late '80s. I recall some rather large differences from national surveys. Maybe it would be worth trying to get some of this information. (p. H–6) [Whicker]

The NRC use of the national averages was considered best available information a few years ago. These values were used with the understanding they would be updated with site-specific survey results from DOE research once that information was made available. NRC has now updated all consumption rates with DOE values derived from the survey results of the local population of Amargosa Valley.

Comment 92: I do not find anything to give me confidence in the accuracy of the DCF values. (p. H–4) I suspect that the values (for DCF) are generally reasonable, but I did not find specific evidence to make one feel entirely comfortable with them. (p. H–8) [Whicker]

Applying the concept of accuracy to these calculations implies that the purpose is to predict actual exposures to individuals near the site. From the perspective of radiation protection, the goal is not so much to accurately estimate the true dose but to provide assurance that the doses have not been underestimated, and safety is maintained. The extensive documentation of the parameter selection and the justification for selection of the code are provided to enhance confidence that the dose conversion factor calculations are reasonably conservative. Given the code has been tested to verify it is performing as intended, the parameter selections are comprehensively documented and appear reasonable, and the output has been checked for errors by the original modelers and technical reviewers, staff believe that work conducted to date are sufficient to provide confidence in the calculations for use in reviewing DOE biosphere modeling efforts. Because the NRC and CNWRA effort is focused on preparing to review the DOE dose calculation work, the NRC and CNWRA dose calculations and documentation are not intended to be accomplished at the level of detail and rigor as the DOE license application analyses, which should include more extensive documentation and rationales to support the modeling.

Comment 93: Not considering the potential use of agricultural products from the Amargosa Valley and home gardening by the non-farmer resident may not be reasonable. (p. H–8) [Whicker]

See the response to Comment 81 in this section.

Comment 99: There is no coupling between the volcanic deposits and soil characteristics for the groundwater exposure pathway. (p. F–3) [Thompson]

The distribution coefficients used for the volcanic ash have been made consistent with those used for the soil in groundwater pathway dose conversion factor calculations. The implicit assumption is that the volcanic ash is assumed to have the same properties as the sandy soils of Amargosa Valley. This assumption is necessary because no distribution coefficients could be found for volcanic ash for the radionuclides considered. The assumption is reasonable because the volcanic ash is expected to fall on the surface and be plowed into the soil prior to farming. The leach model for the volcanic ash is the same as the model used for soils in the groundwater release scenario except the distribution coefficients are sampled for all radionuclides in the groundwater release scenario and fixed at the mean values for all radionulides in the igneous activity scenario. This procedure is reasonable because the radionuclides (e.g., Am-241 and Pu-239) important for the igneous scenario are nearly insoluble and will not be greatly affected by leaching. The radionuclides important in the groundwater scenario (Np-237, Tc-99, and I-129) are more soluble and, therefore, are more affected by leaching, justifying the need for sampling distribution coefficients.

Soil characteristics for the groundwater exposure pathway following igneous release are not altered to represent changes due to the tephra deposit because of the long transport time associated with the groundwater pathway. This long transport time will allow time for eroding of the tephra and plowing of the deposit into the surface soil such that characteristics of the surface soil will not be significantly changed from nominal conditions when groundwater releases reach the location of the receptor group.

Comment 111: Biosphere data could not be found for any climate state applicable to the critical group behavior for the groundwater pathways compatible with the extensive (e.g., soil) data listed for the volcanic pathway. (p. F–5) [Thompson]

The biosphere modeling for groundwater pathway has been updated in the TPA Version 4.0 Code to include calculation of dose conversion factors in the code rather than using dose conversion factors calculated outside the code. Therefore, the input data related to biosphere been substantially increased for the groundwater pathway. The treatment of soil leaching is consistent for soil (igneous activity) and groundwater pathways and, therefore, the level of detail of parameter inputs is now also consistent.

Comment 154: I would recommend also to calculate consequences of other release scenarios, both natural and 'human induced,' e.g., (1) for a release by groundwater in Death Valley, which is the location for release if the water is not abstracted by wells; and (2) for a release by free flowing wells in Amargosa Valley, if the groundwater table is higher than at present due to a climate with more rainfall. (p. G–8) [van Dorp]

The staff considered various potential release and exposure scenarios prior to establishing the regulations and concluded that a farming scenario about 18 km [11.2 mi] south of Yucca Mountain would be protective of public health and safety and consistent with the stated policy goals of the standard setting agencies (both NRC and EPA). For additional information on the regulatory framework, see 10 CFR Part 63 Federal Register Notice, and the EPA Standard 40 CFR Part 197 at 66 FR 32073. While numerous release and exposure scenarios can be formulated, the final regulations issued by the EPA have eliminated further speculation by designating the location of the receptor group (the reasonably maximally exposed individual) and specifying that diet and lifestyle of the reasonably maximally exposed individual are representative of the people presently living in Amargosa Valley. Considering the examples provided, releases to Death Valley and Amargosa Valley are beyond the compliance location defined in the regulations. Considering the issues from a technical perspective, it is unlikely that calculated doses from groundwater-related exposure scenarios would be higher 90 km [55.9 mi] down gradient from the source compared with the location about 18 km [11.2 mi] south of the repository. Furthermore, potential exposure scenarios are limited in the dry and barren Death Valley area. In the other example, free flowing wells would not be able to supply sufficient water to support large gardens or farms, which would eliminate the ingestion of contaminated food as a exposure pathway to the receptor.

Comment 174: Page 4-93, Figure 4-17: the inhalation dose might also depend on the duration. (p. G–15) [van Dorp]

Figure 4-17 in the TPA Version 3.2 Code User's Guide (Mohanty and McCartin, 1998) was intended to show some examples of parameters and not be comprehensive. There is not sufficient room to list all relevant parameters.

Comment 175: Children and infants are not considered. I agree because uncertainties are larger than the effect of including children and infants, however, reasons should be given in the report. (p. G–16) [van Dorp]

The capability to calculate age-dependent doses has been included in the TPA Version 4.0 Code and has been described in the updated user's guide. This capability is primarily intended for testing and side analyses because NRC has chosen to rely on adult dosimetry for assessing compliance with the proposed regulations. NRC staff believe that these dose limits are protective of children. The International Commission on Radiation Protection recommends that the overall annual dose to members of the public from all sources should not exceed 1 mSv (100 mrem), in order to be protective of all individuals. This limit is based on a lifetime exposure to radiation, and includes all stages in life, from birth to old age. Therefore, children are protected by the all-pathways dose limit, which at 0.15 mSv (15 mrem) is a small fraction of the overall dose limit suggested by the International Commission on Radiation Protection.

Comment 177: Ingestion of soil or dust is neglected? (p. G–16) [van Dorp]

Soil ingestion is included in the calculations, but was not included in the documentation. Soil ingestion has been marked for inclusion in the User's Manual for the TPA Version 5.0 Code. Ingestion of inhaled particles is included in the dosimetry used to derive the intake to dose coefficients in Federal Guidance Report Number 11 Oak Ridge National Laboratory (1988). This is also marked for inclusion in the TPA Version 5.0 Code User's Manual.

Comment 213: Discussion on assumptions for DCAGW reflects the large amount of uncertainties, mainly due to social changes. It is of the highest importance to have a very detailed sensitivity analysis, first on the parameters included in DCAGW, and then on DCAGW in TPA. (p. E–16) [Ouzounian]

A detailed sensitivity analysis of the DCAGW parameters has been documented in LaPlante and Poor (1997). The recent inclusion of stochastic capabilities for the biosphere in the TPA Version 4.0 Code allows for future sensitivity analyses of the DCAGW parameters using the TPA Code (e.g., a total system sensitivity analysis). Such analyses are ongoing.

4 SCHEDULE FOR WORK TO COMPLETE RESOLUTION OF EXTERNAL REVIEWERS' COMMENTS

The responses to the comments of the external reviewers include a combination of references to work that has already been completed and work that is planned in future years. The responses either directly address the issue raised, reference sensitivity analyses related to the issue, or indicate that changes are needed in the TPA Code to address the issue. The changes that have already been made in the code and that are being considered for inclusion into the TPA Version 5.0 Code were significantly influenced by the results of this external review. The following sections describe the changes made in Versions 4.0 and 4.1 of the TPA Code that address comments made by the external reviewers, as well as changes planned for Version 5.0 of the TPA Code to address additional comments.

4.1 Changes Made in Versions 4.0 and 4.1 of the TPA Code in Response to External Reviewers' Comments

Many comments made by the external reviewers have been addressed since the time of the review through changes made in the TPA Versions 4.0 and 4.1 Codes. Following the external review of the TPA Version 3.2 Code, development has continued on the TPA Code. In fiscal year 2000, a major update of the code was released, Version 4.0, which has subsequently been updated to the current Version 4.1. The code was updated to model the design that the DOE proposed following release of the Total System Performance Assessment-Viability Assessment (DOE, 1998), which included modifications to the waste package spacing, drift spacing, and waste package design.

One of the most significant changes in Version 4.0 of the code was incorporation of the dose modeling calculations directly within the TPA Code. A modified version of the GENII code (Napier, et al., 1988), called GENTPA, was included as a stand-alone code run by the TPA Code for each realization to calculate the groundwater dose-conversion factors. This change allowed all input parameters to be sampled to address concerns that the true uncertainty in the calculations was not being shown in the results of the TPA Version 3.2 Code because of the use of constant dose conversion factors. Sensitivity analyses now are able to determine the relative importance of the uncertainty in the biosphere sampled parameters. The TPA Version 3.2 Code is now able to include the effects of the buildup of radionuclides in soil due to multiple years of irrigation with contaminated water. In addition, modifications were made to the biosphere modeling to allow the assessment of doses to age groups other than adults to allow sensitivity analyses to be performed on the differences in dose to these other age groups. These were all concerns with the biosphere modeling identified by the external reviewers.

The dripping model was modified to allow the parameters that control that fraction of water that drips from the drift crown slit and enters the waste package to be time-dependent. This modification allows the code to model time-dependent processes that affect dripping, including drift collapse and increases in the quantity of water entering the waste package due to continued corrosion of the waste package following failure.

Additionally, work was completed to improve the range selected to represent these parameters, which is documented in Hughson, et al. (2000).

The volcanism module has been updated to allow an alternative way to specify the number of waste packages affected by the igneous event. In addition to the geometric model currently specified as the base case model, the code now allows a user-specified distribution to be used to determine the number of waste packages affected by the igneous event, both for extrusive and intrusive events. This distribution allows users to investigate the potential effects of magma-repository interactions to understand the significance of different models of how the rising dike is affected by the presence of the repository drifts in the subsurface.

Other changes made in the TPA Version 4.0 Code that address concerns expressed by the external reviewers include the ability to specify different waste package failure modes (bathtub or flow-through models) for different failure types (seismic, corrosion, initially defective, etc.) and the calculation of the rate coefficient for matrix diffusion in the saturated zone instead of using a user-specified value.

4.2 Changes Being Considered for Version 5.0 of the TPA Code in Response to External Reviewers' Comments

Many changes are being considered for incorporation into Version 5.0 of the TPA Code. The primary basis for deciding which technical improvements will be added to future versions of the TPA Code will be improvements in the realism of the models and the effect that the suggested change has on reducing uncertainty in the performance calculation (i.e., dose to the critical group). Additionally, the complexity of the change will be considered when prioritizing those changes incorporated into the TPA Version 5.0 Code. Items relatively easy to incorporate may get added to the TPA Code to improve the overall credibility of the models even if they do not have a significant effect on performance. However, other changes may not be made to the code if further analyses show that the change is not risk-significant. Those improvements requiring additional site-specific data may not be implemented until new data are gathered by DOE during the performance confirmation period. However, NRC staff will continue to insist that DOE models are supported by sufficient and appropriate data. Major changes being considered for the TPA Version 5.0 Code include

- Modifications to allow the code to calculate results beyond 100,000 years
- Correlation of the percolation flux crossing the repository horizon to changes due to shear-induced fracture dilation, vertical tension in the pillars, and excavation-induced rock loosening in the roof and floor areas of the drifts
- More explicit modeling of the effects of water chemistry, including improvements in the representation of the near-field environment chemistry
- Correlation of K_d values in the unsaturated and saturated zones to calculated chemical conditions
- Improvements in the model for dripping and flow into a waste package, including the results of more detailed models of thermo-hydrological-mechanical effects on flow, if significant
- Modeling of the effects of thermohydrology on the development of salts in the near-field environment

- Addition of a model for colloidal transport of strongly sorbing radionuclides
- Improvements in the modeling of saturated zone flow, including the effect of climate change on saturated zone flow processes
- Development of a model to represent the remobilization of ash initially deposited on the slopes of Yucca Mountain to the critical group location

5 SUMMARY AND CONCLUSIONS

The external reviewers were generally positive about the quality of work performed to develop the TPA Version 3.2 Code. The reviewers also were of the opinion the code was suitable for reviewing the DOE Total System Performance Assessment in support of the license application. A common theme in the reviewer findings was the need to continue to improve the documentation in the user's guide for the TPA Code as development continues on the code. Improvements in transparency and traceability of the TPA Code were started during the development of the TPA Version 4.0 Code User's Guide and will continue to be improved while developing the user's guide for the TPA Version 5.0 code. The strategic plan for the TPA Code (Mohanty and Wittmeyer, 1999) strongly recommends that future efforts focus on developing thorough documentation.

There was general agreement that the modules in the TPA Version 3.2 code had solid technical bases, and the model abstractions and data included in these modules captured the important physical processes occurring at Yucca Mountain. Nonetheless, the experts provided many suggestions for improving the technical bases of the code. An overarching theme of many of the experts' suggestions focused on the TPA Version 3.2 Code not including or explaining the exclusion of various coupled processes. In particular, several external reviewers noted the code does not adequately address the coupled thermal-hydrological-mechanical-chemical processes arising from the decay heat of the emplaced waste. Responses to these concerns indicated that plans for the TPA Version 5.0 Code include more explicit tracking of the chemistry of water in different areas of the repository system to more explicitly modeling some of these couplings. Some of the external reviewers also felt that the interdependence of seismicity, tectonism, and volcanism warranted greater consideration. Responses to these comments indicated that developing the probability of seismicity included igneous-induced seismicity, and that the direct consequences of igneous activity caused more indirect processes (such as induced faulting and seismicity) to be negligible. Also, it was stated that correlation between thermally induced fault slip and seismicity are probably weak because the fault slip area will be highly localized and the slip rate relatively slow. The external reviewers proposed many other technical improvements to the TPA modules that are summarized and responded to in Chapter 3. However, there was particular concern that the level of understanding of the saturated zone hydrogeology at Yucca Mountain is insufficient to support development of a credible transport model. This concern was responded to by indicating that although data are limited to support the saturated zone flow model, additional data are being collected by CNWRA staff and the Nye County drilling program staff to be used to improve models and support for models in future versions of the TPA Code.

Many of the technical improvements suggested by the external reviewers have been implemented in Version 4.0 of the TPA Code. Many more will be added or shown to be not significant to performance during development of the TPA Version 5.0 Code. The primary basis for deciding which technical improvements will be added to future versions of the TPA Code will be the effect that the suggested change has on reducing uncertainties in the performance calculations (i.e., at the receptor location). Those improvements requiring additional site-specific data may not be implemented until new data are gathered by DOE during the performance confirmation period.

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APPENDIX A

REPORT OF BARRY BRADY

External Review

Total-system Performance Assessment (TPA) Version 3.2 Code: Module Descriptions and User's Guide CNWRA, San Antonio, Texas Predecisional - September 1998

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Contents

SUMMARY

1. The overall conclusion of this review is that the TPA Version 3.2 Code is a well-conceived and well-produced software product, reflecting its development in a managed software process environment. With some reservations, the code is considered suitable for a performance assessment of a repository at Yucca Mountain provided that the repository geometry is similar geometrically to that described in the DOE Viability Assessment report of 1998.
2. In the course of the review, three sections of the TPA v3.2 code were considered in detail – the SEISMO module, the FAULTO module and the thermal functionality.
3. A notable feature of the TPA v3.2 formulation is the extent to which the various features, events and processes simulated in the code are decoupled. Although convenient in terms of code architecture and efficient in terms of code execution, some further study is required to show that the lack of coupling is consistent with the intention to conduct bounding calculations in the sensitivity studies.
4. In SEISMO, a relatively simple model assuming an unfilled drift is used in the current code to assess WP rupture. A more comprehensive model described during the review will permit a more thorough assessment of seismic effects on WP rupture. Whether or not emplacement drifts are backfilled will have an important bearing on seismic effects on WP rupture, and the unfilled drift model will be conservative.
5. In FAULTO, a conservative criterion for fault displacement is used to assess the possibility of WP rupture. Whether or not emplacement drifts are backfilled will have an important bearing on fault slip effects (which may be aseismic) on WP rupture. The unfilled drift model may not be conservative. However, the result may not be important as only a very small number of WPs are at risk of rupture under aseismic fault slip.
6. Thermal stresses are not taken into account in the code. These may have an important bearing on mountain-scale seismic effects and fault slip, and on the repository scale hydrology, by reducing vertical permeability at the repository horizon.
7. In its current form, the strengths of the code are the simple architecture and the logically consistent functionality, the rigor of the methods used to design and perform sensitivity analysis and the execution speed, which permits multiple executions in acceptable computation time. Its weaknesses are the lack of coupling between some of the controlling processes and possible lack of versatility in analysis of repository layouts different from the standard drift-and-pillar horizontal planar design.
8. From the results of the studies conducted to date, it is difficult to answer definitively the question about the completeness of the formulation of the code. It almost certainly covers the range of FEPs that need to be accounted for in the particular geological setting and the currently proposed repository designs. Decoupling of many of the FEPs raises questions about the extent to which all the possible modes of repository response will be captured in the performance simulations. A qualification study on a repository analogue, such as the Pena Blanca uranium orebody, could provide strong support for an inference of an acceptable level of completeness of the formulation.
9. It is doubtful if the code in its current form is sufficiently flexible to handle possible radical changes in repository layout. These could arise from design developments

intended to restrict the number of WPs subjected to contact with percolating and refluxed water. For that purpose, repository designs based on horizontal drifts arranged in vertical planes or panels are conceivable. In further development work on the TPA code, one objective should be to ensure that generic repository designs, other than those with a geometry based on a drift-and-pillar layout in a horizontal plane, can be simulated.

GENERAL REPORT

1. Scope of Work

Following the remit provided by the Review Coordinator, three areas of the TPA v3.2 code were reviewed in detail. In doing so, the complete set of documentation was considered in order to assess the complete set of features, effects and processes simulated in the performance assessment utility. This was a time-consuming task. However, it provided a basis for evaluating the particular sections of the code in context, and to evaluate the way in which they were integrated in the performance assessment methodology. It was also preparation for responding to questions, for which answers were sought in the remit, about the strengths and weaknesses of the code, its completeness and flexibility and scope for improvement of the code.

The three sections reviewed in detail were those concerned with the SEISMO module (Section 4.4), the FAULTO module (Section 4.10) and thermal effects (Section 4.2.3.1). In the review, it was noted that the implicit assumption made was that many of the processes and consequences were decoupled, while others were treated as coupled. For example, account is taken of thermal loading as a direct effect on rock and pore fluid temperature in the repository near-field domain and the resultant effect on WP corrosion and mineral solubilities. However, no account is taken of the possible changes in rock mass permeability that may be induced by the thermal stresses associated with the temperature field. Treating many of the processes as decoupled certainly simplifies the logical structure and information flow of the code. Although it may well be that effects such as these are second order effects, their role in the overall performance assessment will be referred to at various stages in this report. As will be discussed later, a complete mapping of interactions between various processes would aid considerably in an overview of the performance assessment methodology.

In assessing the modules of interest (and subsequently the overall code), the criteria used are those specified in the remit to the review team, as follows:

- Examine the methods and assumptions embedded in the TPA v3.2 code;
- Identify necessary code improvements;
- Evaluate implementation of conceptual models, including the approach for treating parameters;
- Is the TPA code suitably flexible and sufficiently complete?
  - Are the included features, events and processes sufficient to provide confidence in the Licensing Decision?
- Are the conceptual model abstractions defensible

- Are the conceptual model abstractions appropriate for the spatial and temporal scales being considered and for the selected performance measure?
- Are the model abstractions sufficiently supported by the site data or other related information to ensure the credibility of the results?
- Is the documentation sufficient to provide an understanding of the approach?
- Is the level of conservatism and simplicity of approach appropriate considering the role of the NRC?

- Are the methods used to develop abstracted models and their associated parameters reasonable?
  - Are the parameters used in the TPAv3.2 code appropriate to the abstractions?
- Are uncertainties in model abstractions and parameter values reasonably accounted for by the alternative conceptual models and parameter distributions provided in the code?

The documents considered in the review were:

1. Total-System Performance Assessment (TPA) Version 3.2 Code: Module Descriptions and User's Guide, CNWRA, September 1998.
2. NRC Sensitivity and Uncertainty Analyses for a Proposed HLW Repository at Yucca Mountain, Nevada using TPA v3.1 Volume II: Results and Conclusions, NUREG-1668, October 1998.
3. Other documents considered were:
   a. External Peer Review Meeting Graphics: U.S. Nuclear Regulatory Commission's Total-system Performance Assessment Version 3.2 Code, CNWRA, July 27-29, 1999.
   b. CNWRA Technical Operating Procedure 018 Revision 6
   c. A Parametric Study of Drift Stability in Jointed Rock Mass – Phase I: Discrete Element Analysis of Unbackfilled Drifts. CNWRA 96-009.
   d. A Parametric Study of Drift Stability in Jointed Rock Mass – Phase II: Discrete Element Analysis of Unbackfilled Drifts. CNWRA 97-007.
   e. Vere Jones, D. 1995. Forecasting earthquakes and earthquake risk. International Journal of Forecasting, Vol. 11, 503-538.

2. The SEISMO Module

The function of the SEISMO module is to determine the number of WPs ruptured by seismic events. In the current version, this consequence is conceived in terms of seismically induced rockfalls impacting the WP. The module consists of several components, including the seismic event recurrence relationship for the area, the algorithm for determining the weight of rock released from the crown of the drift and the algorithm for evaluating the loading and possible failure of the waste canister. The conceptual model is a comparatively simple one, and is presented as a basis on which some preliminary evaluations of the potential significance of WP rupture can conducted. The working assumption is that the drift is not backfilled.

It was concluded that the model as described is properly implemented in the TPA v3.2 code. In relation to the terms of reference above, the question that arises is whether the conceptual model is a sufficient representation of the loading conditions which a WP will experience over the 10 kyr TPI. With passage of a seismic wave past a drift, both the near-field rock and the WP will be accelerated by the ground wave. Because the seismic source is relatively remote from the drift, the loading is not impulsive in the way that might be imposed by an adjacent seismic slip, leading to rockburst conditions, for example. However, a more convincing analysis of the consequences of seismic loading would take account of the history of motion during a seismic event of both the WP and the local rock. This would require a more comprehensive representation of the WP and drift near-field rock in terms of both structural detail and time history of motion.

In the course of the on-site review, the engineer responsible for the SEISMO module described work in progress involving 3D dynamic finite element analysis of the drift near field and a WP. Such an analysis could explore other criteria for rupture of WPs under dynamic loading. In particular, it would permit evaluation of some of the assumptions regarding interaction between rock in motion and the WP, and WP damage and rupture criteria based on principles of fracture mechanics. The conclusion is that the relatively simple formulation of seismic effects may be sufficient as a first pass, but the more comprehensive analysis is required to assess seismic effects thoroughly.

As noted earlier, the working assumption is that the drift is not backfilled. If the drift is backfilled, the WP is protected from impact with displaced rock and by the damping capacity of the backfill. Apart from the reservations noted above, if in practice the drift will be backfilled, the assessment of seismic effects as now conducted is therefore highly conservative.

The assumption (which is reasonable) is that natural seismic sources leading to excavation dynamic loading are located outside the Yucca Mountain repository domain. However, an effect that may be of consequence in the evaluation of seismic factors is the possibility that thermal stresses may lead to conditions sufficient to cause slip on existing faults, which may be co-seismic, within the repository domain. Some preliminary evaluation of mountain-scale thermomechanics was conducted during the 1980s but does not seem to have been considered or pursued in this assessment scheme. If the thermally-induced seismic slip effect has been evaluated already and found to be not significant, it should be recorded in the documentation, for the sake of completeness. If it has not, some further work is justified. The effect could be included in a later version of the TPA code by modification of the seismic event recurrence relationship. However, the coupling with the thermal logic may not be compatible with the current code architecture, which relies on a high degree of decoupling. On the mountain scale, a temporal and spatial thermomechanical history which is relatively insensitive to repository layout may mean that direct coupling is unnecessary, and thermal stress effects can be interpolated from a look-up table.

The possibility of mountain-scale, thermally induced seismic events points to the need for comprehensive seismic monitoring of the repository during construction, to establish seismic baseline parameters, and in the pre-closure phase, to characterize seismic response which may bear some relation to the temperature field.

3. The FAULTO Module

The function of the FAULTO module is to calculate the number of WPs that are ruptured by displacement of faults that transgress the repository domain. It takes account of the prescribed emplacement of WPs relative to known faults, in which the WPs are assumed to be set back from the trace of a fault across the host drift boundary. Thus, the problem is also to evaluate the possibility that new faults will be generated in the repository domain in the TPI. In assessing the possibility of WP damage under fault displacement, no seismic impulse is assumed. In this way, a FAULTO event is distinguished from the effect of seismic loading, in which dynamic loading of WPs is the operative mechanism.

The analysis is developed in terms of a Critical Simulation Region, devised to include the range of fault orientations and fault lengths mapped in the vicinity of the repository domain. The application to mapped faults of PDFs derived for faulting in this region is intended to include future faults which could conceivably intersect the repository, although the faults may originate outside the repository footprint. The method used to estimate the recurrence time for faulting in the CSR and the way in which this is applied to the repository domain are considered to be scientifically sound, although it is noted that recurrence times for coseismic faulting is a topic of active research (Vere-Jones, 1995). The result in the current formulation is a very large recurrence time (197 kyr) for faulting within the repository footprint. The representation of fault displacement data and fault zone width data in terms of log-normal distributions is shown to be quite consistent with the current data set for these parameters.

The arbitrary factor in the assessment of WP rupture in FAULTO is the setting of a threshold value of fault displacement at which rupture will occur. It is probably reasonable at this stage to resolve the issue by setting the threshold to a low value of 25 mm. The resulting CMD attributed to faulting is found to be very low, because the number of WPs indicated in the analysis as ruptured is quite small. At this stage, the rupture threshold can be taken as a reasonable working hypothesis. However, as noted in the User's Guide (p. 4-106), the code takes no account of possible loss of strength of the WP with corrosion and other modes of damage. While the current displacement threshold figure for rupture seems conservative, at some stage some hard data derived from experimentation would be useful in determining how corrosion and other modes of damage affect WP resistance to rupture under various types of imposed deformation.

As was discussed for the SEISMO module, the effect of thermal stresses on the mountain scale may be important in assessing fault displacement in the repository domain. Figure 4-9 (p. 4-29) indicates the significant zone of influence of the thermal load at the repository horizon. Some earlier mountain-scale scoping studies of thermomechanical response suggest that significant changes in the state of stress in the repository domain and on the mountain scale arise from the thermal stresses. If faults in the repository domain are close to a state of limiting equilibrium in the existing state of stress, the perturbations arising from the thermal stresses may be sufficient to initiate fault slip. Figure 4-9 suggests the effect will be of most interest within a TPI of about 1000 years of repository performance. If the effects of thermally induced fault slip are found to be significant, they can be evaluated directly and recorded in a look-up table for subsequent inclusion in the complete FAULTO calculation sequence.

Considering both seismic effects and fault slip, the results presented in the TPA v3.2 User's Guide and NUREG 1668 suggest it is difficult to conceive of conditions where a sufficiently large number of packages could be ruptured to cause a substantial increase in TEDE at the candidate 20 km site for the 10 kyr TPI. Nevertheless, because the objective is to conduct a bounding calculation on TEDE, the possibility of thermally induced fault slip and associated seismicity (even though the slip may indeed be aseismic) is worthy of further consideration.

It is conceivable that backfill could affect WP rupture under conditions of faulting. On the one hand, backfill will restrict acceleration, inter-WP collisions (for the EDA II design) and potential damage of WPs if faulting occurred co-seismically. On the other, backfill could result in localized deformation of WPs and a higher incidence of rupture under even aseismic faulting conditions.

4. Significance of thermal effects and thermomechanical analysis

In Section 4.2.3.1, thermal analysis is reported for the repository for both the mountain scale and the drift scale of reference. The formulations are derived from the unit solutions derived by Carslaw and Jaeger. An inspection of the formulations suggests that they could be readily extended to calculation of the thermally induced stresses at both scales. As noted earlier, the mountain scale stresses may be important in evaluation of fault slip and induced seismicity on the repository scale.

The drift scale thermal analysis is important in the current formulation of the TPA code in evaluating thermal effects and thermohydrological effects in the vicinity of the repository horizon. Refluxing is a particular issue in near-drift behavior. However, for the reasons noted below, the thermomechanical response may also be important.

In the course of the on-site review, it was learned that bomb-pulse H3 and Cl36 had been detected at the repository horizon, indicating that the rate of percolation of water from the surface is somewhat higher than expected initially. That being the case, increased attention has been focused on the design of the repository in terms of fluid flow past the repository horizon. Relative to the TSPA-VA design, the Enhanced Design Alternative (EDA) II design posits a reduced AML (60 MTU/acre versus 85 MTU/acre), an increased drift spacing (81 m versus 28 m), a smaller longitudinal gap between WPs (0.1 m versus 5.5 m), different ground support (rock bolts and steel sets versus concrete liner and steel sets), a drip shield, 50 years of ventilation and C-22 as the outer (rather than inner) barrier of the WP. All these changes reflect a better realization of the need to control water flow and related phenomena at and above the repository horizon. An important concept incorporated in the wider spacing of the drifts is 'shedding' of reflux water from above the drifts to the pillars between the drifts. The success of such shedding is dependent on the vertical permeability of the pillars generated between the emplacement drifts. That in itself is determined by the thermal stresses, which are generated in the period of active heating of the repository near field and which are compressive in the horizontal direction. The period of reduced vertical permeability of the pillars therefore coincides with the period in which reflux water can accumulate above the repository.

This analysis indicates that incorporation of the shedding concept as a feature of the repository operation and the posited diversion of flow requires evaluation of the extent to which vertical permeability is retained in the core of the pillar. This could be determined readily by extension of the drift scale thermal analysis to provide calculation of the thermal stresses. As noted later, concerns about the effectiveness of shedding as a method of controlling WP exposure to percolating and refluxing groundwater could conceivably lead to changes in repository layout more radical than those expressed in the EDA II design.

5. Strengths and weaknesses of the TPA v3.2 code

Conduct of a PA study over the possible ranges of FEPs, scenarios and parameter values involves multiple executions of the TPA code, requiring speed of execution as a critical code performance parameter. This implies a compromise between model simplicity and efficient implementation on one hand and comprehensive simulation of all the FEPs which bear on repository performance on the other. The question that arises in the model simplification procedure is whether the final TPA code formulation can generate results which represent bounds on the complete range of possible modes of response of the repository. As a general principle, it is accepted that a capacity to calculate reliable bounds on TEDE at the locations of interest which is important, not the detailed simulation of individual FEPs or complex scenarios.

Considered in that context, a significant strength of the current code is the capacity it provides to conduct large numbers of performance assessment calculations in a timely way. The value of this attribute is expressed in the ability to evaluate the many possible scenarios which need to be considered over the prescribed TPIs.

A further strength is the rigor which has been developed in the procedure of sensitivity analysis. Development of an engineering procedure such as this is seen as a notable achievement and deserves to be published widely in the refereed literature.

The code user's documentation is seen as a strength of the TPA code. It provides a clear description of the code architecture and the functions of the various routines which implement the abstractions of the suite of FEPs. The documentation is presented in a logical and consistent way for each module. The logical modular structure of the code and the clear relationship of the functionality to the FEPs are also seen as considerable strengths of the code. From TOP-018, it is assumed that code development is supported by a complete and archived file of documents which define in detail the code design, acceptance tests, analysis, assumptions, code review and alpha and beta testing. As described in the review, the code is developed in an environment of rigorous configuration management.

As implied above, the weakness of the code arises directly from the need to achieve acceptable execution times in performance assessment calculations. In creating a relatively simple model of repository performance, many interactions between individual FEPs have been ignored, either explicitly or implicitly. Some of these have been considered in this review in relation to thermomechanical effects and their impact on repository scale hydrology and fault slip, for example. However, it is possible to identify many other such interactions. While many of the possible interactions might not be important in the final analysis, it is important that there is an explicit evaluation of them individually. The documentation of the code would be improved considerably if the interaction or coupling between the FEPs was mapped as an influence diagram or a matrix, and the strength of each interaction was evaluated explicitly. Such an approach would permit an analyst to affirm the correctness or acknowledge the limitations of the TPA procedure. An independent reader would be made aware that, in formulating the TPA utility, the developers had deliberately ignored certain interactions, and that these had not been omitted by oversight.

In the course of the on-site review, the panel was advised that the TPA v3.2 code has been developed in a software process environment defined by CNWRA Technical Operating Procedure (TOP) 018. According to CNWRA management and in the assessment of this reviewer, this is probably equivalent to a level of maturity of the software process between Level 2 and Level 3, as these are defined by the CMU Software Engineering Institute. For the purpose for which the utility is intended, this is probably a sufficient level of maturity. For purposes of completeness of documentation of the code, this information should be included both internally in the code and in the User's Guide.

6. Completeness and flexibility

To some extent, the question of completeness of the TPA v3.2 code has been addressed in the preceding discussion. The code almost certainly simulates the complete suite of FEPs which are conceivable for the geological setting and the repository design. However, the simulation of the full suite of FEPs is not a sufficient condition for completeness, as demonstrated by the decision in model formulation to decouple some of the FEPs, with the objective of achieving execution speed targets for code application. In adopting this approach, it was recognized explicitly by the developers that the code would not capture the full range of FEP interactions which are involved in a complete simulation of repository behavior.

This reviewer proposes that the answer to whether the code is sufficiently complete cannot be answered from the studies reported to date, in either NUREG 1668 or the code documentation. Verification and validation studies are reported to have been conducted for the various modules of the code. However, qualification of the complete utility, to demonstrate its overall suitability for the purpose of TSPA, might be best accomplished by a study of a prototype repository or an analogue which incorporates the suite of FEPs to be considered in a repository and which are represented in the TPA code. A prototype repository could be represented in a yard test which was constructed purposely to represent the many elements of an actual repository. This would be a difficult and expensive exercise, and would still leave residual questions about the time and length scales in the test bed relative to those of a repository. A possible alternative approach might be to use the Pena Blanca uranium orebody as an analogue for a repository. It could be treated as a qualification test site rather than a source of radionuclide transport and retardation data, as has been done in the studies to date. With a suitable choice of parameters defining the geochronology and mineralogy of the orebody (or any associated structures) and its geological setting, it may be possible to conduct bounding calculations of radionuclide mineral distribution, for comparison with the observed field values. This exercise would undoubtedly require many approximations in deriving the analogue repository. However, the capacity to simulate computationally a rock mass response consistent with the observed field condition would provide a strong inference that the TPA simulator is sufficiently complete to be qualified for the purpose of repository performance assessment.

A qualification exercise on a natural analogue of a repository would probably involve time scales significantly longer than those considered to date. Whether consideration of such time scales is justified from the regulatory viewpoint depends on the details of the regulations themselves.

The issue of flexibility of application of the TPA v3.2 code arose in the review in the context of the change in the DOE reference design, from that considered in the VA document to the EDA II description. This reviewer was left with the impression that the design change was not accommodated readily by the current TPA code functionality. Whatever the case, flexibility in application is a feature that must be provided intrinsically in further development of the code. One reason for this is that one can readily conceive of design changes for the repository more radical than those experienced in the change from the VA reference design to the EDA II design. As an example of this, both repository designs considered to date are based on a horizontal planar layout of WP emplacement drifts. These result in literally all the WPs being subjected to passage of water from the percolation and reflux processes. It has been noted earlier that the rate of percolation is somewhat higher than expected and thermomechanical reduction of vertical permeability raises questions of the soundness of the shedding concept. One possible design response to reduce exposure of WPs to water contact is to change the layout of drifts from a drift-and-pillar, horizontal planar layout to a widely spaced array of horizontal drifts arranged in vertical planes or panels. In this configuration, probably only the top drift would experience significant water penetration, and lower drifts would be shielded from water influx to some extent. The right conditions of vertical permeability would be preserved in the large pillars between the vertical planes of the repository drifts for the shedding concept to operate satisfactorily.

In responding to or anticipating changes in DOE thinking on repository layout, further development work on the TPA code may be conducted which will improve the functionality supporting flexible application of the code. As suggested by the discussion above, one objective should be to ensure that a generic repository design, with a geometry not necessarily tied to a drift-and-pillar layout in a horizontal plane, can be simulated. In particular, a capacity to simulate multiple vertical panels, consisting of horizontal drifts arranged in vertical planes, would be valuable.

7. Conclusions

The preceding discussion is summarized in terms of the remit for the review as follows:

- *Examine the methods and assumptions embedded in the TPA v3.2 code;*
  The methods are accepted as generally sound. The consequences of specific assumptions (particularly in terms of de-coupling of processes) need to be tested.
- *Identify necessary code improvements;*

Several code improvements have been proposed, the main ones being a capacity to handle repository geometries different from the reference horizontal drift-and-pillar planar layout and improvement of the SEISMO module.

- *Evaluate implementation of conceptual models, including the approach for treating parameters;*
  The software implementation of the conceptual models was conducted in accordance with a prescribed software process. The method of treating system parameters is a notable achievement of the TPA development exercise.
- *Is the TPA code suitably flexible and sufficiently complete?*
  The code is probably sufficiently flexible provided the DOE repository design concept does not change significantly. The condition of completeness is limited by the assumption of de-coupling of many processes. The formulation is therefore incomplete, but it may well be sufficiently complete for the intended purpose. A suitable qualification exercise would provide a clearer fix on the sufficiency of the degree of completeness.
  - *Are the included features, events and processes sufficient to provide confidence in the Licensing Decision?*
  - The suite of features, events and processes included in the simulator provides confidence that the complete range of conceivable scenarios can be analyzed. The statistical treatment of parameters is accepted as a valid approach in the probabilistic analysis of performance. Taken together, these factors lend confidence to a Licensing Decision derived from application of the TPA code.
- *Are the conceptual model abstractions defensible*
  - *Are the conceptual model abstractions appropriate for the spatial and temporal scales being considered and for the selected performance measure?*
  - Some reservations have been noted in relation to the SEISMO module, but seismic rupture of WPs is not expected to represent a major source of radionuclide release.
  - *Are the model abstractions sufficiently supported by the site data or other related information to ensure the credibility of the results?*
  - For the modules reviewed here, the model abstractions are well supported by the site data to ensure credibility of the results.
  - *Is the documentation sufficient to provide an understanding of the approach?*
  - The logical and ordered documentation is one of the strengths of the code, and is sufficient to provide an understanding of the approach.
  - *Is the level of conservatism and simplicity of approach appropriate considering the role of the NRC?*
  - The approach adopted, in terms of simplification of models and conservatism in application, is accepted as consistent with the role of the NRC.
- *Are the methods used to develop abstracted models and their associated parameters reasonable?*
  - *Are the parameters used in the TPAv3.2 code appropriate to the abstractions?*
  - For the modules considered in detail, the methods of model abstraction and parameter definition are sound, provided account is taken of reservations about the mechanics embedded in the current SEISMO module.

- *Are uncertainties in model abstractions and parameter values reasonably accounted for by the alternative conceptual models and parameter distributions provided in the code?*
  The uncertainties in model abstractions are handled adequately and appropriately by the process of informed scientific and engineering judgement. The uncertainties in parameter values are handled well through the use of bounding values and the application of a well-conceived sampling procedure.

APPENDIX B

REPORT OF PAUL DELANEY

September 1999

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External Review Meeting:
U. S. Nuclear Regulatory Commission's
Total-system Performance Assessment
Version 3.2 Code

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Summary of Comments

The dispersal of radionuclides by igneous disruption has never been observed and so there is no possibility of testing with data models that are fully capable of being falsified. The physics of host-rock entrainment during magma ascent and of dispersal in ash clouds, moreover, remains rather poorly understood even in the absence of contaminant transport. Yet, the assumptions and handling of the entrainment processes used in the present TPA code seem entirely defensible. Although the basis for and the implementation of the empirical ash-dispersal model proposed by Suzuki (1983) was extremely well defended by CNWRA staff, it is imperative that the underlying physical processes be better understood through focused field and theoretical studies. Although better models may be obtained, at great cost to computer time, I expect the improvements would have a marginal effect, at best, on the total population of outcomes. More importantly, increased confidence in the parameterization will probably be crucial to the eventual acceptance of the results by both scientists and the general public.

My primary concern with the present TPA code is its failure to estimate dosages due to fluvial dispersal from the vicinity of a volcanic vent to the critical population.

Objectives

It is my purpose to discuss the physical basis for and implementation of the volcano-hazard components of the TPA version 3.2 code developed by the Center for Nuclear Waste Regulatory Analyses, Southwest Research Institute (CNWRA). In particular, I will focus my report on:

1. implementation and ease of use of volcano-related code modules
2. integration of volcanic processes with other dispersal processes
3. strengths and weaknesses of volcano-related theoretical models
4. potentially important volcano-related processes not yet treated.

Due to a scheduling conflict, I was unable to attend the sessions of the TPA Review group during 27-29 July 1999. Rather, I was briefed during 13-14 July on a range of subjects somewhat narrower, and probably, in instances, somewhat more abbreviated than was the case for the balance of our review group.

I should emphasize that even though this report maintains a rather narrow focus, I was free and even encouraged during my briefing to range widely into any topic and to offer comments in this report on any concerns I may have.

The Briefing

Prior to traveling to the CNWRA offices in San Antonio, I studied the *Module Descriptions and User's Guide* for the TPA version 3.2 code, paying particular attention to sections on seismic and volcanic hazards and hydrologic processes. I also examined *Results and Conclusions* for the TPA version 3.1 code.

I was briefed by G. Wittmeyer, T. McCartin, S. Mohanty, B. Hill, J. Firth, and R. Codell, supported by a number of their colleagues, on the scope, purpose, and perspective of the External Review, on igneous activity and airborne release and its subsequent dosage consequences, and on the incorporation of volcanic scenarios with others and the uncertainties and sensitivities of the many parameters involved in the code. Much effort was devoted by all in explaining the licensing procedure, particularly the concept of the *critical group* and the *compliance point.* I was, and remain, impressed by the excellence of the work that has gone into to the TPA code. I did not have the impression that the code is so much a black box as a tool requiring considerable use before it can be mastered.

I also came away from the briefing with the impression that any TPA code, even one with capabilities far stronger than version 3.2, would require a strong body of fundamental scientific research to justify the parameterizations.

Implementation & Ease of Use of Volcano-related Code Modules

CNWRA staff have been instrumental during recent years in development of probabilistic methodologies as the apply to volcanic hazards. Spatially and temporally, these methods nicely handle the possibilities for entrainment of radionuclides from the repository during eruption and for their subsequent transport in an ash cloud. The model, implemented in the ASHPLUMO module, contains few parameters not used by other volcano researchers and would generally be understandable and usable to most all of them.

Integration of Volcanic Processes with Other Dispersal Processes

Volcanic eruption through the repository, if it were to occur, would have an effect that would overpower other dispersal processes. It would distribute the radionuclides directly to the earth's surface where they would be subject to further transport and more readily able to supply a significant dose to nearby populations. The TPA version 3.2 code seems to handle this quite well, particularly through the ASHMOVO module.

I should note that the possibility of a combined seismic and volcanic event may be judged rather high as one might be thought capable of triggering the other. I see this as very unlikely, especially in view of the great depth from which magma must ascend before it is capable of eruption.

Strengths & Weaknesses of Volcano-related Theoretical Models

The probability of direct volcanic disruption now appears to be about as well determined as can be expected. (Congratulations to Connor and Hill.) I doubt that continued development of probabilistic models will be so beneficial as focused study of geologic analogs of the expected Yucca Mountain magmatic system.

While the particle distribution of the fragments carrying the radionuclides from the repository to the atmosphere seems empirical, the basis is probably acceptable to all but the harshest critics. Most would accept that it will be very difficult indeed to estimate from physical principles how much material will remain underground, even if their cannisters are destroyed.

The Suzuki (1983) model for ash dispersal is largely empirical, which explains in part why it can be implemented in such a simple and straightforward fashion in the ASHPLUMO module. While this model can be defended by its numerous successful applications at volcanoes worldwide, the underpinning of the dosage calculation is nonetheless weakened by its empirical nature. I suggest that a research program to develop more sophisticated models be undertaken to document more fully the viability of Suzuki's model.

Data on wind direction and speed, along with atmospheric structure to the expected heights of the ash clouds would provide considerable comfort to the eventual users of the TPA version 3.2 code. If such data were available, it may be found worthwhile to properly integrate the ash-fragment paths temporally and spatially through changing wind conditions.

Potentially Important Volcano-related Processes Not Yet Treated

Deposition of ash near a critical group in the Amargosa Valley is unlikely to exceed greatly exceed several millimeters under most volcanic-eruption scenarios, causing doses often not exceeding 10^0 mrem/yr. Yet, the ash thickens toward the volcanic vent where doses may well be quite toxic. A relatively small area of several square kilometers near the vent may have deposits with average thicknesses of several meters. The fine-grained components of these deposits would, inevitably, be washed during rainstorms into the drainages, where debris flows and flash floods would carry it to the Amargosa Valley.

I believe, therefore, that some assessment needs to be undertaken of doses caused by fluvial transport to the critical group of radioactive volcanic debris.

APPENDIX C

REPORT OF GHISLAIN DE MARSILY

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August 99

Review of Total System Performance Assessment (TPA) Version 3.2 Code (Predecisional) Module Description and User's Guide Sensitivity and Uncertainty Analysis

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Introduction and objective

This review was made for the Nuclear Regulatory Commission (NRC) at the request of the Center for Nuclear Waste Regulatory Analyses, Southwest Research Institute (CNWRA) in July and August 1999. The terms of reference of the review, as described in the CNWRA memo of June, 4, 1999, "External Review Plan for the TPA Version 3.2 Code", can be summarized as follows :

- examine the methods and assumptions embedded in the TPA Version 3.2 code;
- recommend improvements;
- evaluate implementation of conceptual models including the approach for treating parameters;
- determine whether the NRC approach to TPA is suitable for achieving its objectives of reviewing the DOE license application and TSPA.

This review will mostly focus on the **hydrology** portion of the TPA, which is my field of interest, but will also comment on the general approach of the TPA, and on some specific points.

The review process included four successive steps :

(i) Initial review of two CNWRA documents, which were distributed in advance to the review committee :
   (1) Total System Performance Assessment (TPA) Version 3.2 Code, Module Description and User's Guide, prepared for NRC by CNWRA, September 1998
   (2) NRC Sensitivity and Uncertainty Analyses for a proposed HLW Repository at Yucca Mountain, Nevada Using TPA 3.1. Volume II : Results and Conclusions. NUREG-1668, October 1998

(2) External Peer Review meeting at CNWRA in San Antonio, Texas, July 27-29, 1999, where the CNWRA and NRC staff presented orally the content of these two documents, and of some supporting documents, and answered the question of the Peer Review group. In attendance in that group were Drs. Barry Brady, Robert Kelly, Gérald Ouzounian, Brian Thompson, Fritz van Dorp, F. Ward Whicker. Dr. Paul Delaney, member of the group, could not attend.

(3) Further analysis of additional supporting documents which were distributed at the meeting, at the request of each reviewer. The documents which I asked to review are :

1. Stothoff, S.A., Castellaw, H.M., Bagtzoglou, A.C. (1997) Simulating the spatial distribution of infiltration at Yucca Mountain, Nevada. Submitted to WRR.
2. NRC (1997). Issue resolutions status report on methods to evaluate climate change and associated effects at Yucca Mountain (KTI : Unsaturated and saturated flow under isothermal conditions). Staff of the Division of Waste Management, Office of Nuclear Material, Safety and Safeguards, US NRC, June 1997.

3. Fedors, R.W. and Wittmeyer, G.W. (1998) Initial assessment of dilution effects induced by water well pumping in the Armagosa Farms area. Center for Nuclear Waste Regulatory Analyses, Revised, July 1998
4. Basse, B. (1990) Water Resources in Southern Nevada. Center for Nuclear Waste Regulatory Analysis Task Activity 3702-002-305-604, Final Technical Report, August 3, 1990
5. Flint, A.L., Hevesi, J.A., Flint, L.E. (1996) Conceptual and numerical model of infiltration for the Yucca Mountain area, Nevada. US Geological Survey, Water-Resources Investigations Report, Draft ???, September 20, 1996, 174 p. + Figures
6. Luckey, R.R, Tucci, P. et al (1996) Status of understanding of the saturated-zone ground-water flow system at Yucca Mountain, Nevada, as of 1995. US Geological Survey ,Water-Resources Investigations Report 96-4077.
7. D'Agnese, F.A., C.C. Faunt, A.K.Turner, M.C. Hill (1997) Hydrogeologic Evaluation and Numerical Simulation of the Death Valley regional Ground-Water Flow System, Nevada and California, USGS Water Resources Investigation Report 96-4300, Denver, Colorado, 124 p.
8. Baca, R.G., Wittmeyer, G.W., Rice, R.W. (1996) Analysis of contaminant dilution in groundwater. Draft report, SRI, San Antonio, 28 p.
9. Murphy, W.M. (1998) Commentary on studies of ^{36}Cl in the exploratory studies facility at Yucca Mountain, Nevada. MRS Symp. Proc., 506, 407-414.
10. Murphy, W.M., Pabalan, R.T. (1994) Geochemical investigations related to the Yucca Mountain environment and potential nuclear waste repository. Southwest Research Institute, CNWRA, Report NUREG/CR-6288.
11. LaPlante, P.A., Poor, K. (1997) Information and analyses to support selection of critical groups and reference biospheres for Yucca Mountain exposure scenario. Southwest Research Institute, CNWRA, Report 97-009.
12. CNWRA (1998) Technical Operating Procedure. Development and control of scientific and engineering software.

(4) Independent writing by each reviewer of his comments based on the above information.

General Summary Comments

This reviewer is quite impressed by the excellent level of the work in the two TPA code documents that were distributed for review, as well as in all the additional supporting documents that have been prepared by CNWRA. I consider indeed that the models that have been developed for the TPA code, and the general structure of the code, are of very high quality and have sufficient flexibility to account for most, if not all, of the features, events and processes likely to occur at Yucca Mountain. This clearly demonstrates the very high level of expertise and scientific understanding of the team that developed the TPA code.

Furthermore, the quality of the reporting is also in general excellent, complete and precise, and this makes it possible for the reader to understand how the final outcome of the TPA (the expected dose to man) is related to the ensemble of processes going on in the repository and in the environment. In other words, the reader does not get the impression that the code is a "black box" in which the on-going processes are poorly explained.

I have, however, some fundamental criticisms, that I list here in decreasing order of importance, and which I will further develop below.

1. I have very strong reservations on the present level of understanding of the hydrogeology of the saturated zone at Yucca Mountain (YM). These reservations are based on the analysis of the two USGS reports R95-4077 and R96-4300 (items 6 and 7 of the list of reviewed documents above), on the second of which I also have severe reservations. I consider that the Conceptual Model of the saturated zone hydrology at YM is at present so uncertain, with so many alternatives and unknown transport properties, that it is not at this stage possible to derive a representative model to be included in the TPA code, even with a range of uncertainties for its parameters. The Conceptual Models of transport in the saturated zone that have been developed in the TPA code are of good scientific level, and may eventually be proved to be correct, but they are based at present on a series of unproved assumptions, not supported by the available data, and therefore underestimating the uncertainty. The only viable alternative at this stage and with the present level of data

seems to me to be the use of a much more conservative saturated zone model, which I will describe; I consider the present models not defensible today.

2. I have minor comments on the assumptions made for the transport in the unsaturated zone, that can be easily accounted for by changing some parameters in the TPA code. It concerns the distinction between matrix transport and fracture transport. The net effect of these suggestions should not have a major impact on the over-all results.
3. I also have minor comments on the estimate of the infiltration flux above the repository, which could be taken care of by some parameter changes.
4. One of the most conceptually complex models is for me the one that determines the percolation flux that reaches the canisters, as a function of time, also accounting for the effect of the thermal phase. Although I do not have significant disagreements on this model, I find it very difficult to justify the assumptions made and the values of the parameter used. What I mean is that the model is probably quite reasonable, but that it will be very difficult to defend it if NRC is asked to justify these choices. I did not find any source of external information to support them.
5. The TPA code does not address a number of potential couplings of the various processes active in the repository. For instance, the coupling between the thermal loading, the mechanical behaviour, and finally the hydrology of the infiltration (role e.g. of potential additional fracturing) is not addressed. The rationale for not considering these couplings is not given. One coupling mechanism will be suggested (the "cold wall" effect) that could significantly change the flux of liquid water reaching some canisters, and therefore their corrosion rate.
6. In a similar way, the TPA code is based on an earlier selection of a list of Features, Events and Processes (FEPs) that are included in the approach. It is however not clear which FEPs were excluded, and based on what reasons. The IAEA has developed, for instance, a standard list of FEPs, which can be used as a starting point, each irrelevant FEPs being screened out, and those considered negligible being shown to be so in a documented and defensible way. The previous comment on the lack of coupling may be part of this screening process, which was not available to the review team. More generally, I did not find in the documents a clear picture of which "internal FEPs" are included in what is generally called "the Process System" (the ensemble of FEPs which are simultaneously accounted for in the modelling of the behaviour of the system), and those "external FEPs" which may or may not act on the system, depending on the scenario. As an example, the change of climate is sometimes considered as an "internal FEP", and is modeled in the Process System in two areas, the change in the infiltration rate, and the living habits of the recipient critical group, but is not considered as a change of the temperature of the system, nor as a change of the elevation of the water table. A more rigorous classification of the FEPs, of their roles and of the consistency of their introduction in the Process System or the Scenarios would be desirable.
7. The TPA code is clearly a very complex code and engineering achievement. In order to build confidence in its results, a very important issue is the level of QA that was used during its development, and the level of validation that was achieved (e.g. by comparison with other codes) either for each individual module, or for the entire code. This issue was not adequately covered by the documents made available to the review team, and may have to be made more visible.
8. Some very minor comments are listed at the end.

These different points will now be developed in more detail, in the same order. In particular, the four issues assigned to the reporting of this review will be addressed :

- description of areas of the TPA Version 3.2 code reviewed;
- weaknesses of the TPA Version 3.2 code in these areas;
- strength of the TPA Version 3.2 code in these areas;
- recommendations for improving subsequent versions of the TPA code in these areas.

1. Comments on the hydrology of the saturated zone

These comments are relevant for the transport of radionuclides in the saturated zone (SZFT) and the annual dose calculations (DCAGW).

My major concern is not that the codes are inadequate, but that the database on which they are built is inadequate to make a credible defense of the assumptions made for developing the corresponding modules of the TPA code. In Appendix 1, I have provided detailed comments on the two USGS reports that were presented to me as the most recent basis on which the hydrogeology of the YM site could be based. These are R96-4300 by d'Agnese et al. and

R6-4077 by Luckey et al. The first one describes the regional hydrogeology in the YM area, and the second the local hydrogeology. I have several reservations about the analysis presented in the first report, which I found inadequate to answer the relevant questions on the groundwater flow in the regional area. The second report presents a better perspective, but is still preliminary and does not include the development of a local model of the groundwater flow in the local area, on which a TPA module could be based.

My conclusion after reading these two documents is that the flow system at YM in the saturated zone is really very complex, and not sufficiently understood to propose a conceptual model on which scenarios of transport of radionuclides released by the repository can be made with any degree of realism. The major issues seem to me to be:

(1) the role of the paleozoic carbonate (is water coming from or going to the carbonate, or both, as suggested in the R96-4077 report to explain the zones of high and low gradients);
(2) the horizontal anisotropy of the fractured volcanics, to determine the direction of flow, the velocity in the fractures;
(3) the connectivity of the fracture network, to determine how much mixing could occur in the system;
(4) the relation between the volcanics and the alluvium : How layered are the alluvial deposits ? Is there vertical mixing in the alluvium ? At the contact between the volcanic tuffs and the alluvium, how is the flow distributed ? Along the whole thickness of the alluvium ? Over a fraction only ? Mostly at the surface ? At depth ?
(5) What is the exact geometry of the alluvium in the area lying between YM and the Amargosa Farms area ? Where are community wells likely to be drilled, in other words, are there reasons to dismiss the 5 km well scenario and only keep the 20 km well scenario ?

In the presence of these unanswered question, the assumptions made in the TPA are that the local flow system is isotropic, therefore flow lines can be drawn orthogonally to the head contour lines; that flow tubes can therefore be drawn to describe the flow path from beneath the repository down to the Amargosa Farms region; that an assumption of continuous equivalent porous medium can be made both for the fractured volcanics and for the alluvium; that the dilution in the wells drilled downstream from the repository (at 20 km or perhaps 5 km) can be calculated for a homogeneous medium, using concepts of hydrodynamic dispersion and vertical anisotropy.

Within the framework of these assumptions, the TPA code development and the supporting CNWRA documents that I reviewed (items 3 and 8 in the list of documents listed above, Fedors & Wittmeyer, 1998 and Baca et al, 1996) are excellent and provide very reasonable models and parameters to perform the TPA calculations.

However, I do not believe that the above assumptions are supported by the available documents. First, the volcanics are almost certainly anisotropic; Luckey et al (1996, R96-4077) mention only one attempt at estimating the horizontal anisotropy, giving a value of 5 to 7. It is therefore not defensible to assume isotropy and determine in that way the flow lines and flow tubes. Second, it is necessary to determine if transport can occur through the fissured (?) carbonates, and in what direction, before the potential recipient zone can be outlined. Third, the fraction of the pathway, which is situated in the volcanics, cannot be treated as a continuous equivalent porous medium, particularly if abstraction wells may be drilled directly in the volcanics. But to determine if wells are likely to be drilled in the volcanics downstream of the repository, it is necessary to first know the real direction of flow, anisotropy and role of carbonates being taken into account. Fourth, the potential layering in the alluvium must be

determined, its exact geometry, and the manner in which the flux leaving the volcanics is distributed over the vertical when it enters the alluvium must be known before defensible dilution calculations can be made.

I fully realize that answering these questions requires a large amount of fieldwork, which is not the responsibility of NRC to perform. But if such work is not done, I seriously question the feasibility of analyzing in a defensible way the DOE licensing application when it is submitted, if any credit is to be given to the saturated zone transport.

One very minor comment on the suite of codes used in the saturated zone in the TPA is about NEFTRAN. The NEFTRAN code allows for including matrix diffusion, with a linear exchange coefficient. It is not clear to me if this option is used in TPA. It is a rather crude approach; the usual approach in fractured media is to solve a 1-D diffusion equation in the direction orthogonal to the fracture. But more importantly, one limits in general the thickness over which matrix diffusion can occur, either as the half distance between two fractures, or by an *a priori* defined length, assuming the porosity to be "closed" at larger distances. Such a limitation of matrix diffusion should be included in the TPA, if the matrix diffusion option is used.

Coming back to the main issue of conceptual model uncertainty, the only recommendation that I can make, apart form expanding the data base on which the TPA is based, is to replace the present modules of the TPA Version 3.2 code representing transport in the saturated zone and well dilution by an extremely conservative estimate, and the only one I can suggest is to assume that the entire flux of water and of radionuclides which seeps into each one of the infiltration sub-areas of the repository can be transported with no or little retardation into one single community well, without any additional dilution. In this flux of water, for each sub-area, the flux of radionuclides is determined by the relevant part of the TPA code, as a function of the number of breached canisters. The rationale for this conservative model is that in a fractured system, a few fractures can convey to a given well the flux from a given area of the repository. Selecting the entire repository area seems to me non-conservative, since if only a few canisters leak, then the flux of the entire repository would act as a diluting flux, for those leaking canisters, which may not be defensible given the size of the repository. At the other extreme, the flux from one single canister is definitely too small to support a community well. But the flux form one infiltration sub-area is on the order of $5.x10^3$ m^3/y during a humid period, which is not unreasonable for a small community drinking water well. This scenario is really the only one at this stage that is fully defensible. Any additional dilution should be based on a real understanding of the saturated zone hydrogeology.

2. Comments on the hydrology of the unsaturated zone

These comments are relevant for the transport of radionuclides in the unsaturated zone (UZFT).

In general, the approach used seems adequate, and its results seem consistent with the observed Cl-36 data. It is also noted that the continuing investigations on the Cl-36 data may induce a revision of the model. One question however is related to the passage from matrix flow to fracture flow as a function of the hydraulic conductivity of the strata compared to the flux. Let us assume that fracture flow occurs in a given low-permeability unit. When this water reaches the next unit with e.g. a higher hydraulic conductivity unit, the model would predict matrix flow. But this can be debated. If the fracture continues in the lower section (which is a very likely assumption, I believe), one could imagine that the water would continue to flow in the fracture. The mechanism, which would prevent this and restore matrix flow, is the "suction" of water by the negative pressure in the matrix adjacent to that fracture. But it has been assumed that there is very little exchange of water between the fracture and the matrix (matrix diffusion is neglected, as supported by the difference in water chemistry between the fracture and the matrix). If this were true, would this "clogging" of the fracture walls also prevent the "suction" of the water into the matrix ? In that case, once fracture flow has started at a given stratum, all fractures below it could also have fracture flow. It seems to me that the geochemical data, as discussed by W. Murphy in items 9 and 10 above may provide the evidence of such behaviour. Changing the TPA code to account for this mechanism is trivial.

Another issue is the neglecting of the influence of the thermal phase on the UZFT. This is justified by the fact that few if any canisters will have failed during the thermal phase. I believe that this is not consistent with the assumption (page 4-40 of the user's guide) of the existence of a type 1 failure of the canisters at time t=0, representing initial manufacturing defects. This is related to comment 5 on coupling.

3. Comments on the Infiltration in the unsaturated zone above the repository (UZFLOW)

The study of the present infiltration into YM and its possible variations with the climate are very interesting contributions. I believe the infiltration rate both for the present and the humid conditions are reasonable. The on-going field studies at YM may also help confirm the present-day rates. For the future rates, my comments are as follows :

The Climate Cycle (Page 4.11) that is assumed seems rather simplistic to me. Although I am not an expert on climate change, I know that the Milankovitch theory assumes that three orbital parameters with different periodic variations influence the climate on earth : about 21, 41 and 100 k years. Obviously, the assumed temperature changes are only based on the longest period, and not the two shorter ones. In Sweden, where glaciations are a very important issue for a waste repository, a number of climate predictions have been made, and, roughly speaking, predict a gradually colder cold climate from now to 10,000 years, with a brief recovery but then reaching a first cold peak around 20,000 y, then warming, then cooling again, etc., with two minima around 60,000 and 100,000 (the coolest period), and warming again with a new climatic optimum in 120,000 y, see e.g. McEwen and Marsily (1991), Boulton and Payne (1993), King-Clayton et al (1995, 1997), SKI-Site 94 (1996). It may not change the order of magnitude of the increase in infiltration, but its timing. I have also read the "issue resolution status report" on methods to evaluate climate change and associated effects at YM (KTI : Unsaturated and saturated flow under isothermal conditions, NRC, June 1997, item 2 in the list of reviewed documents). I see that the two shorter periods of 21 ky and 41 ky, representing tilt and precession, are considered unrelated to climate change, but I may just mention that this is not accepted in Europe. I also know that the Milankovitch theory is occasionally challenged. The action to correct this point would be a reassessment of the climate change theories by an appropriate expert.

A second issue is the calculations performed by Stothoff et al (1997, item 1 of the list) to estimate the infiltration as a function of the properties of the soil cover, which are really interesting. The order of magnitude that they reach for a more humid climate seems reasonable, however there are a number of assumptions that may be questioned and which could lead to other values, if they were changed. Among them :

-In case of climate change, the AAP may increase, but also the distribution of this rain during the year, or the variability form year to year. The authors assumed the same pattern as today, and only increased the rain depth. This may not be conservative : a different pattern could produce higher AAI, either if it is more concentrated in time, or occurring at a different season.

-Runoff is not considered anymore when it occurs. This is also not conservative. Runoff in one area can infiltrate into another area downstream. I know that this is very difficult to predict and estimate, but it occurs in nature. The runoff ratio to the rain depth is known to decrease with the size of the surveyed area, because of that. This can also result in localized much higher infiltration rates, in areas where this runoff water re-infiltrates (e.g. in local ponds, or locally more permeable areas, or in outcropping fractures...).

-Vegetation is neglected, and it is assumed that this is conservative. It may well be. But vegetation may also increase the permeability of the soil cover. So may biota : one of my students is studying in a semi-desert area in Burkina-Faso, Africa, the role of termites on the infiltration rate. He was able to show that the presence of termites can increase by a factor of 10 the infiltration, and he is presently testing a rehabilitation program for degraded soils where termites are brought in just by spreading straw on the surface of the soil !

I would therefore recommend that spatially variable infiltration rates with possibly higher values should be considered by incorporating these neglected phenomena in the infiltration model.

A third issue relates to the question of coupling. Nowhere did I see that natural fault movements could result in an infiltration increase, by opening new fractures or widening the existing ones. Similarly, the thermal loading of the repository will induce dilation of the rock. I have calculated long ago that for a 500 m deep repository, the ground surface may move upwards on the order of 1 m or more. But this is for a smaller thermal loading than at YM. This number should be calculated, and mechanical calculations made to estimate if these movements are likely to create new fractures in the rock. Their potential impact on the infiltration rate should then be assessed.

4. Comments on the failure of the engineered barrier system (NFENV, EBSFAIL and EBSREL)

This part of the TPA code assembles calculations that can be done with very little uncertainty (e.g. the thermal response) and others that are highly uncertain.

Concerning the thermal calculations, I found that there are a few simplifications that would not be difficult to remove, by using a 3-D heat flow model with all the required complexities in order to correctly represent the exact geometry of the system, including gaps, convective transport in the drift, etc. Since these thermal calculations are deterministic (there is little uncertainty on parameters such as thermal conductivity, etc.), the calculations could be made once and for all. In other words there is no real justification for simplifying the calculations in order to speed up the stochastic analysis. The only valid reason to simplify them is in view of the uncertainties on the other parts of the system, but then it would be necessary to evaluate the error made in the simplified models, by comparing them with the 3-D ones. My suggestion is therefore either to derive conservative estimates with the simplified models, or to develop the more complex 3-D ones, as is also suggested on page 4.37 of the user's guide. Here are a few examples.

Equation 4.13 in 1-D assumes a uniform distribution in space of the heat flux. Since the heat flux is localized in the canisters with a prescribed spacing, the temperature estimated by 4.13 is probably correct at some distance from the source (on the order of a few times the distance between canisters), but is an underestimation close to the canisters. When this temperature, called T_{rock}, is used as the reference against which the increase in temperature at the WP is calculated (equation 4-16), this WP temperature will be underestimated (see also comments in section 5 below, on coupling).

Page 4-22, I do not understand why the effective axial length for convective and conductive transfer from the WP to the drift should be larger than the actual length of the WP, and why two times the length was selected. This is again an unbounded approximation, the effect of which is unclear.

For the calculation of the percolation flux, the physics of the processes as long as the boiling isotherm is above the repository level is indeed complicated, and the results of the on-going heater test may be very important to improve this model. The existence of three different Reflux models makes it difficult to determine which is the best option. I have some difficulties figuring out how much water can be stored above the boiling isotherm, and what happens when this storage capacity is reached. Rapid flow in fractures, perhaps avoiding the vaults, seems a possibility. The proposed models to estimate how much water comes into contact with a canister seem to make a significant number of assumptions that are hard to justify. I understand that the model is very flexible, and that the values of the parameters, which determine this amount of water, can easily be changed. But I do not see on what kind of experiments these parameter values can be realistically based. See also one additional mechanism for bringing water to some canisters, in the following section (5) on coupling.

On the corrosion model, I am not competent. One mechanism which I did not see mentioned is the potential effect of a rock debris or dust on the surface of the canister, or even rock blocks if the drifts are, at least in some areas, partly backfilled with fallen rocks from the roof. The question is then : would the presence of the piece of rock, on which water would drop, have an influence on the corrosion rate of the metal beneath it ? Another question concerns the parameters of the corrosion models, I wonder how well founded are their assigned range of uncertainty, given that the corrosion experiments on the various metals composing the WP have probably lasted for a few years, and need to be extrapolated for several orders of magnitude longer durations.

Concerning the waste release model, my only concern is whether the amount of early release of radionuclide from those fission products that accumulate at the fuel grain boundaries is well accounted for. I have seen percentages much greater than those used in the present TPA code. The basis for the selection of this parameter should be explained.

5. Comments on the couplings

Very few coupling mechanisms have been included in the TPA Version 3.2 codes. This may be correct, but needs to be justified by additional calculations or explanations giving the reasons why these couplings can be neglected. Among them are :

-Couplings between the thermal loading of the medium and resulting effects. Apart from the existence of a vapor zone above the drifts, and the effect on the chemistry, which are taken into account in the TPA, other mechanism could be envisaged. One is the mechanical effect, and the potential consequence on rock blocks fall, fracture aperture opening and closing, fracture displacement, etc., and the resulting effect on focusing/diverting the infiltration flux on/away from the canisters. The thermal experiment presently going on at YM may be important to assess such potential effects.

-One mechanism which may need examination is the following : sometimes after the peak of the thermal phase, the temperature on the canister surfaces will fall below 100°C. The liquid water which will seep in the repository is most likely to be in a quantity sufficient to maintain the humidity in the air of the drifts at saturation at the average temperature of the rooms. There will be natural convection of the air inside the drift to mix and homogenize the air in the drift and its humidity. So far, nothing new. But let us assume that there are some differences of the temperature distribution on the canister surfaces. This could be due to unequal burn-up of the fuels in the different canisters, in fact such differences, not necessarily very large, are bound to occur. It is then clear that there may be a "cold wall" effect within the repository, in competition with the effect of the walls of the drift : those canisters above the average drift temperature will be dry, and those below it may serve as condensation surfaces, and may thus be dripping with water. This may need to be taken into consideration in the calculation of the flux of water on the canisters, and their corrosion rate. To assess this mechanism, a better 3-D thermal model will be needed, where unequal thermal loading of canisters could be simulated, to see if a "cold wall" canister can exist or if the walls of the drifts are always cooler.

-The coupling between the change in climate and the saturated flow is ignored. This may be irrelevant, given my earlier comments on the lack of sufficient understanding of the hydrogeology of the site. But if eventually this hydrogeology becomes better understood it seems necessary to me that the TPA code should couple the variation of the infiltration rate with the changes in elevation of the water table and of the groundwater velocity. When I read that the water-table elevation could rise as much as 100 m in a humid climate (NRC, 1997, item 2 on the list of reviewed documents), I have doubts about the velocity not varying. Basically, when the recharge is increased during a climate change, the increased amount of water flowing into the aquifer can be taken care of by increasing the saturated thickness, as well as the hydraulic gradient, i.e. the velocity. In general, both mechanisms occur. Not to account for this likely increased gradient is not conservative.

-Another coupling is the effect of new fault movements. This is a scenario which generates mechanical breaching of some canisters, but the additional effects on the infiltration rate are not considered. It is indeed likely that the new fractures may induce increased infiltration on top of the breached canisters. Or if this is not so, it should be justified.

-Similarly, the effect of a volcanic eruption on those canisters that are not included in the explosion is not considered. Incidentally, I wonder if the open drifts will not be used as conduits for gases and/or magma, since they are not backfilled. Even if the number of canisters involved in the explosion is not affected, the behaviour of the repository regarding the groundwater pathway may be quite altered, this needs to be, at least, estimated.

More generally, to evaluate the potential role of coupling in a performance assessment, one useful tool is to build an "influence diagram", in which all the FEPs taken into account both as internal or external are linked to all the relevant processes on which they may have an effect. An additional document then describes, for each link, the reason why this link is not considered important in the TPA, or, on the contrary, how it is incorporated in the Process System. Such an analysis would be of interest to support the decisions made in neglecting a number of potential couplings in the TPA Version 3.2 code.

6. Comments on FEPs screening

Most of this comment has already been made in the summary. It is very clear that to develop the TPA Version 3.2 code, the phase of FEPs screening and scenario development, of definition of the internal and external FEPs, of the Process system, and of the Influence Diagrams, has necessarily been made. However, in the documents that have been made available to the review team, this step is not described nor is it justified. It therefore leads to some questioning about the potential role of FEPs, which are not analysed. The section 5 on coupling is an example of these concerns.

One brief comment is that human intrusion scenarios in the repository, and criticality issues are not addressed.

7. Comments on Quality Assurance and Validation

The documents available for analysis to the review group did not include any information on the Quality Assurance (QA) program under which the code was developed, nor on the verifications and validations attempts that have been made. During the July 27-29 meeting, some information was given to the review group, and a QA Procedure Memo (item 12 in the list of reviewed documents) was made available. It appears that the level of QA in code development used for TPA Version 3.2 was around 2, in an engineering QA scale of 1 to 5. It is to be noted that DOE prescribes a higher level of QA to its contractors in the preparation of the Viability Assessment and Licensing Application, or for the WIPP Compliance Application. The question then arises on whether the NRC should use a different level of QA than DOE. This is not a question for me to answer.

Concerning code verification and validation, it appears that a number of test cases and comparisons for each of the modules of the TPA Version 3.2 code have been made during the coarse of the code development. These verifications should perhaps be better documented to provide evidence of the confidence that can be placed on the TPA code.

When it now comes to the validation of the Total System approach, i.e. the linkage of the different modules, and the driver for the sampling of the stochastic parameters, it is clear that it becomes a very difficult task to validate such a global code. The present level of verification has been to check the plausibility of the outcome of the simulations, and also of the sensitivity results. While this is a valid and necessary step, I suggest making an additional attempt at verifying the TPA Version 3.2 code by comparing its results with those of the DOE TSPA code. It is my understanding that the DOE TSPA code has been (or will be) made available to NRC. I recommend therefore that a test case be developed, where the two codes should be given parameters and assumptions as close as possible to each other, so that the outcome of the two Total System Performance Assessments would be expected to be quite similar (it may never be possible to make the two cases identical, since the processes represented in each code are different, together with the modules used to treat them). Nevertheless, if the codes are asked to simulate very similar systems, it may be possible to either obtain very similar results, or to be able to explain why the answers of the two codes are different. If not, then this may raise questions on the existence of errors in one or the other of the two codes, and help identify these errors.

8. Minor remarks

-On page 2-1 of the TPA Version 3.2 user's guide, it is said that "detailed simulation models that include all the couplings, heterogeneities, and complexities **cannot be incorporated into PA models** and still maintain reasonable computer execution times and meet hardware requirements". This decision must be re-evaluated periodically, as a function of the evolution of hardware and also numerical resolution techniques. The present trend in PA in Europe seems to be to use more and more sophisticated models in PA. The comment made in section 4 about the potential use of a 3-D thermal model goes in this direction.

-For doses calculations, I wonder is a drinking water consumption of 2 L/day is reasonable for an arid climate. One suggestion for a particular pathway that may need to be considered is the use of contaminated water in a swamp cooler.

-I have some comments on the dilution factor, but these are overwhelmed by earlier comments on the hydrogeology of YM, which prevents, in my view, to start studying well dilution, until a better understanding of the hydrogeology is available. These comments are given in Appendix 2.

-For the sensitivity analysis, the results are very interesting and informative. I have only one suggestion for another method to perform the Sensitivity Analysis for one parameter at a time : a deterministic approach in one point of the parameter space was used, and different values of the parameter of interest were tested, all other parameters being fixed. Another method is to fix one parameter, and to perform a full stochastic analysis, all other parameters being sampled in their distribution function. The analysis is then repeated with a different value of the same fixed parameter. The two distributions of the outcome (e.g. the CCDFs) are then compared. This has the advantage of not using a single point in the parameter space, but is of course more demanding in terms of computer time. This approach was proposed by Lions in Canada using SYVAC, and applied at WIPP.

-I was also surprised to see Np and Am as the major dose contributors. In most PA results that I have seen for spent fuels, I and Tc are in general the major contributors, sometimes with Cs-135. I would like to understand what is particular about YM for the actinides to be more important than I and Tc. I understand however that the on-going sensitivity study using the 3.2 version of the TPA code, with different sorption constants, provides different results.

References used :

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McEwen, T, G. de Marsily (1991) The potential significance of permafrost to the behaviour of a deep radioactive waste repository. SKI 91 :8, 1991

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SKI-Site 94. Deep Repository Performance Assessment Project. Volume 1 and 2. SKI, Stockholm; Reports 96:36, 1996.

Appendix 1

Comments on the Hydrogeology of the Yucca Mountain Area

This appendix is a critical comment on the present level of understanding of the hydrogeology at YM, based on the reading of the following documents, which I understand form the basis of the information available today on the hydrogeology of the site, used in the TPA 3.2 code :

1. *Hydrogeologic Evaluation and Numerical Simulation of the Death Valley regional Ground-Water Flow System, Nevada and California, by F.A. D'Agnese, C.C. Faunt, A.K.Turner, M.C. Hill, USGS Water Resources Investigation Report R96-4300, Denver, Colorado 1997, 124 p.*
2. *Status of Understanding of the saturated-Zone ground-water flow system at Yucca Mountain, Nevada, as of 1995, by R.R. Luckey, P.Tucci, C.C. Faunt, E.M.Ervin, W.C. Steinkampf, F.A. D'Agnese, G.L. Patterson. USGS Water Resources Investigation Report R96-4077, Denver, Colorado 1996, 71 p.*

In the framework of a potential Licensing Application of the YM site for high-level nuclear waste disposal, I find in general that the level of understanding of the hydrogeology of the site, if based on these documents, is extremely low, unclear, and vastly insufficient to support a Performance Assessment, if <u>any</u> credit is to be assigned to the saturated groundwater pathway in the TPA. It seems to me that in all cases, there will be at YM a potential pathway to man through the saturated zone, even with very long-lasting canisters, because of the unavoidable percentage of initially defective canisters, the scenario of fault displacement breaking canisters, or early breakthroughs of canisters because of unexpectedly rapid corrosion. Furthermore, if the Licensing Authority extends the TPA beyond the expected lifetime of the canister, then transport of radionuclides to the accessible environment through the groundwater system is certain to occur.

A better understanding of the flow through the saturated zone is necessary for three reasons :

-locating the zones where the radionuclide plume will be accessible to man, and designing a scenario for groundwater abstraction consistent with this location, both in present-day conditions, and in a more humid climate;

-estimating the groundwater travel time, and the nuclide travel time, taking into account potential retardation mechanisms;

-estimating the potential dilution which could occur between the repository and the selected abstraction zone.

From the documents that I have read, and above all the USGS reports R96-4300 and R96-4077, it seems to me that none of the above three objectives can be met today, with any degree of confidence. It is a question of Conceptual Model Uncertainty, not yet of parameter uncertainty. Therefore, the essence of the TPA, which is to assume that a lack of exact knowledge can be compensated for by assigning a range of parameter uncertainty to a selected conceptual model assumed to represent the uncertain mechanisms, is yet inapplicable : the Conceptual Model of flow in the saturated zone at YM is, in my view, vastly undefined and uncertain.

I may have missed some other important documents that may sufficiently allay my concerns, but based on what I have read, the hydrogeology of the site is not, in my view, quantitatively well enough known to permit today the building of a local model of flow and transport to address the three questions listed above.

The site is obviously very complex, and the series of stratigraphic units in which flow is taking place is interbedded, fractured, very variable both vertically and horizontally, and undersampled. The USGS Report R96-4300 analyses the regional hydrogeology of the Death Valley system, and will be reviewed first. The USGS Report R96-4077 addresses the local hydrogeology of the site, imbedded in the regional setting. The first report is at best a very preliminary attempt at quantifying this regional system, on which I have some severe reservations. It and cannot be viewed as a framework in which the local hydrogeology can be understood nor constitute the scientific basis on which to understand the flow system. The second report is more comprehensive and offers a better view of the local hydrogeology. However, it raises a very large number of issues and presents several alternative conceptual models of the site, which cannot be judged at the present level of knowledge. This second report concludes that some of these alternatives may be chosen based on the building of a local model of the site, an effort which I believe is on-going at this time. I am not sure that I agree with this conclusion, as some of the alternative models could only be accepted or rejected, in my view, based on a much larger site reconnaissance effort. Furthermore, since I have rather strong reservations about the regional model presented in the first Report R96-4300, and since this regional model should provide the boundary conditions for the local model to be built, I seriously doubt that the hydrogeology of the site can be sufficiently well understood even after this new modelling, so as to provide a reasonable database on which to base the TPA 3.2 assessment.

In general, the development of a conceptual model of the hydrogeology of a given area goes through the following steps :

1. Determination of the boundaries of the system.
2. Description of the major lithofacies in the domain, with their geometry, major properties, measured heads, etc.
3. Estimates of the recharge and discharge fluxes.
4. Development of a numerical model of the complex system.
5. Calibration of the model on all existing data.
6. Sensitivity studies.

We will follow this logic when reviewing both Reports.

A) <u>Review of Report USGS R96-4300</u>

1. <u>Boundaries</u>. In the USGS Report, the selection of the boundaries of the system seems relatively appropriate, although it is not a closed system. It would have been more satisfactory to extend the limits up to the actual physical boundaries of the system being drained by Death Valley, i.e. no flow boundaries, but the studied area is already very large, and the fluxes that have to be estimated on some parts of the boundaries which are not "no flow" must be relatively small, and should probably not affect too much the global hydrologic balance and the understanding of the system.

2. <u>Lithofacies</u>. The description of the lithology is good in broad general terms, and the building of a Geoscientific Information System to store and represent all the information on the 3-D geology of the site is a very good step. There are serious gaps in the knowledge because of the existence of large areas with few or no borehole data, or insufficient depth of the boreholes. One very surprising absence of data is on geophysics : there is not a single mention of geophysical data in the report, nor of the existence of such data. It seems to me that a lot of information could be gathered by aeromagnetic surveys, gravimetric maps, and seismic profiling, electromagnetic soundings, electric resistivity maps, etc. On each site that I have seen studied for regional and local hydrogeology, particularly in nuclear waste disposal projects, such geophysical surveys have been made and used. This is all the more true as the second report R96-4077 mentions the existence of a large number of geophysical surveys of the area, none of which was used in this first report. The 3-D geologic model should have been made consistent with the borehole information, the surface geology, and the geophysics.

The information on the head distribution is unfortunately lumped into one single "average" system. There is only one piezometric map for the ensemble (Figure 27), and no attempt was made to present information on the difference in head between the various units. I understand that this is difficult, as the position of the screens in the wells is not well known, but some attempts at describing the head differences between hydrogeologic units should have been made. Are there vertical head gradients, which are the units receiving water by vertical leakage, or giving water, are there low-permeability layers separating the various units ? Only one such layer is mentioned, the Eleana formation separating the upper and lower carbonate aquifers (paleozoic rocks). The analysis of the piezometric data is not detailed enough to obtain an understanding of the vertical exchanges between the different lithologic units nor the physics of the system. When such important data are lacking, a detailed geochemical analysis of the water composition can help to understand the importance of leakage (particularly when there are rocks as different as volcanics, carbonates, alluvia, etc. The geochemical signature of the waters could help to understand the flow system better. None of this is done in the report. By contrast, the second USGS Report R96-4077 puts a lot of effort into analyzing the difference in head between the various hydrogeologic units, and particularly between the volcanics and the carbonates, which seems to me a very important issue. The use of the geochemical data are also mentioned and used in this second report.

3. Recharge/Discharge. Concerning recharge and discharge, I understand that the problem is difficult, since neither can be easily measured. But the work presented is not convincing. For one thing, direct evaporation of water from the water-table, even without any vegetation, is not discussed nor estimated. In arid areas, it is well known that evaporation can withdraw water even if the water-table is very deep, there are measures available with water-tables as deep as 10 m below ground, and empirical rules that relate evaporation to depth; in some areas, in Africa, in the 200 mm/y rain depth area, there are closed depressions where the water-table is more than 70 m deep (it is not however proven that evaporation is the only cause of these depressions). Similarly, the estimation of recharge as percentages of rainfall which vary with altitude or classification of vegetation, slope or soils, looks very arbitrary. Furthermore, in arid climates, recharge often occurs by runoff followed by re-infiltration in wadis or gullies. This is not discussed in the report, nor is it evaluated. Furthermore, in such systems, the recharge is often episodic, and occurs only in a few extreme years (e.g. every 30 years in North Africa, on average). If these episodic recharge events are not considered, the global water balance of a large system may be totally biased. By contrast again, the USGS second Report R96-4077 mentions both the infiltration in the Fortymile Wash, and the importance of major flows, the last major flow was in 1969, but extreme events occurring at frequencies such as every 500 years are mentioned.

When such uncertainties on recharge and discharge are present, it is necessary to use additional sources of information to try to estimate fluxes. Environmental tracers are used (e.g. the salt balance, the ensemble of natural tracers, and the "age" of water is used to determine velocities and hence fluxes and hence recharge. Temperature anomalies in borehole profiles are sometimes used to estimate fluxes, both vertically and horizontally. None of these are used here.

Finally, the hypothesis is made that the system is in steady state. Until calculations have been made that show that a steady-state is relatively rapidly established in such a large system, which I do not believe, the assumption of equilibrium seems largely arbitrary, the system may still be reacting to climate changes in the past. By contrast again, the second USGS Report R96-4077 specifically points out that the regional system may not be at equilibrium, and that Winograd and Doty (1980) or Claassen (1985, references in USGS R96-4077) have precisely suggested that the system is still in transient conditions resulting from pluvial cycles during the Quaternary.

4. Modelling. The modelling attempt that follows is really very unsatisfactory to me. Even if it may be an improvement over previous models, by being partly 3-D, the work presented is extremely rudimentary. For modelling this complex system, two options were available :

(1) to construct a very detailed grid in 3-D from the Geoscientific Information System, enhanced by all the available geophysical information, using millions or even billions of nodes. In general, this grid is very thin in the vertical direction (e.g. 10 cm) and on the order of 10 m horizontally. This scale was for instance used in the study of the London Basin. The exact (or assumed) geometry of each lithologic unit is thus finely described and discretized. Each unit is assigned its anisotropic estimated hydraulic conductivity value. Then, a 3-D calculation grid is superimposed on the previous one, with as many nodes as feasible given the computing power available (but currently closer to a million cells than on the order of 75,000 cells used by the USGS). A rigorous upscaling of the detailed model cell hydraulic conductivities to the scale of the flow model is made, giving the anisotropic hydraulic conductivity of the flow model, see for instance Renard and Marsily (1997). Calibration of such a model is made by changing the hydraulic conductivity of lithofacies of the detailed model, and upscaling again, not by adjusting the flow model conductivity. Thus, the importance of each layer can be individually assessed.

(2) to construct a very detailed multi-layer model, where each lithologic unit is represented by a layer of meshes, and vertical links representing leakage are introduced between layers, with estimated vertical permeabilities. The extent of each layer is not necessarily continuous, and each layer is not necessarily present at all sites. It is common to use up to several tens of superposed layers, if necessary. The fitting of such a model is then based on treating each layer as a more or less homogeneous zone, (or subdividing it if it has large known variations e.g. in thickness, density of fractures, etc) and also calibrating the vertical conductivity between layers. This approach is consistent with for instance the detailed description of the hydrogeologic units at the site scale given in USGS R96-4077.

USGS R96-4300 used none of these two options. Instead, a totally arbitrary coarse mesh of three continuous layers was built, and the hydraulic conductivity was assigned to each mesh in a very crude fashion, by using the 50 percentile K value for each of the zones in the model, each zone having been defined by limiting to four different classes the permeability in the whole domain. These permeabilities were used as initial guesses, and then an automatic inverse procedure based on linear regression theory was used to improve the hydraulic conductivity distribution in the model. The selected grid size is very elementary, uniform squares over the whole domain, whereas it would have made much more sense to have variable size meshes, e.g. nested squares meshes, and to focus the grid on the areas of interest, i.e. the Yucca Mountain area and also the downstream area towards Death Valley. This was not done.

The transmissivity in the model is assumed constant, and not a function of the saturated thickness of the aquifer. While this may be an acceptable starting point, it is not sufficient and should have been turned into a variable saturated thickness model, in order to study (as a complementary calibration exercise) what happens in the model for a humid period, when the recharge is higher. Such a calculation is for instance suggested in the second USGS Report R96-4077. Since a few indications of past elevation of the water-table are available, this would have been a second independent test of the plausibility of the model. This was not done.

At this stage of the development of the model, an automated calibration method used to improve the fitting is really worthless. It may well decrease the discrepancy between observed and calculated heads, but the structure of the model is so poor that it does not improve in any way the understanding of the actual functioning of each of the lithologic units of the system (whereas the methods (i) or (ii) above would have done so). I also have strong reservations on the method of calibration The hydraulic conductivity values have been grouped at the start into four zones, each zone being assigned an initial hydraulic conductivity, as indicated above, and then this value is improved by automatic calibration. But the pattern of each zone is kept constant in space. These patterns are given in Figures 44, 46 and 47 for each of the three layers of the model. In fact, more than four zones were introduced, to account for some local complexities, a maximum of nine zones were selected. But the essence of the fitting is the following : if two areas of the model, tens miles apart or more, happen to belong to the same zone, the model calibration is forced to assign the same hydraulic conductivity to both zones. This does not make any sense to me, and could be called "underparametrization". If a zone could be identified with a lithology, this might have been a defensible approach, but given the arbitrary uniform discretisation that was used, a "zone" is a complex assemblage of different lithologies. When the role of faults, the variability of facies, the depth of each layer is so variable, this arbitrary calibration constraint does not make any sense to me. The grid used is inappropriate, but even with this grid, an initial manual trial-and-error fitting would have been more sensible than this automatic calibration. It should also be noticed that the fitting of the model is very poor, the head residuals are large; 20 m is considered a good fit, a moderate fit is between 20 and 60 m of residuals, and a poor fit has residuals larger than 60 m. The same applies to spring flow.

5. <u>Sensitivity</u>. The sensitivity study that follows adds very little, given all the reservations on the structure of the model, the parametrization, and the fitting. Its only merit is that it is concluded from this analysis that the model is highly nonlinear, and that the linear regression analysis which is presented is only a rough indicator of simulation uncertainty. It does not give any clues about the important pathways for the water in the system (e.g. is most of the water flowing in the Paleozoic carbonate ? How important is vertical leakage ? Are the alluvial sequences draining the system ? What is the role of faults ? Are the volcanic rocks anisotropic ? etc.).

B) <u>Review of Report USGS R96-4077</u>

This report is a much better description of the hydrogeology of the site (at the local scale) than the previous report (at the regional scale). It provides a comprehensive description of the major hydrogeologic units, their relations, and the various conceptual models that have been proposed to explain the observations. I agree with most of the statements and conclusions made in this study. My areas of concern about this report are as follows :

-Page 3, I disagree with the statement that "because ground-water travel time in the saturated zone probably is much shorter than travel time in the unsaturated zone (US DOE, 1988) (...) only limited characterization of it may be appropriate". For one thing, the transfer in the unsaturated zone is no longer considered to be very long, and second, the dose to man will occur essentially through abstraction wells, and the dilution in these wells cannot be determined if the hydrogeology is not understood.

-Although the existence of geophysical data is mentioned (page 7), it is not clear how much of it was used to construct a detailed geological model of the site at the local scale. To prepare for a model of the site, a Geoscientific Information System would be needed, as was done for the regional scale, but with a finer scale and intensive use of geophysics.

-It seems to me that the existence of an impervious layer (or semi-pervious) between the volcanics and the carbonates is a very important issue in understanding the site, and that the presence or absence of the Eleana formation needs to be more firmly established. I realize that this is a costly analysis.

-On page 36, it is mentioned that the fractured volcanic rocks are probably anisotropic. The work by Erickson and Waddell (1985, page 24-29, reference in R96-4077) is reported and gives an anisotropy ratio of 5 to 7 in the only case where an attempt was made at measuring this anisotropy (well USWH-4). This seems to me an extremely important issue, because with such an anisotropy, the direction of flow may be very different from what is assumed today based on the head gradient direction.

-Concerning the interpretation of the well tests, it is surprising that the dimensionality of the flow tests was never determined. I refer to the work by Barker (1988) who showed that the analysis of pumping tests could be done by also fitting the spatial dimensionality of the medium being investigated (this spatial dimension may vary between 1 and 3, and is sometimes referred to as fractal). Such an analysis is particularly relevant for fractured media, and can indicate the degree of connectivity of the fractures, and whether or not the assumption of equivalent porous medium is applicable to the fractured system. This method has been very successively applied in Sweden to characterize fractured granite.

-I fully support the statement (page 44) that "hydrochemical and isotopic data, where adequate data are available, can provide qualitative information for checking numerical flow models", and would have liked to see this done, e.g. at the regional scale.

-I disagree with some of the suggestions (page 55 and following) that some of the uncertainties about the conceptual model of the site can be lifted with adequate numerical simulations. For instance, I disagree with the statement page 56 that "investigations as to whether the system can be treated as an equivalent porous medium or if discrete features need to be accounted for can best be carried out using a series of numerical simulations". If one type of model may give better numerical results compared with the existing data, it will necessarily deal only with flow, and not with transport. Since the objective of the numerical simulations will, in the end, in the TPA, be to predict transport of nuclides, I do not believe that numerical simulations can adequately answer that question, with the existing data.

-I fully support however the statements about the need for additional data.

C) <u>Conclusion</u>

My conclusion after reading these two documents is that the flow system at YM in the saturated zone is really very complex, and not sufficiently well understood to propose a conceptual model on which scenarios of transport of radionuclides released by the repository can be made with any degree of realism. The major issues seem to me to be (i) the role of the Paleozoic carbonate (is water coming from or going to the carbonate, or both, as suggested in the R96-4077 report to explain the zones of high and low gradients); (ii) the horizontal anisotropy of the fractured volcanics, to determine the direction of flow, the velocity in the fractures; (iii) the connectivity of the fracture network, to determine how much mixing could occur in the system; (iv) the relation between the volcanics and the alluvium : How layered are the alluvial deposits ? Is there vertical mixing in the alluvium ? At the contact between the volcanic tuffs and the alluvium, how is the flow distributed ? Along the whole thickness of the alluvium ? Over a fraction only ? Mostly at the surface ? At depth ? (v) What is the exact geometry of the alluvium in the area lying between YM and the Amargosa Farms area ? Where are community wells likely to be drilled, in other words are there reasons to dismiss the 5 km well scenario and only keep the 20 km well scenario ?

Until these questions are answered, I do not see how a realistic conceptual model of the site can be developed, and how the TPA code can use a description of the saturated flow that is defensible. Unless a better characterization of the hydrogeology of the site is available, the only defensible approach seems to be a "worst case" description, which would in fact assume fracture flow with very little mixing, injection into a layered alluvium, and therefore very little dilution in the receptor well. The resulting doses need to be evaluated, but might be much higher than those currently calculated in the sensitivity study.

The extreme complexity of the YM saturated zone hydrogeology reminds me of the recent decision taken in December 1998 in France for the selection of a potential site for further studies for a potential high-level waste repository : a complex granitic site was dismissed, not because it was necessarily a "bad" site, but because the feasibility of convincingly proving that the site was safe was considered much too low.

References :

Barker, J.A. (1988) A generalized radial flow model for hydraulic tests in fractured rock. Water Resour. Res., 24, 10, 1796-1804.

Renard, Ph., Marsily, G. de (1997) Calculating equivalent permeability : a review. Adv. In Water Resources, 20, 5-6, 253-278.

Appendix 2

Comments on the calculation of the well dilution

In order to study the well dilution, I have already stated that the hydrogeology of the YM site must be better understood. Nevertheless, I provide below some general comments on the methods that have been used in the TPA version 3.2 code to address this issue.

I have read Fedors and Wittmeyer (1998). I generally agree with the approach that the dilution factor must be based on the flux of radionuclides divided by the pumping rate of the well. This is something on which I worked a little with the Swedish SKI, for fractured granite, and we concluded that, contrary to what could be found in the literature, this dilution can be very small, and that the limiting case is to take the entire annual flux of nuclides leaving the repository, and dilute it in the annual volume of water pumped by the well. But this is probably excessive here, because the granite in Sweden is not very permeable, the flux of nuclides is transported in a few conductive fractures, and one is forced to assume that the well will be drilled in the same conducting fractures, otherwise the well would not produce water...! In Sweden, the surveys showed that the local community wells, for a single family, would have a very low production, like 2 to 10 m^3/d. Diluting in such a low volume the flux of nuclides from the repository could yield very high concentrations and doses...!

In the TPA version 3.2 code, I failed to understand the meaning Page 4-91 of "the volume of water into which the released radionuclides are diluted is the greater of the flow rate of water within the uppermost producing horizon in the pumped aquifer and the volumetric flow rate of the water pumped...". To determine the flow rate in the uppermost producing horizon, I need a thickness and a width. Which are these ? Furthermore, it is said that this is the greater of the UZ or SF flow rates. Again, in which area ? Later on, the sentence "enough to capture all released radionuclides" is unclear. Is this for each stream tube, or for all four stream tubes taken together ? From the rest of my reading, I tend to think that DCAGW considers the four stream tubes as one, and lump the fluxes. Since these four tubes come from different zones of the repository, which may have different WP failure rates because of different infiltration, etc., this lumping does not seem adequate, it creates a dilution from one tube to the other. I make this statement as on line 1 of page 4-99 it is said : "the width (of the radionuclides plume) is equal to the width of the four stream tubes".

Let us first take the case of the community well, which can be as close as 5 km from the repository, i.e. in the fractured part of the saturated tuff aquifer. I do not think it makes any sense to use an equivalent continuous medium approach in a fractured aquifer to calculate dilution. This is not defensible. The flow coming down from the repository in the UZ can very well be focused in a few fractures, and not "spread" in the width of the stream tube, which is on the order of 1 km on Figure 4-16 page 4-84. In the limiting case, all nuclides can be transported by a single conducting fracture, with very little dilution. Now when a well is drilled in such an aquifer, the lucky driller (or the experienced one who can locate the good fractures, e.g. by geophysical methods) will drill the well in the same high conductivity fracture. For a simple comparison, we can calculate the infiltration flux beneath the repository. I take a surface area of 4.8 km^2, and the maximum infiltration rate of 80 mm/y during a high pluvial climate. The repository infiltrates a volume of 3.8×10^5 m^3/y. And the smallest community well ($1.5\ 10^4$ gpd) produces about 2.1×10^4 m^3/y. These numbers are one order of magnitude apart. One can thus pretend that, in the limiting case, the entire flux of nuclides from the repository can be recovered into a few wells each producing on the order of $2\text{-}4 \times 10^4$ m^3/y. This would produce a very low dilution, much lower I believe than what has been assumed in the TPA. To be more realistic, fracture flow and dilution in a fracture network must be examined, not in an equivalent porous medium.

When the radionuclides enter the alluvial aquifer, the continuous equivalent porous medium approach is reasonable. But, although I am very impressed by the quality of the work done in Fedors and Wittmeyer (1998), I do not totally agree with the approach. In alluvial deposits, there is a very strong heterogeneity both vertically and horizontally. The analytical calculations to estimate the capture zone, depth and width, of a well depend really very strongly on the homogeneity assumption. The existence of such layering is mentioned e.g. page 5-1 of Fedors and Wittmeyer (1998), but is only included for limiting the transverse vertical dispersion. Some rough calculations give however some orders of magnitude. The Darcy velocity is taken as 0.46 m/y (page 4.98 and 4.101). For the lowest flow rate in the alluvial aquifer of 40,940 m^3/y, this means, for an average thickness of the aquifer of 55 m (both values from page 4-91), that the width of the capture zone of a well is 1.6 km, assuming the well to be screened over the whole saturated thickness. This is one half of the width of the four stream tubes. The order of magnitude of the dilution is thus to inject the radionuclide flux from two stream tubes into these 40,940 m^3. For the other flow rates, all the nuclides arriving at the 20 km distance are to be injected into the pumped water volume. I would like to see that this is approximately the result obtained by TPA version 3.2 code. I assume here that the well is in the plume, and a random position of the well in the whole area transverse to the plume would give higher dilution.

I noticed in the sensitivity study that the dilution factors in the wells downstream from the repository are very sensitive parameters for some TPI and scenarios. This gives importance in my mind to my comments on the way the TPA code evaluates this dilution factor.

APPENDIX D

REPORT OF ROBERT KELLY

External Review of

Total-system Performance Assessment (TPA) Version 3.2 Code Predecisional

CNWRA
San Antonio, Texas

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NOTE: This document contains my personal assessment based upon the materials made available to me and the time allotted. It does not necessarily reflect the opinion of the University of Virginia or the Commonwealth of Virginia.

SUMMARY

The Total-system Performance Assessment (TPA) Version 3.2 Code represents an excellent example of engineering analysis. As a tool, it should be sufficiently flexible for the NRC to use as part of its evaluation of the DOE repository license applications for a high-level waste repository at Yucca Mountain. It also provides a basis for similar analyses of alternative sites if necessary. The team that has developed this code has performed an outstanding service. Nonetheless there are areas of the code that need enhancement, as would be expected for a code that is still under development. In the area of corrosion of the waste packages (WP), there is a pressing need for a more realistic abstraction of the development of the environment on the WP surface. In addition, several modules required more extensive coupling of processes between them. Finally, documentation that allows a full analysis of the entire structure of the code needs to be assembled.

1. Scope of Work

In assessing the modules of interest (and subsequently the overall code), the criteria used were those requested by CNWRA, as follows:

- Examine the methods and assumptions embedded in the TPA v3.2 code;
- Identify necessary code improvements;
- Evaluate implementation of conceptual models, including the approach for treating parameters;
- Is the TPA code suitably flexible and sufficiently complete?
  - Are the included features, events and processes sufficient to provide confidence in the Licensing Decision?
- Are the conceptual model abstractions defensible
  - Are the conceptual model abstractions appropriate for the spatial and temporal scales being considered and for the selected performance measure?
  - Are the model abstractions sufficiently supported by the site data or other related information to ensure the credibility of the results?
  - Is the documentation sufficient to provide and understanding of the approach?
  - Is the level of conservatism and simplicity of approach appropriate considering the role of the NRC?
- Are the methods used to develop abstracted models and their associated parameters reasonable?
  - Are the parameters used in the TPAv3.2 code appropriate to the abstractions?
- Are uncertainties in model abstractions and parameter values reasonably accounted for by the alternative conceptual models and parameter distributions provided in the code?

Most of my comments focus on the areas of materials science and engineering with which I am most familiar, that is, those involving corrosion of materials. I have made comments in other areas which affect the corrosion of metals due to coupling.

Issues not addressed, as they were beyond the scope of this review, include:

- Appropriateness of the US regulations. This review group was not asked to address this issue. Although my review is based on the current regulations, I would encourage the CNWRA to continue to perform calculations out to longer times and use of other receptor models as time allows as part of a sensitivity analysis.
- Reasonableness of tentative DOE designs, assumptions, and models. The scope of the review was limited to the ability of the code to provide scientific input on whatever license application may be presented to it, not to comment on current or proposed designs. The TPA code must be sufficiently flexible to assess any reasonable design proposed by DOE for Yucca Mountain.
- The usability of the TPA ver. 3.2 by those outside CNWRA and NRC. The primary users of the code are members of the NRC with the aim of evaluating repository license applications. Although it is likely that outside individuals or groups will be interested in using the code to test alternative scenarios, version 3.2 is not meant for such application.

The documentation provided included:

1. Total-System Performance Assessment (TPA) Version 3.2 Code: Module Descriptions and User's Guide, CNWRA, September 1998.
2. NRC Sensitivity and Uncertainty Analyses for a Proposed HLW Repository at Yucca Mountain, Nevada Using TPA 3.1 B Volume II : Results and Conclusions, NUREG-1668, October 1998.
3. Additional documents consulted:
    a. External Peer Review Meeting Overheads: U.S. Nuclear Regulatory Commission's Total-system Performance Assessment Version 3.2 Code, CNWRA, July 27-29, 1999.
    b. Inconel Alloy 622 Data Sheet, Inco Alloys International.
    c. G. A. Cragnolino, et al., Factors Influencing the Performance of Carbon Steel Overpacks in the Proposed High-Level Nuclear Waste Repository, Paper 147, Corrosion '98, NACE International, Houston (1998).
    d. G. P Marsh, K. J. Taylor, An Assessment of Carbon Steel Containers for Radioactive Waste Disposal, Corrosion Science, v. 28, 289-320 (1988).
    e. K. A. Gruss, et al., Repassivation Potential for Localized Corrosion of Alloy 625 and C-22 in Simulated Repository Environments, Paper 149, Corrosion '98, NACE International, Houston (1998).
    f. T. Tsuru, et al., Electrochemical Studies on Corrosion under a Water Film, Materails Sci. & Engr., A198 161-8 (1995).
    g. D. Dunn, C. Cragnolino, The Effect of Galvanic Coupling Between Overpack Materials of High-Level Nuclear Waste Containers – Experimental and Modeling Results, CNWRA 98-004, CNWRA, March, 1998.
    h. P. Lichtner, M. Seth, User's Manual for Multilo : Part II, CNWRA 96-010, CNWRA, September, 1996.
    i. S. Mohanty, et al. Engineered Barrier System Performance Assessment Code : ESPAC Version 1.1, CNWRA 97-006, CNWRA, June, 1997.
    j. N. Sridhar, et al., Experimental Investigations of Failure Processes of High-Level Radioactive Waste Container Materials, CNWRA 95-010, CNWRA, May, 1995.

The User's Guide was the primary source of information before the review meeting. Although suitable for its original purpose, it was inadequate for a comprehensive review of the approach being taken by NRC to analyze the eventual DOE license application. It is strongly recommended that a document that provides a traceable overview of all aspects of the TPA code be developed and maintained. Such a document would provide an important roadmap for those interested in understanding the approaches used and the limitations inherent in the code. The document would have a layered structure; the overview would show the approach taken with links to additional information on the consequence modules which would have links to any external codes used as the basis for the abstractions which would have links to the documents that provide the data used for the analyses. This structure would allow an individual to delve into any area of the code was to as little or as much depth as needed. Influence diagrams would show the framework clearly while also indicating what issues are **not** considered. These can be discussed in separate documents that are the result of CNWRA side analyses which were discussed at the review meeting.

Although the construction of such a document will be a formidable task, the effort will be rewarded not only by allowing improved analyses in later reviews, but also in helping the CNWRA and NRC staff to see the forest for the trees. A User's Guide will be only one part of such a documentation system, and one that is used by far fewer people than the overview document. In reviews of future versions of the TPA code, such a document would be indispensable to a review team to understand both the general framework of the code and the monumental amount of work that underpins that framework.

One issue that arises repeatedly throughout the review is the issue of coupling between and among modules. Although coupling increases the computational load, in some cases it would likely be very important. In addition, whereas it is stated in the User's Guide that the extent of abstraction needed is determined by the computational power available, the massive increase in computational power occurring in the past several years is not considered.

The remainder of this review focuses on the modules that touched on my area of expertise (corrosion of metals and materials science): NFENV, EBSFAIL, EBSREL, VOLCANO.

2. The NFENV Module

The Near Field Environment (NFENV) model is critical to the success of the code predictions. The corrosion of the WP canisters will be directly coupled to the nature and evolution of the environment present around them. As the NFENV module is currently constructed, there exists a large gap which needs to be addressed. As presented in the Users' Guide, the NFENV describes the composition of the environment within the pore solutions of the rock at the rim of the drifts. This environment is then used to calculate the corrosion conditions (T, solution composition) on the WP. There is a pressing need for an improved estimate for the container-surface environment. Although the container-surface environment will be influenced by the environment calculated by NFENV, it will also be influenced by other factors, including dripping and previous corrosion of the containers. In addition, the temperature of the WP would be expected to be higher than that of the walls at almost all times. Unfortunately, it does not appear that either MULTIFLOW or REFLUX3 can capture the concentration of solute that would appear in the flow of water to the WP.

Because much of the WP life prediction depends on an accurate assessment of the corrosion of the containers, an improved consideration of the surface environment is required. In large part, experimental work will be needed to determine the connection between NFENV and WPSURF (to coin a module name). As shown by the observation of refluxing, unexpected physical phenomena can occur that can have substantial impact on the corrosion conditions. Additional experimentation and modelling efforts should be put forth on determining (a) the local environment on the WP surface under refluxing conditions, and (b) the corrosion parameters (E_{corr} and E_{repass}) in this environment.

The dripping abstraction presented at the review meeting is a good start/place holder, but it represents another area where substantial effort needs to be applied. The coupling of the dripping abstraction to fracture flow should be considered as it will have an impact on the nature of the container-surface environment. The sensitivity analyses indicate that the fracture flow is a parameter that affects dose. Thus, it is important to get these abstractions as close to realistic as possible. At present, the "F" factors in the dripping abstraction are better than ignoring the effects, but are not defensible in any scientific way.

Consideration of WP corrosion is generally limited to attack on the upper ½ to 1/3 of the waste package circumference. It was pointed out by one of the review team members that after rockfall, there may be sufficient material on the floor of the drift to collect runoff from the walls and wick solution to the bottom of WP, leading to corrosion there. Such a scenario should be considered, possibly through allowing rockfall and the area of a WP deemed susceptible to corrosion to be linked. This effect would lead to the flow-through model of release being more likely than the bathtub model (see below).

3. The EBSFAIL Module

In general, the EBSFAIL module is outstanding. It represents one of the most noteworthy achievements in corrosion engineering in the last 50 years. By using the threshold concept of the repassivation potential, the process of localized corrosion, often considered to be too complicated to model effectively, has been successfully abstracted to allow it to be in the TPA code. The experimental demonstration of the accuracy of this concept to date has been extremely encouraging. The abstraction of the localized corrosion rates is reasonable, based upon current understanding. More work needs to be done in this area due to the sensitivity of the predictions of dose to the rate at which the WP are compromised, but the essential framework is in place to handle these data.

Although the EBSFAIL module in TPA ver. 3.2 represents the state of the art, a substantial amount of work remains in its refinement and expansion. These needs are in large part driven by the continued evolution of the EBS design strategy. A series of questions resulted from the reading of the documents and papers supplied as well as the presentations and discussions at the review meeting. These are listed below:

a. In the EBS design considered in TPA v3.2, the thickness of the container walls is such that the production of peroxide via radiolysis is deemed negligible. It is important to keep this option flexible to allow for assessment of alternative designs that could involve the use of a double wall of corrosion resistant alloys (CRAs). In such a WP design, the wall thickness would be greatly reduced, and the possibility of radiolytic production of peroxide or other oxidants must be carefully considered. CRAs are highly polarizable in their passive condition. The presence of peroxide could elevate their corrosion potentials to much higher values, which could lead to localized corrosion initiation. I suspect that propagation would be slow due to the diffusion limitation on the reduction rate of peroxide, but this issue would need addressing.

b. There were some reports of chemical analyses from the test drifts at Yucca Mountain that indicated the presence of sulfur in an undetermined oxidation state. If elemental sulfur or reduced sulfur species are present, the nature of the corrosion could change from the expected localized process to a rapid, more uniform corrosion. The code as constituted should be able to handle such a change, although the data needed to assess the corrosion rates must be developed in the proper environment. The importance of this effect would be the increase in the amount of spent nuclear fuel (SNF) available for dissolution. Although pure nickel is most susceptible to sulfur effects, nickel-based alloys are not immune.

c. Another area of coupling that must be considered is that of rockfall-induced defects/stresses to corrosion via the possibility of SCC. One might attack the problem by assuming, conservatively, that any rockfall that impacts the canisters leads to a stress at yield. If SCC is possible in the canister-surface environment, immediate failure by SCC should be assumed. As the stress intensity, K, is already calculated for the outer steel overpack assuming the stresses are at yield to determine if mechanical failure occurs (*i.e.*, when $K = K_{IC}$), comparison to K_{ISCC} should be fairly straightforward as well.

d. In addition, the possibility of either rockfall-induced or backfill induced capillarity should be considered. If areas of the WP are in contact with either rockfall or backfill, those areas will be more susceptible to corrosion attack via crevice corrosion.

e. For water intrusion into the canister, it is not clear how the code will handle the issue of pit area density. In the current code, it seems that one pit is assumed to form and when it penetrates, a hole is formed that leads to either flowthrough or bathtub filling of the canister. It seems that there is no direct connection between pit area density and the important parameter in EBSREL of q_{in}. The release rate is dependent on the *total* area of perforation, so a means to estimate this area based on the localized corrosion characteristics of the material is needed in the TPA.

f. The presentations indicated that the effects of the welds on the corrosion behaviour of the materials will be studied. As these often represent areas of reduced corrosion resistance, such studies should be given high priority. In addition, the possibility of dissimilar metal crevice corrosion between the construction materials should also be studied. Although it is generally assumed that a deformable crevice (as used in most of the experimental studies of WP canister materials) is the worst-case scenario, for some CRAs, a far worse situation is one in which a less corrosion-resistant material is in intimate contact.

4. EBSREL Module

The model of the release of radionuclides from the SNF after the breaching of the canisters seems reasonably well-developed. The use of data from the natural analog at Peña Blanca increases the confidence in its predictions. Two issues arose during the analysis:

a. In the bathtub model of SNF dissolution, it would seem that there could be either humid air corrosion or dripping corrosion of the SNF above the water line. As the water enters the canister, it will continually rinse along the outer surface of the SNF until it reaches the water line. Currently, only the fraction of SNF below the water line is considered available for release by dissolution. This approach would seem to be non-conservative. Within the canister above the water line, the relative humidity would be expected to be that in equilibrium with a saturated solution of SNF dissolution products. The effect of constituents from the container materials might also need to be considered.

b. A related issue involves the need to estimate the chemistry that develops inside the WP during corrosion of the SNF. As the corrosion of SNF is electrochemical in nature, the local cathodic reactions may lead to alkalinization of the solution within the WP. The effects of this rise in pH on the dissolution rate and nature of the SNF should be considered. For example, equilibrium may be achieved for one component of the SNF that dominates that local pH. Incongruent dissolution of other components may follow.

5. VOLCANO Module

My expertise in volcanism is extremely limited. Nonetheless, there was discussion during the review meeting that the temperature of the magma would reach 1100 C. The question arose as to whether this temperature would lead to melting of the C-22 outer container. The importance of this issue data lies in the assumption of uniform dispersion of the SNF throughout a volcanic plume. If the C-22 were to melt, it would be likely that the SNF would be distributed uniformly throughout the plume, diluting its impact to some degree.

Data from Haynes International indicate a melting range of 1350-1390 C for C-22. Thus, melting is unlikely during a volcanic event. Creep of the containers could occur rapidly at this temperature however, leading to failure. Although the accuracy of the temperatures in the magma is unknown, and the interplay between the stresses during an eruption and the creep rates are unknown, some study of the possibilities is warranted. If the canisters are expelled intact, it is likely that they would fail on contact with the ground, leading to a very different release scenario. If they fail in the magma by creep, then dispersal of the SNF throughout the magma is much more reasonable.

6. **Strengths and weaknesses of the TPA v3.2 code**

Strengths:

a. The descriptions of abstractions used in the modules are clear and the assumptions/conservatism are clearly outlined.
b. The underlying process-level modelling (although not apparent in the User's Guide) is truly impressive.
c. The abstractions for the most part capture the critical aspects of the physical processes in a reasonable and conservative way.
d. In particular, the EBSFAIL module represents an accurate abstraction of a tremendously complicated process, and one that will have far-reaching consequences in other applications of corrosion engineering.
e. The consideration of different scenarios seems quite comprehensive. Although the methodology behind the selection of the features, events, and processes (FEPs) could be clarified, it does not appear that any plausible scenario has been neglected.

Weaknesses:

a. Documentation of the origins of many of the modules, data, and side analyses needs to be more traceable. The methodologies used for the selection and rejection of different FEPs are not clearly outlined in the documentation available.
b. Coupling amongst modules is sometimes missing. In some cases, this coupling could be expected to have significant effects as the results are cascaded.
c. The reflux effects need increased attention. The current abstraction must be compared to experimental results that need to be generated.

7. **Completeness and flexibility**

As noted above, the comprehensiveness and flexibility of the TPA code are two of its major strengths. The presentations at the review meeting made clear that as new scenarios were considered, the code was able to include them. Combinations of events are handled well.

8. **Conclusions**

Returning to the criteria for assessment:

- Examine the methods and assumptions embedded in the TPA v3.2 code;
  The methods and assumptions are reasonable. The assumptions are clearly delineated and appear conservative.
- Identify necessary code improvements;
  These have been indicated in the descriptions of the individual modules. The most pressing are those involving an improvement in the determination of the canister-surface environment. In addition, more direct coupling between modules should be investigated.
- Evaluate implementation of conceptual models, including the approach for treating parameters;
  The implementation seems reasonable, although a review of the actual code text was not performed. The approach for treating parameters is outstanding; it allows the user immense flexibility in assigning either variability or uncertainty to the parameter values.

- Is the TPA code suitably flexible and sufficiently complete?
  - Are the included features, events and processes sufficient to provide confidence in the Licensing Decision?

  One of the strengths of the TPA code is its flexibility. I believe that it will provide the basis for an informed decision by NRC on the repository license application. For the present state of knowledge, the code is as complete as possible in terms of the nature of the processes expected to occur. The ability to provide statistical estimates of the likelihood of doses under different scenarios is critical to the mission of the CNWRA and the TPA code is clearly capable of handling such "what-if" scenarios.
- Are the conceptual model abstractions defensible
  - Are the conceptual model abstractions appropriate for the spatial and temporal scales being considered and for the selected performance measure?
  - Are the model abstractions sufficiently supported by the site data or other related information to ensure the credibility of the results?
  - Is the documentation sufficient to provide and understanding of the approach?
  - Is the level of conservatism and simplicity of approach appropriate considering the role of the NRC?

  The conceptual models are in large part defensible. Some of the models rely on extremely limited data and/or experience (e.g., corrosion rates over millenia for modern alloys). As indicated above, there are aspects of some conceptual models that require more effort to make them more defensible. Nonetheless, overall the abstractions are excellent. The documentation system needs substantial improvement to allow newcomers to the code to efficiently develop a grasp of what factors are and are not being considered, the process by which the selections were made, and the influence of the selection of the various parameters. The level of conservatism is quite appropriate considering the role of the NRC and the likely regulations under which it must operate.
- Are the methods used to develop abstracted models and their associated parameters reasonable?
  - Are the parameters used in the TPAv3.2 code appropriate to the abstractions?

  For the modules analysed in detail, the methods use to develop abstract models and their associated parameters are very reasonable.
- Are uncertainties in model abstractions and parameter values reasonably accounted for by the alternative conceptual models and parameter distributions provided in the code?

  In general, the estimation of parameters through expert elicitation and the development of alternative conceptual models do an excellent job of accounting for uncertainties. In some cases, the present level of scientific and engineering knowledge is such that rigorously defensible parameter values are not available. In these cases, the code is able to take the best estimates provided.

APPENDIX E

REPORT OF GÉRALD OUZOUNIAN

Center for Nuclear Waste Regulatory Analyses

External Review for The TPA Version 3.2 Code

August, 1999

Gérald OUZOUNIAN
ANDRA (France)

Contents

Center for Nuclear Waste
Regulatory Analyses

External Review for
The TPA Version 3.2 Code

August, 1999

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1. Introduction

The TPA Version 3.2 review has been performed upon request of the Center for Nuclear Regulatory Analysis (CNWRA), which supports the U.S. Nuclear Regulatory Commission (NRC) for reviewing the license application which will be submitted by the U.S. Department of Energy (DOE) for construction and operation of a high-level radioactive waste disposal at the Yucca Mountain site.

As the research and development program as performed by the DOE is going on, options for the concept of disposal are evolving with increasing knowledge. Thus tools for performance assessment and safety assessment must be able to take account of the different design options, and allow for reliable analyses of the different cases. The TPA 3.2 version code, an improved version of the previous TPA 3.1 code, has been designed by the CNWRA with the capability to consider the different situations to be simulated. It is assumed to give enough flexibility to comply with the successive different requirements corresponding to the evolution of the disposal design at Yucca Mountain.

The present review has been performed according to the plan submitted by the CNWRA :

1. Documents reviewed :
    - Total-System Performance Assessment (TPA) Version 3.2 Code: Module Descriptions and user's guide, CNWRA, September 1998
    - NRC Sensitivity and Uncertainty Analyses for a Proposed HLW Repository at Yucca Mountain, Nevada Using TPA 3.1 – Volume II: Results and Conclusions, NUREG-1668, October 1998
2. Questions and comments (Appendix 1) submitted previously to the External Peer Review Meeting in San Antonio, Texas, containing a request for additional documents
3. Additional documents consulted:
    - Barnard, R.W., M.L. Wilson, H.A. Dockery, J.W. Gauthier, P.G. Kaplan, R.R. Easton, F.W. Bingham, and T.H. Robey. 1992 TSPA 1991: An initial total-system performance assessment for Yucca Mountain. SAND 91-2795. Albuquerque, NM: Sandia National Laboratories
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- Wilson, M.L., J.H. Gauthier, R.W. Barnard, G.E. Barr, H.A. Dockery, E. Dunn, R.R. Eaton, D.C. Guerin, N. Lu, M.J. Martinez, R. Nilson, C.A. Rautman, T.H. Robey, B. Ross, E.E. Ryder, A.R. Schenker, S.A. Shannon, L.H. Skinner, W.G. Haley, J.D. Gansemer, L.C. Lewis, A.D. Lamont, I.R. Triay, A. Meiker, and D.E. Morris. 1994. Total-system performance assessment for Yucca Mountain – SNL Second iteration (TSPA-93). SAND 93-2675, Vols. 1 and 2. Albuquerque, NM: Sandia National Laboratories

4. External Peer Review Meeting: July 27-29, 1999, San Antonio – TX
5. Review report

2. General comments

Most of the questions addressed from the first lecture of the two reviewed documents had answers either in the additional references consulted or during the external peer review meeting in San Antonio. Documentation seems appropriate to provide an understanding of the approach, and additional information is referenced which can be consulted. This documentation can be improved, specially by adding a logical flow-chart for each module, as given for some during the EPR meeting.

Among the aspects to be considered by the External Review Group (ERG), the following were of primary interest to the NRC and CNWRA:

- Flexibility of the TPA 3.2 Version code
- Completeness
- Reliability and defensibility of the model abstractions
- Treatment of uncertainties

Flexibility for a code designed to simulate the expected behavior of the repository is understood as the possibility to take account of different processes which may affect the safety of the system, as well as different pathways for the released radionuclides, in order to represent various options of the proposed disposal concepts. The TPA 3.2 Version code appears to be extremely flexible as it can accommodate many situations and computational possibilities. The flow diagram for TPA Version 3.2 (fig.3.1) summarizes the very modular structure of the code, with a succession of transfer boxes from the waste package to the biosphere, and optional disruptive events. Moreover, another aspect of flexibility is the capability to incorporate processes with different formats, as shown on figure 3.2 for the consequence modules.

The design and structure of TPA 3.2 allow for the requested flexibility. The overall assembly appears very efficient and previous sensitivity analyses have demonstrated its capabilities. The quality assurance program as presented and performed, with its validation test plan and the various controls grounds reliability and confidence in the document. The pending questions about completeness, reliability and defensibility of model abstractions and treatment of uncertainties need to analyze the consequence modules, and their underlying models which are considered, data and parameters.

Keys for defensibility are legibility and transparency of the information. Justification of choices are given all along the reports, with a strong scientific support and a precise description for abstraction approaches. When the level of information was not enough, as mentioned previously, it could be completed. However, I assume that it was easier to reach additional information in the framework of this review. A basic recommendation will be not only to have a control of configuration of the TPA 3.2 Version, but also to make sure that all the underlying work, models, data and assumptions are made traceable. One of the keys for understanding and confidence is that links between the phenomenological or process level and the performance assessment level are described in a comprehensive and accessible way. On the organizational point of view, having teams in charge of describing the processes, and mirror teams performing sensitivity analyses gives certainly all chances for an efficient work.

In the frame of this expertise, the overall project has been investigated, with a priority on the following areas:

- Initial inventory (INVENT)
- Near-field behavior with special focus on chemical aspects (NFENV and EBSFAIL)
- Radionuclide release (EBSREL)
- Radionuclide transport in the saturated zone, with special focus on chemical aspects (SZFT)

As dose is calculated from a series of successive reactions and transfers, water chemistry is a determining factor for the behavior of the disposal system. An illustration has been given during the ERG meeting with the presentation of the TPA 3.2 Version Code, and specially the introduction of alternative conceptual models of water composition for release. The water chemistry controls:

- Conditions in the near-field for short time periods,
- Corrosion,
- Radionuclide release,
- Transport.

Most of the comments given in this report are focused on chemistry and interactions between water and solid materials involved in the disposal. A strong recommendation is given in the conclusion, to develop as initiated in CNWRA, a methodology through which chemical pathways of water are analyzed and described all along its hydrodynamic path from infiltration in YM to the alluvium.

Before entering detailed comments, importance of scenarios is to be remembered. Most of choices which have been done or which drives the analysis will depend on the nature of the scenarios. The level of required science also depends on scenarios, as well as scenarios description depends on available science.

Flexibility must allow for the capability to consider different types of scenarios. The base case was issued from conceptual models, from which different alternatives can be derived. In any case, description must be given about how scenarios have been generated and how they are adjusted to the new acquired knowledge, or to the evolution of the disposal design. Another important step in scenario development is to explain how decision is made to take account of a disruptive event, and with which level of detail.
The scenario development methodology must be explained and documented. Sensitivity studies may also be used to focus some of the scenarios. QA and traceability are important in order to record how decision was made at each step, to include or not an event or a process. For those scenarios which have not been analyzed, justification must be given.
In order to allow the NRC having an independent review of DOE's approach, it is also needed to have its own capability to generate a set of FEPs and scenarios. For each of the scenarios, definition of the range and boundaries of the given set of models and data is requested in order to prove that computation was not performed out of the validity domain.

3. Inventory (INVENT)

A set of 43 radionuclides has been selected as input for the TPA 3.2, based on a literature review. During the meeting, it has been mentioned that the main origin for this selection was the work performed by U.S.DOE. The impact to man given by the release from a waste disposal will depend on many parameters, including the initial disposed of inventory, and then the environmental conditions.
The starting point must be the total inventory, from which a selection can be extracted, based on criteria which must be defined. As an example, a first criteria can be to consider those radionuclides which can allow for an impact after closure of the disposal, and which typical half-life time is greater than 10 years. Other criteria like radiotoxicity (activity x dose factor) can also be considered.
The behavior of radionuclides selected from the first set in the disposal is then studied. Some of the selected radionuclides will be retained in the environment and will not result as dose to man. On the other hand, some of the radionuclides may have higher mobility and give rise to higher dose to man. In order to avoid any misfit, the behavior of those radionuclides which were not retained from the preliminary first selection must also be checked.
Each iteration between a new selection and calculated dose to man will lead to a new ranking of radionuclides, and selection as to be reconsidered for each step. Thus, exercises performed with TPA 3.2 would have benefited from previous results.
As the TPA code allows for analysis of the behavior of the different radionuclides contained in the waste package, it is suitable to test all relevant radionuclide initially contained in the disposed of WPs. As the same level of effort is not possible, nor useful, selection and ranking of radionuclides must be performed. This will also help in defining further research requirements.

Selection given by the DOE cannot be suitable to achieve the objectives of reviewing the DOE license application and TSPA. A specific methodology, starting from the total inventory of radionuclides to be disposed of must be defined and described. It can lead to the same selection as the one used, but will be justified.

4. NFENV

Heat transfer and temperature are calculated at different scales, which allow for useful information at various space and time scales. Most of the provided information is used as input data for other modules, dealing with reflux, corrosion or radionuclide release. This information can also be valued in considering the different stages of the disposal life, and specially to determine the chemical composition of the water allowed to react with the disposed of materials:

- The first period, during which the highest temperatures are reached, giving rise to evaporation and condensation; due to coupled processes with a two-phase behavior in a porous system, with flux and reflux cycles, chemical composition of waters reacting with materials is difficult to predict.

- The second one, at temperatures below the boiling point, and during which waters slightly modified by thermal effect are involved.

The disposal concept is designed according to the thermal load of the waste packages. Temperature reached at the drift wall, and even at the waste package, decreases under the boiling temperature after 10^3 years in most cases, and after a few 10^3 years for 80 MTU/acre (MULTIFLO results). During the first period, the REFLUX model describes the thermodynamical behavior of the water phases. Physical evidence of thermal reflux has been shown through the drift-scale heater in Yucca Mountain, as well as with the CNWRA laboratory-scale heater test. Data have been derived about thickness and duration of dry-out zone, duration of reflux, fraction of water that escapes cycle and depth of penetration of boiling isotherm. However, chemical composition of water is difficult to predict during the reflux cycle, and except a sludge recovered during laboratory experiments, no data is available (care must be taken about early results, which in such a context are difficult to understand; as the system is complicated, processes need to be analyzed separately before being considered as coupled. In this context, the disk-shaped uniform representation as homogenized over the entire repository will certainly not give reliable results, as chemical reversible, as well as non-reversible reactions will occur at a reduced scale, in adequacy with the amount of water available in the UZ. In the case of the laboratory experiment, chemical quality of the concrete used for the test may have determined formation of sludge). An upper bound on the chloride concentration has been derived assuming equilibrium with halite (NaCl). However, this upper bound appears quite speculative, and alternate conceptual models can give rise to very different results. As an example, if concentrate moves down it will dissolve salts previously deposited during vaporization, thus giving rise to a composition of water close to the initial one. On the other hand, to keep a conservative approach, pure concentrates can also be considered. How reliable are the different chemical models at this stage? It seems that there is a lack of grounds for a chemical model during the reflux cycle. A theoretical approach can be considered for the coupled two-phase hydrodynamical-chemical system, but will have to be validated against experiments. In all cases, specific experiments could be considered in order to better define the chemical composition of water, and its evolution, during reflux cycles. Moreover, specific experiments could help in assessing effects of irreversible chemical changes due to thermal period, mainly phase changes with correlative porosity and permeability changes.

For the cooler second period, chemical composition of the water can be derived in an easier way, just taking account of the thermal effect on the chemical reactions in the liquid phase.

In both cases, a clear knowledge of the initial water is needed in order to derive the modified water composition. The initial near-field chemical composition is described based on the general knowledge, and a few data. Reference is made to the data compiled by Perfect et al. And screened by Turner (1998). However those data were generated and given for the saturated zone, for another purpose than that of the near-field chemical composition in the unsaturated zone. Same remark is made about J-13 well water, often used as a reference water, even for the unsaturated zone. As water chemistry will constrain further behaviors of the system, a reliable knowledge is requested. This assumes that the chemical pathway of the water is described, from meteoric waters, then modification when it infiltrates, and during its transfer to the disposal level. Several evolution can then be considered to represent temporal variations in near-field chemistry, depending on the stage of the disposal system:

- The thermal effect,
- Contact with materials used for construction of the disposal
- Both coupled effects

Limitations of the present approach have been well identified in the discussion of assumptions and conservatism. However, reliability and confidence in the model will be gained if a clear process is described for chemical composition of the water.

Other processes described in NFENV are relevant, but have to be applied in the context of each time scale, as for the two periods, the two-phase and the liquid phase period. As example, some of the corrosion figures presented during the meeting dealt with a life-time of more than 10,000 years for the waste canister. This means that except for early failure, which also has to be considered, there will be no release before at least 10,000 years. A detailed analysis in order to define the main processes occurring at each space and time situation is suggested.

5. EBSFAIL

The three processes recorded for corrosion of waste packages match with the successive thermal situations:

- Oxidation by interaction with gaseous oxygen in dry air at relatively elevated temperature
- Humid-air corrosion as a result of the air containing water vapor at intermediate RH values
- Aqueous corrosion

All three processes are well described, in spite of an empirically approach. Discussion about assumptions and conservatism is very clear, and respective role allowed to each of the three processes seem reasonable.
As the third process appears to be the main one to be involved in WP failure by corrosion my comment will be focused on characteristics of aqueous medium contacting the WP. A great uncertainty is associated to the composition of water, as it is not known along the pathway from surface to the WP. Assumptions are made on some of the characteristics, about the chloride content as well as the carbonate system, and conservatism is also retained based on unfavorable pH values (above 9 for pitting) for the considered alloys.
Sensitivity analysis is a way to manage this lack of knowledge. However, reliability and confidence can be improved with a reasonable description of the chemical evolution of water all along its interactions with the successive materials. This requires a detailed analysis of the involved processes, also taking account of time dependent properties of the system, the thermal phase as an example. In the case this step is not get over, any other hypothesis about boundaries of chemical properties to be examined for the sensitivity analysis can be opposed to the approach.

6. EBSREL

Mass transfer out of the WP is represented by advection, with 2 factors, the first one describing the concentration of radionuclides in the WP water and the second one the amount of water leaving the WP.

Concentration of radionuclide is directly derived from the spent fuel dissolution rate, which depends on the quality of water. Below solubility of limiting mineral phases, concentration of radionuclide will depend on the residence time during which water interacts with the spent fuel. This means that both terms C_i and q_{out} are not really independent in the advective mass transfer out of the WP (w_{ci}).
On the chemical point f view, congruent release with dissolving SF matrix for immersed fuel seems a reasonably conservative assumption for the considered radionuclides. Flow-through tests as reported from Gray and Wilson (1995) give a good upper limit for the radionuclide release, as limited by intrinsic solubilities. However, this conservatism is very far from reality. The very important role of secondary minerals is neglected in this approach; as illustrated with further works in the laboratory as well as on the field, it could account for orders of magnitude .
Dissolution rate as expressed by Gray and Wilson (1995) makes an assumption on chemical composition of the water in the near field. Previous comments on quality of water, at present also modified by products from WP corrosion, still remain valid. Nevertheless solubility limits have been assigned for nuclides, which gives an upper limit to their release. Some variability was accounted from 900 runs performed with EQ3/6 to take account of variability of the water composition. Does that means that there are at least 900 different types of waters, as a result of 900 different chemical processes, giving rise to the waters allowed to react in the near field? As processes are not described, confidence is looked for by multiplying the number of calculated tests in order to define wide boundaries. In the TPA 3.2 Version, near field chemistry is also based on Multiflo 1.0 calculations, with 2 important input data:

- J-13 as initial fluid
- Equilibrium with calcite, which is allowed to precipitate

As previously noticed, the J-13 water is from the saturated zone, with a chemical composition reached after several thousand years of interactions with the rock matrix. Even if in some cases equilibrium is achievable within a few days, some reactions will require more than the flow-time through the upper UZ, and overall equilibrium condition will require much more time. The same chemical composition of solution has been derived to simulate interaction with the WP and the waste form. There is a great uncertainty about the quality of water, and the extent of this uncertainty is also illustrated through the alternative release models or through some remarks reporting that in the presence of Si or Ca ions, dissolution rate will decrease by about 2 orders of magnitude. Those Si and Ca ions are in any case present in the YM site water, even in the unsaturated zone. For model 2, different types of water have been considered and are estimated to cover all possibilities and ranges. Conservatism of the approach is acknowledged, but its level is certainly to far from realism. Even with this very high level of conservatism, a lack of description reflects a lack of understanding, a lack of confidence about the environmental context, and hence the right data to consider.

My understanding about conservatism is that it is not intended to cover all possibilities, and lack of knowledge, but to reasonably take account of margins of variability and uncertainties, in such a way as to be penalizing.

Natural analogs from which low release is derived certainly gives reliable result. A very nice illustration is given from the Peña Blanca case, showing that even under oxidizing condition the uranium oxide remains stable. As part of the release process will rely on their solubility, secondary minerals and their role must also be underlined (Schoepite in the case of Peña Blanca). Presentation of the model based on schoepite solubility gives a strong scientific basis, supported by natural analog field observations. As 3 orders of magnitude remain between model 1, which is recognized to be very conservative, and the schoepite solubility model, efforts to reduce uncertainty margin can be valuable and help increase confidence by improving the overall knowledge and thus reducing the overall uncertainty.

Thermodynamic based approach, as the schoepite model, does not depend on surface area of the exposed fuel, so another succession of assumptions on the geometry of grains in the SF is avoided. However, mineral phases involved in SF need to be well characterized as dissolution rate of the irradiated SF is higher by about 100 X than for fresh fuel.

Among the pending questions, a few are very relevant:

- Which are the secondary phases which can occur upon SF leaching, what is their stability and what is their ability to trap FP or other radionuclides?
- A level of inventory of grain boundaries and gaps up to 6% has been considered for the prompt release. According to different experiences this value seems reasonable. It must be noticed that the fraction for the different radionuclides in grain boundaries and gaps may differ. However, a sensitivity analysis would show that even a factor of 2 on this value will not modify the final result. Nevertheless, it is important to describe a methodology about how values have been derived, how values have been selected for the model, and make sure the traceability.
- The weight of radiolytic effects has not been considered in the document. Either a comment explaining that they are not relevant on the considered time scale, taking account of the width of the overpack, or on the other hand that those effects may be important and will have to be considered in further developments.
- Cladding accounts in the model for the geometrical protection it provides. The reduction of release of radionuclides from a SF with its cladding compared to that of the bare SF accounts for orders of magnitude, depending on the nature of the radionuclide, as shown during the review meeting. Due to the various mechanisms involved in its long term behavior, it is very difficult to predict the evolution of its characteristics and its confining role. Thus keeping role of cladding as a margin seems reasonable.

- Remarks given on materials used to construct the invert, allowing for sorption properties, are fully supported. This type of solution , easy to reach, may lead for results at relatively low cost.

The work presented and reported for the chemical part of EBSREL is very impressive, with a very high quality analysis. The most important is to show that relevant processes have been identified and understood. Then it becomes easy to explain and justify the simplified approaches, or range of values to be considered for the calculation.

About the second term, the q_{out}, dripping has been introduced as the source for the amount of water involved in SF dissolution. The conceptual model for water dripping from the drift to the WP is very attractive, as well as the analysis which has been performed, and the way consequences are taken into account through the three factors F_{wet}, F_{ow} and F_{mult}, as abstracted from the stochastic process-level model. One of the basic assumptions is that dripping occurs when I>Ks. Validity of this assumption depends on the homogeneity of the system, without rough patches at the wall of the drift, on surface interaction between materials and water, possible capillary forces, and other. Nevertheless, the probabilistic sampling may implicitly take account of those heterogeneities at a scale consistent with the size of droplets, making the approach valid. This type of abstraction can be expressed, and enrich the approach. Questions remain about the model: does opening of the drift divert fluxes preferentially to the drift? On the other hand, isn't there any diversion along the walls of the drift?
Again, the analysis is very attractive, with an in depth analysis of the processes taken into account with an abstraction model, which appears to be in adequacy with the level of the requested representation. Any other approach, like a deterministic one, would require a very detailed characterization of the system, at a scale which is consistent with the size of the droplets. As suggested during the review meeting, additional observations will increase knowledge and confidence in the model. Some mock-up tests, first with non-reactive materials to avoid chemical interaction, and then with tuff would also help to increase knowledge.

However, even if the model is valid for representing dripping, it becomes highly speculative to interpret the information which it produces in terms of water influx into the waste package, and of water outflow. Conservatism is retained with a 3% value for the plan area of waste package to determine the potential quantity of water getting into all waste packages. The very over-conservatism here assumes that all drops get into all WPs. At the beginning of WPs leakage, only a very small fraction of the area submitted to dripping will allow for water penetration into WPs. Then corrosion will progressively open the exposed area, inducing a full exposure corresponding to the 3% of the plan area. The time scale between the first drop getting in contact with the spent fuel, and full opening may also be an important factor in the case of pitting or in the case of a very long time scale between first opening and full opening. This aspect may be considered, on conjunction with corrosion models, and may give rise to a model representing a progressive exposure which result may be significant on the final dose result.

EBSREL is a very dense module, with many processes which are involved. Faced to this complicated situation, approaches have been split off in more simple situations, helping a more precise analysis. The work as performed is considerable, and has a very high quality. Each answer to a specific question bears a new question addressed in order to better understand and describe the involved processes. Discussions reported about assumptions and conservatism are very important and well managed. Boundaries of the approaches and limitations are well known and clearly explained. Remaining work is also well known. The most important remains to report methodologies, describe approaches and explain how models and data have been selected. It is then possible to share, accept or discuss any approach when information is available. It is why exhaustive analyses are looked for, to make sure that the different aspects of a process, or of a situation, have been considered. Abstraction models can be accepted when, as it has been reported for dripping, a detailed analysis is given; in this case, signification of the different parameters, and how those parameters are adjusted to take account of specific processes is important.

One of the risks with such a complex module was to not be conservative. On the other hand, in order to avoid this risk, some over-conservatism appears; it can be favorably reduced. The aim for NRC and CNWRA is not to achieve a demonstration for a license, but reliability in their analysis, and confidence will also rely on the quality of the scientific grounds supporting their appraoch. This quality is measured by comparison with the representation we may have of reality. Conservatism must be defined according to some realism. The major uncertainty remains in ENFREL in the chemical behavior of the system.

7. SZFT

SZFT is the consequence module which calculates transport in the saturated zone. Some complications are reported. Those complications linked to spatial variability in the geochemical properties of fracture surfaces and rock matrix, heterogeneity of pore-scale to formation-scale transport pathways may be overcome with a proper methodology to select, from the characteristic dimensions of the system, sampling scale according to the formation-scale representation requirement.

Variability in the rate at which radionuclides transiting the UZ reach the water table may be an important factor if time required is significantly important compared to the time in the SZ; however this can only be possible if retardation is demonstrated in the UZ, for which discussion shows limitations.
Other complications like temporal variations in the flow field is mainly constrained by hydrological properties, much more than by chemical properties.

Resolution of transport processes is matched to the use of results from SZFT. This choice is very important and must be explained, maybe with more details in the paragraph about assumptions and conservatism, in order to avoid any over-dimensioned request in the process analysis and in the data precision.
Another choice is made about dimensions of description of the system, and only variations in geochemical properties along the transport path are taken into account. In fact the only variation is the change of formation, from tuff to the alluvium, at about 10km from the YM disposal. Into each of these two formations, chemical regulation of the water must be driven by homogeneous processes. Even if variability has been recorded for a few data, it would be interpreted according to the major chemical processes occurring in each of the formations. Other variability than from a formation to the other will not be significant if chemical regulation processes are described.

A very interesting abstraction approach has been presented for deriving Kd values. This approach which seems to correctly represent sorption processes has been derived for actinides, but limited or no information was reported about FP. For all cases, literature reported values have been used to develop the approach.

However some data generated specifically for the purpose of validation of the model would be helpful in gaining confidence. All data are not possible to generate, but availability of a few will enhance reliability in all. Are data available for the alluvium as well as for the tuff? As distance increases from the disposal level, concentration in radionuclides decreases. Nevertheless, even alluvium is allowed to retain some species by sorption, and it will need a certain level of characterization in order to derive reliable Kd values.

8. Conclusions

The TPA Version 3.2 Code has a very impressive structure with a very wide range of capabilities. Requirement for flexibility is achieved through various ways :

- Simple input set of data
- Specific subroutines
- External stand-alone program

and abstractions which are analyzed with support of sensitivity computation.

Organization and accompanying QA structure seem adapted to the high level of requirement. The main message about the overall structure deals with documentation and traceability. Reviewing the TPA 3.2 Version

Code, the most sensitive point was to make understandable how and why options were selected. Documentation is very rich and can better be valued by focusing on methodology and process of modeling in some instances. Most of the information has been spontaneously given during the ERG meeting. Links between different levels of modeling have been clarified in all cases. Thus it's just a matter of reporting, maybe with a road-map for each module, with a logical flow-chart and with documentation and steps to understand relations between data, models, results, abstraction and integration in the TPA 3.2 Version Code.

A lot of work has been performed to develop the code. The very high quality of analyses must be underlined and acknowledged. However, a lot of work still remains, not only to take account of new acquired knowledge or evolution in the concept design of YM, but also to bring the level of the consequence modules at a level of sophistication which is in adequacy with the requirements. Some of the modules are much more mature than other. All the modules must be sustained by process modeling and are to be considered in well defined boundaries, and specially when simplifications or abstractions are used.

Among those aspects which have been reviewed, it appeared that there is a need to give a consistent view of the chemical pathway of water, and an analysis of the different interactions. It is not possible to only consider a wide range of possible water compositions without boundaries defined by field knowledge, based on a strong scientific ground. It is also not possible to only consider water which has been sampled and analyzed. How to justify that water sampled and analyzed from the SZ is used to qualify interactions with the WP or the SF occurring in the UZ?

Chemistry below the WPs is very well analyzed and described, with a very high level of conservatism:

- According to schoepite or natural analogs for SF release
- With a very well defined and bounded approach for Kds in the SZ.

However time required for release to occur is a determining factor upon which final result will depend. This time is strongly constrained by the water chemistry which infiltrates, and which will interact with the WPs and then with the SF. Chemical processes and chemical pathways must be described in a logical way, according to the different period of time situations:

1. Characterize the chemical composition of infiltrating water
2. Have a good characterization of the water flow through the UZ, to the disposal level, and describe reactions occurring during water-rock interactions
3. Take account of major processes when relevant for the time period (reflux, temperature effect), and identify consequences on the water chemistry
4. This water will be allowed to react with the EBS materials; analyze behavior of the materials (aging, corrosion, alteration) as well as the evolution of water composition during interactions
5. Consider the water as modified through step 4 to interact with the SF, even according to a range of models giving rise to a range of chemical compositions
6. Assess the chemical evolution of this water during transfer through the UZ and then the SZ, taking account of the relevant parameters.

Such an approach, which has been initiated in CNWRA, will help to focus the chemical composition of water, based on a logical pathway and a recorded methodology. First results from CNWRA tend to show that water getting into contact with WPs has pH values lower than 9. I feel much more confident in those values which have been derived from a clear and logical approach than with values which have no link with reality except that they are considered as conservative. If such a result is demonstrated and confirmed, it will help simplifying the analysis of behavior of the system, based on a strong scientific basis. Confidence will then be based on objective results rather than on a very open analysis from which link with field values are not perceptible.

Two other points need to be risen for these conclusions:

- The first one deals with a need to have a proper methodology described for scenario developments, as mentioned in the previous general comments
- The second one is about independence in performing the review of DOE's licensing application. For an independent assessment, the NRC needs to have its own approach. Two points of weakness appeared in this context during this review: the first one is that selection of radionuclides was that determined by DOE, and the second one about FEPs to consider

All comments given in the report are intended to help CNWRA improving its approach, as requested for this review. Those comments do not prejudge about the very high quality of all the work which has been performed or which is going on. A summary is presented in appendix 2, according to questions from the statement of work as asked by the CNWRA.

APPENDIX 1

Question and comments for the ERG meeting
July 27-29, 199927-29, 1999

(Dr. Gérald OUZOUNIAN)

The following comments and questions are given according to the structure of the documents under review, with numbers referring to the page.

VOLUME I

1-2 A comment is given about deterministic and probabilistic approaches. Those 2 types of approaches are complementary. The deterministic one is suitable as a driving force, to help ranking processes, uncertainties and parameters to be addressed by R&D programs. It can be useful for a project under development, and typically in the present case, for the DOE. The role of the probabilistic view is much more static, and is well suited to an analysis which has to be performed at a given stage, as that which has to be performed by the authority.

2-6 What is the signification, in the last paragraph, of "a statistically sampled parameter" to scale the chloride history? Is the range of measured chloride known ?

2-8 The conceptual model for radionuclide release seems to be a leaching process of the spent fuel, and then precipitation of limiting phases. Why isn't it clearly stated, instead of having an "adjustment to ensure consistency"? In case of adjustment, can we be clear about which of the end-members was good, or wrong. But after having read chapter 4, I'm not sure that this conceptual model was used (see questions on chapter 4, 4-72).

2-8 Two models are considered for failure of the WPs. For the bathtub model, the outlet height is statistically sampled. What is the signification of such a statistical sample? Is there any implicit assumption that we are faced to a uniform process, such as those given in 2-7, dry air oxidation or humid air corrosion? In the case of aqueous corrosion, as flow model is driven by gravity, the model can be refined to take account of gravitational forces. At least two different behaviors can constrain the statistical distribution: drip on a given emplacement on the upper half area of the canister and local hole on this part, or flow of the droplets to the bottom of the canister and accelerated corrosion in the bottom. Besides, this type of behavior has been considered among the limitations for the corrosion model (4-49). Comments given later, in 4-69, also indicate that many configurations can be imagined. Sensitivity analyses as performed, are clearly useful to consider the lack of determinism. Nevertheless, the improvement of the result from a more deterministic approach will be limited, but confidence will increase if a more reliable description of the physical process is given.

2-9 How has the list of 43 radionuclides been derived?

3-15 Same question.
It seems, according to 3-20, that selection was performed based on decay equations, and that environmental condition (i.e. retention, retardation, migration) were not taken into account for the second and third iterations in the calculation process.

4-26 What is the signification of the silica concentration from J-13 well (0.0011M) compared to the values given for equilibrium with quartz, chalcedony or cristobalite?

4-27 Calculation show that a liquid phase is always present, and complete dryout does not occur following emplacement of WPs. Is this result due to the scale of representation which is homogenized in the disk-shaped uniform heat-source?
With MULTIFLO, or any other model/code, has a profile for the presence of water been drawn in the case of a single drift? Such a profile, as a function of time, would offer a better resolution to understand the crucial point of the presence of water in contact with the WP.
In the same way, with the disk-shaped uniform representation, pH increase and chloride increase are homogenized over the entire repository. A detailed profile at the scale of the drift would be helpful to discriminate local effects from large scale effects, and to determine at which time scale homogenization can be considered. At the drift scale, the process described by MULTIFLO (4-26) of suction followed by vaporization and then condensation with a correlative salinity increase close to the heat source, and a dilution at the condensation zone could also be described. But once adjusted on the above suggested profiles, due to the mass balances between high salinity waters and low salinity condensate would lead to the original water (except diffusion and mixing which can slightly modify the scheme). Quality of water getting into contact to the WPs depends on the involved time scales for the respective processes (heat generation, resaturation). Such an analysis could lead to avoid large overestimates of the consequences.

4-28 What is the relationship between the pH value set at a constant value of 9 (highest value obtained from simulations), the pH increase in the vicinity of the repository at approximately 10 (4-27), and values given for J-13 between 6.8 and 8.3 (table 4-1)? With such a set of values, final results may differ at least by 3 orders of magnitude.

4-28 About the reflux models, it is said that water that penetrates the dry-out zone would be available to contact the WPs, possibly accelerating the corrosion of WP materials and facilitating transport of radionuclides released from the failed WPs. But according to figure 4-9, after 1,000 years temperature decreases below boiling point. However, the lifetime of the WP overpack is designed to stand more than 1,000 years even in the base case with 620 or 825. Synchronism between invoked processes needs to be explained. This shift among specific time periods for different events has been considered in the discussion of the EBSFAIL approach for corrosion.
Moreover, the time for the water begins to drip into the drift has to be considered, taking account of the near-field groundwater infiltration (REFLUX in 4-30).

4-39 How is the multiplication factor for chloride concentration derived to take account of the difference between groundwater chemistry and brine resulting from evaporation from the WP surface?

4-50 Is time taken into account for ageing of the WP, for example for corrosion and mechanical resistance decrease, in the conceptual model? (time of occurrence has been taken into account to determine the radionuclides release) . Has the thickness of the WP been taken as a constant over time for the I parameter (4-52)?
There are many assumptions, with a very detailed development. Is this at the scale of the question? Are the relevant parameters taken into account? The example given above could be considered as a non conservatism assumption.

4-62 Sensitivity to the height of holes in the bathtub and flow through models is crucial.

4-63 What support is available to the selection of radionuclides (justification for Tc99; why other radionuclides such as Nb, Se or many other were not included in the list?)

4-63 to 4-66 Assumptions given to represent UO2 solubility seem reasonable. Nevertheless, the validity of these assumptions have been checked against more sophisticated and complete geochemical codes. This needs to be mentioned in order to support the simplified models.

4-67 and 4-73 "The surface area available for leaching is conservatively held constant ". Leaching can lead to a higher fragmentation of the SF. In this case, the "conservatively constant" needs to be demonstrated, or at least justified.

4-67 Remarks on ionizing radiation are right, and the point really needs to be clarified because it can lead to orders of magnitude differences. In the same way as for thermal effects, synchronism of the different effects over time periods will be useful to analyze. If the ionizing radiation only occur before WPs have been corroded, consequences will not be the same as in the case it occurs over a very long time period.

4-71 As flux is mainly driven by gravity, the remark about the role given to the invert and the opportunity to improve its performance is relevant.

4-72 About the discussion on assumptions, when writing "if solubility controls the release, the fraction of fuel contacted is unimportant", isn't it the intrinsic dissolution rate (4-63, ref. Gray and Wilson) rather than solubility?

4-85 to 4-89 Transport of radionuclides is said complicated by, among others, spatial variability in the geochemical properties of the fracture surfaces and rock matrix. But reading this chapter, it appears that the system is made of 2 formations, the tuff and the alluvium. Except if those formations have variable properties regarding the chemical regulation of the water (but is there any reason for that?), the process must be homogeneous in each of those 2 formations. That means that even if variability is measured, it only reflects dilution effects, except for the very short times of contact between water and rock. A certain level of equilibrium must be reached (10km at 4m/yr=2500yrs). If it is characterized and the process described, then spatial variability will no more be significant, all the more conservative approaches have been reasonably taken into account for differences between fractures and matrix.
On the other hand, during the first stages of field studies, measuring and characterizing the chemical variability will help in understanding the processes.

4-92 to 4-102 Discussion on assumptions for DCAGW reflects the large amount of uncertainties, mainly due to social changes. It is of the highest importance to have a very detailed sensitivity analysis, first on the parameters included in DCAGW, and then on DCAGW in TPA.

4-107 In FAULTO, same comment as for SEISMO. Intensity of consequences on release will depend on the quality of the WP (corrosion) at the time of occurrence of the faulting event.

4-112 to 4-118 Why ASHPLUMO is not weighted by a 10^{-7} probability, as done for the VOLCANO event?

VOLUME II

General questions:

1 Why fission products, such as Cs, Nb, Sn, Se are not considered at a large extent?

2 What about instant release of iodine once water gets into contact with the SF?

Detailed comments and questions

3-2 For the base case, alloy 625 is used for the inner overpack, and carbon steel for the outer overpack. In the conceptual model described in volume 1, reference is done to pitting, but with those 2 materials, is there any analysis of the risk for galvanic coupling, and faster consumption of the carbon steel overpack after it started to fail?

3-2 J-13 wall water chemistry is used for dissolution of SF. How relevant is it to consider this water, while just infiltrated rain is supposed to reach the waste package?

3-4 In the flowthrough alternative, does the Fmult value simulates solubility limited contaminant release by limiting direct solubility of spent fuel (intrinsic as defined in volume I), or is there a solubilization step followed by reprecipitation of a more stable phase, in which case depending on the phases, some contaminants can be released.

3-4 Flowthrough with higher fuel dissolution: what is the signification of the J-13 water for SF dissolution? How much is it relevant to consider an increase in carbonate? What is its effect? What is the full set of data for this alternative? Is it relevant to consider a reduction in silicate, whereas J-13 silica content is quite low, close to equilibrium with chalcedony, and that if we consider a just infiltrated rain, it can reach a very fast equilibrium with amorphous silica, at higher dissolved silica values?

3-4 Natural analog: does the process consist in a congruent dissolution of U from the SF, or is there a non congruent dissolution, or a 2 steps process (with dissolution and then reprecipitation of secondary more stable minerals, and release of some of the fission products)?

3-5 Immediate WP failure: all assumptions in WP failure are that failure occurs by the top of the canister. But as mentioned from volume I, there is also a possibility to have droplets flowing to the bottom of the canister and reacting (corroding) the lowest point. In such a case, if there is a short cut between top and bottom, release occurs immediately, by leaching, but probably with small amount of radionuclides released.
Isn't there an instant release for some radionuclides, once the WP fails?

3-8 It would be interesting to measure the contribution to the TEDE peak of the main radionuclides in each of the cases.

3-17 "radionuclides providing the majority of dose are probably release rate limited" for the alternative conceptual model where infiltrating water is focused to one quarter of the WPs. Needs to be explained.

4-11 At 10kyr, the use of C-22 makes the WP unsensitive to Chloride and to OO-Coflc. However, new critical parameters appear like WPDef% and those related to pumping at 20km and retardation (ARDSAV).
But this has to be weighted by the fact that the TEDE peak is lower by a factor of 40 between the base case and the C-22 case (table 3-2 in page 3-8). Thus erasing effects from the major phenomena or processes contributing to the TEDE by the use of a more robust device will shift down the ranking.
Transport related parameters become important at 50kyr.

5-2 Some of the parameters listed in table 5-2 can be found in the appendix, but where not recorded in chapter 4. Are they so important for uncertainty or sensitivity?
InnOvrEI was not recorded and is not defined
SSMOHeF did not appear previously
InitRSFP did not appear previously

5-3 For 10kyr and alloy 625, the peak TEDE resulting from the volcanism scenario class is comparable to the nominal case, after being weighted by its probability. What is the significance and validity of such an approach? Saying that it's the same, it's a good opportunity to loose confidence.
Volcanism occurs or not. In the case it occurs, its consequences cannot be weighted by anything. There must be a class of consequences for the nominal case, and classes of consequences for the volcanism scenario, depending when the event occurs.

6-1 Conclusions given for the analysis are fully supported.

A-4 The RT and RDTME KTIs did not conduct process-level sensitivity analyses because they were not funded to do so. Does that mean that the concept is robust enough to do not suffer a sensitivity study?

A-7 Spent fuel dissolution:
Matrix dissolution is derived from dissolution rate experiments, in pure carbonate solutions. What is the signification of this approach, is it conservative, by how much, and of what is it representative?
. Does the J-13 water have a stable chemical composition? Was the process of its chemical regulation understood? Is it at equilibrium with the rock matrix?
. Are analog studies or drip tests representative of the spent fuel dissolution? To what extent, what are the limitations?

A-10 Dissolution rates did result in peak TEDEs similar to those calculated for J-13 water, for dissolution rates 100 times less than the default value. What are the conclusions of this? Are the dissolution tests representative of the involved processes, are the main parameters known, is the J-13 water the good representative?

A-10 Redistribution of infiltrating flux: why are the differences in sensitivity attributed to solubility limited radionuclides dominating the peak TEDE for the TPI at 5 km and release-rate limited radionuclides controlling the peak TEDE for the TPI at 20 km?

Is this justified by a change of process along the time (but this was not recorded previously in the documents)? Is it because high flow rates on the SF have been assumed for the 5 km case, and lower flow rates on the SF for the 20 km case?

Needs explanation.

A-11 What is the stability of the secondary precipitating CHS compared to that of the primary CHS , which dissolves?

A-12 The balance between transport into the fractures and into the matrix needs further comments, as it is not really clear to me.

A-14 How do you justify the assumption that a release rate for each individual radionuclide to be equal to the oxidation rate of SF?

A-16 Comments from ENFE Process-Level Analyses:

TPA works more like a simplified representation of the total system , than like a mechanisms or phenomenology based model. Thus its limits can be overcome by implementing processes via a transfer function approach, which advantage will be to keep a clear and easy analytical tool, as it appears now. This approach assumes to have a 2 stages analysis, the first being at the phenomenological level (process level), in order to determine those parameters which will have to be analyzed in the second stage with the TPA code.

The other alternative is to fully couple phenomenological models to TPA, but analyses may become more difficult, and this can result in a loss of transparency.

A-17 "Short duration events result in a more concentrated ash deposit at 5 km. Longer-lived and larger eruptions dilute the dispersed inventory over a large area". Is it correct to take account of a fixed same amount of inventory released for both cases?

A-19 Faulting is not a significant WP failure mechanism. This result is given by the sensitivity analysis, but as for seismicity or volcanism, does it have to be matched to the physical properties of the WP system?

APPENDIX 2

Statement of work
Scope of the review

Goals of the external review

Examine the methods and assumptions embedded in the TPA Version 3.2 code ;
Most of the comments given in the report directly concern methods and assumptions embedded in the TPA Version 3.2 Code.

Recommend improvements ;
Two series of improvement lines have been issued from the present review:

- Define a clear chemical pathway for the water composition
- Maintain the independence between the analysis and the approach used to determine input data like initial inventory or FEPs

Another recommendation is made about documentation and traceability, with a need to present, explain and develop methodologies for the different choices, as for example for scenario generation.

Evaluate implementation of conceptual models, including the approach for treating parameters (i.e., lumped parameters) ;
Implementation of conceptual models is carried out using different approaches which are very well explained, and which appear well supported by good science. When abstracted models are used, assumptions and conservatism give rise to very precise discussions. Most of the comments deal with presentation and explanation of methodologies, maybe with a requirement for explanatory flow-charts.

Determine whether the NRC approach to TPA is suitable for achieving its objectives of reviewing the DOE license application and TSPA.
The NRC approach is suitable for achieving its objectives of reviewing the DOE license application and TSPA. Organization and QA accompanying the modeling process is in adequacy with the high level of requirement. However, reviewing a license application or assessing an approach would benefit from independent approaches and analyses. Specially in case of input data such as those mentioned above (inventory or FEPs), it will be useful to have its own approach.

Questions to consider includes

Is the TPA code suitably flexible and sufficiently complete ?
Flexibility of the TPA code is one of its intrinsic characteristics. Experience as illustrated from analysis performed with TPA 3.14, or with the present guide for TPA 3.2 and related illustrations confirm this flexibility, and capability to take account of various processes or situations, either through direct subroutines or through abstractions.
Are the included features, events, and processes sufficient to provide credible results and meaningful insights ?
Included features, events and processes seem sufficient to provide credible results and meaningful insights. However there are important differences in the level of detail among modules describing and analyzing the various processes. Another point which has been noticed, is that the set of FEPs to be used, and the scenarios to be analyzed must be generated in an independent way, with an own explained methodology.

Are the conceptual model abstractions defensible ?

Grounds for conceptual model abstractions are very strong, and can be defensible. However, abstractions need an involvement in the details of the processes and in the method used to understand what happened between a detailed model and its results through adjustment of a single parameter. Most important is to clearly show the process of abstraction, and have a clearly described methodology.

Are the conceptual model abstractions appropriate for the spatial and temporal scales being considered and for the selected performance measure ?
Most of the reviewed model abstractions appear appropriate for the spatial and temporal scales being considered and for the selected performance measurements. Nevertheless, there are certain incoherence in the time scale of the different processes, the reasons for which do not appear very clearly in the presentation, as this has been reported for the thermal phase.

Are the model abstractions sufficiently supported by site data or other related information to ensure the credibility of the results ?
Credibility of the results is a point of weakness, which can only really be overcome with some field data (water composition in the UZ for example) or with some laboratory scale tests (dripping for example). Those type of data, by giving some realism in the range of considered values, will strengthen confidence.

Is the documentation sufficient to provide an understanding of the approach ?
Documentation is very rich and provides an understanding of the approach when read in detail. Some very simple flow-charts would be helpful in facilitating understanding of approaches.

Is the level of conservatism and simplicity of approach appropriate considering the role of NRC ?
Considering the role of NRC, some over-conservatism is required. However in some cases, the level of over-conservatism is so far from reality that in my opinion it reduces confidence. A better knowledge will help focusing the range for some parameters, specially for water interacting with materials, and determination of radionuclide release.

Are the methods used to develop abstracted models and their associated parameters reasonable ?
Methods used to develop abstracted models and their associated parameters look reasonable, and have been very well explained during ERG meeting. Such a level of presentation would also be useful in the documentation of TPA 3.2.

Are the parameters used in TPA Version 3.2 code appropriate to the abstractions ?
Parameters used in TPA Version 3.2 code abstractions reviewed have been derived from well described processes, and thus are appropriate.

Are uncertainties in model abstractions and parameter values reasonably accounted for by the alternative conceptual models and parameter distributions provided in the code ?
Uncertainties in model abstractions and parameter values are well accounted for by the alternative conceptual models and parameter distributions, as illustrated by the very impressive work analysis in volume II, based on TPA 3.1.4.

What are the strengths and weaknesses of the TPA Version 3.2 code as a tool in supporting NRC's licensing decision ?
Strengths of the TPA Version 3.2 Code are its flexibility, and its capability to take into account in a very simple way many different processes and situations. Another strength is the organization implemented for development of TPA, with a very strong scientific support.
Among weaknesses, the main one would be a lack of a clear presentation for certain specific methodologies. A few simple logical flow-charts would be useful to understand links between sophisticated models and parameters as extracted for abstractions.

What improvements to the code would the members of the External Review Group recommend, taking into consideration the intended application of the code to support NRC's licensing decision ?

Main improvements are in documentation, traceability, and presentation of methodologies. Supporting science is good enough in most cases, but could use improvement in certain others. Very large over-conservatism is not always a factor increasing credibility and confidence. Introducing more realism in defining over-conservatism would be recommended.

APPENDIX F

REPORT OF BRIAN THOMPSON

External Review of
Total System Performance Assessment (TPA) Version 3.2 Code:

Module Descriptions and User's Guide,
CNWRA
San Antonio, Texas.

Predecisional - September 1998

And related Sensitivity Analysis applications
Documented in NUREG-1668, Vol.2 (unpublished) October 1998.

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1. SUMMARY

The NRC are the leading practitioners of independent regulatory performance assessment, centred on Monte Carlo simulation to account for the uncertainty inherent in long term forecasting over the 10,000 years (or longer) postclosure period. Staff credibility during the Licence Application Review for Yucca Mountain is deserved through the considerable 'hands on' experience of developing and applying TPA versions jointly with CNWRA. Unfortunately, this story could not be told effectively in the documents submitted formally by CNWRA for review and the **priority** now is to produce a comprehensive, structured, set of documents covering the entire Yucca Mountain assessment programme, the process of assessment and review, and also the suite of software, comprising the assessment 'toolkit' that supports TPA. A 'Knowledge Management' system to coordinate all data, models, simulations etc..., together with records of decisions, assumptions and omissions that led to a particular PA result, should be implemented. This system must support intelligently the production of the documents in different styles and detail appropriate to the various stakeholders concerned about PA and regulation of Yucca Mountain.

If the results of the sensitivity studies reviewed are taken at face value, extensive enhancement of TPA seems unnecessary if 10CFR63 recommendations are adopted, but, should the time period of interest be extended beyond about 100,000 years (say), then considerable further development is likely to be needed.

2. INTRODUCTION

The stated objective of the External Peer Review is to provide a 'formal, independent evaluation and critique of the Total Performance Assessment (TPA) Version 3.2 code for the NRC '.

Following an initial familiarisation period to develop questions for NRC and CNWRA staff beforehand, the External Review Group (ERG) attended a meeting at CNWRA during 26-29 July 1999 to consider relevant aspects of the TPA code and its regulatory context.

There are eight members of the ERG and the present reviewer was nominated to consider 'Overall Performance Assessment'.

The specialist members of ERG considered primarily the following aspects:

- **flexibility** of TPA code;
- **completeness** of the TPA system representation;
- **defensibility** of the model abstractions;
- clarity of **documentation** for intended users;
- treatment of **uncertainty** throughout, and the
- appropriateness of TPA approach to NRC role in reviewing the DOE(YM) licence application.

The scope of work for the present reviewer is less clear and has been assumed to require not just consideration of technical detail of a particular version of a particular TPA code but also (and it is judged more important) to consider its setting within the entire process of NRC licensing and PA, especially in the need to ensure credibility and trust in the minds of a wide variety of stakeholders and their technical representatives.

NRC have committed themselves to a fully independent, integrated, performance assessment capability at level (iv), see Thompson (1999). Their explicit account of uncertainty using, primarily, probabilistic methods is required in existing regulations and in their proposed new rule 10CFR63, NRC (1999), for Yucca Mountain. The two documents for review and especially the presentations during the Review Meeting, confirmed the very favourable opinion of staff commitment and capability in PA that this reviewer had from exposure to their work at OECD Nuclear Energy Agency (NEA) Committee Meetings and through the published literature since about 1986.

However, the documents for formal review do not and cannot by themselves explain the NRC work to an audience outside the Yucca Mountain programme, nor do the bulk of the unstructured mass of potentially supporting references which, in the time available, were only possible to consult superficially. Appeal to the summary volumes (Vols. 1, 3 and Chapters 4+ of Vol. 4) of the DOE Viability Assessment, DOE (1998), revealed some of the task facing TPA. Despite their elegant style and graphical presentation even these documents failed to make it clear at an early stage how specific aspects of the work, for instance the development of an abstracted model from sources, could be traced. The two NRC reports for formal review would form only a small part of the structured set of documents that are required to explain the YM programme from their standpoint. The beginning of each constituent report should explain visually its place in this structure. As NRC staff may be required, under oath, to present their work in 'discovery' sessions well before the formal License Application (LA) hearings in 2005, Reamer (1995), better communication of their work should be the priority.

Congestion of milestones in the DOE programme just before submission of their TPSA-LA, see Fig.7.2 of Vol.4, DOE (1998) raises fears that much of the three years for NRC review may be eroded by responding to many updates, especially as much hydrogeological information downstream of Yucca Mountain has still to be collected and analysed, Bell (1998a) for instance.

The second major concern underlying this review is the absence of clearly defined site-specific standards and regulations for Yucca Mountain. As will be seen, this could have a major effect on future work related to TPA. Subject humbly to the deliberations of the other members of the Expert Review Group, it is suggested that the results from the sensitivity studies using TPA, notwithstanding honourable caveats by the authors, show that little further work is needed for TPA if the 10,000 year period is confirmed but that a very different conclusion may be reached if this were to exceed about 100,000 years to judge from performance estimates from TSPA-VA, Bailey et al (1999), especially when 'defence in depth' is considered through barrier degradation studies.

3. COMMENTS UPON SELECTED ISSUES

3.1 System representation and completeness

The reasons for including the present combination of features, events and processes in the TPA system model are not stated nor the procedure followed to decide what should be left out. Therefore, it is not possible to be sure that the representation is sufficiently comprehensive for purpose. Indeed there are many potential interactions between processes that appear to be shrewdly omitted to give an economic computational approximation for Monte Carlo simulation over a 10,000 year time period of interest. For example,

(a) There is no link, at present, between faulting, seismics and volcanism, or indeed between these phenomena and the regional groundwater system

(b) The effect of climate change upon the regional groundwater system is ignored but not justified.

(c) There is no coupling between the volcanic deposits and soil characteristics for the groundwater exposure pathway.

(d) There appears to be no overall mass or activity balance maintained throughout the entire system.

Thompson (1999) cautions against oversimplification in PA modelling, from experience in two UK regulatory assessments.

3.2 Model abstraction and justification

3.2.1 Traceability and transparency

The TPA 3.2 User Guide provides exemplary descriptions of each of the abstracted models and their links to the remainder of the system, as implemented. The clear listing of assumptions and limitations at the end of each description is particularly appreciated. The three methods of abstraction outlined in Section 3.1 are all acceptable, in principle, but it is impossible to say from the present documentation if they have resulted in sufficiently precise approximations to observation and/or the results of calculations at a more detailed level. Evidence of quantitative verification/calibration is required, under conditions that lead to the higher dose realisations in TPA simulations, rather than for realisations based upon expected values of the independent variables.

In order to independently reproduce the models (and their associated data) from fundamental source information the entire chain of reasoning needs to be recorded, together with the uncertainties and biases accumulated at each stage, and the evidence used, for instance in expert elicitations. See Thompson and Williams (1997), for example. Such a record typically may be distributed over several supporting documents and a 'roadmap' diagram, see Sumerling (1992), provided in each section of Chapter 4 would then enable the reader to recover the abstraction process. Appealing to a Bibliography indexed solely by author's names is inadequate and does not satisfy fundamental requirements of traceability or transparency. NRC so far have not, it seems, achieved the justifiably high standards that they apply to DOE, Bell (1998b), in their own PA documentation.

3.2.2 Checking model abstraction by high risk reanalysis

An important, but not well rehearsed, stage in the HMIP assessment procedure, see Thompson and Sagar (1993), for instance, was termed 'high risk reanalysis'.

Realisations found to contribute most of the high doses at the time of greatest risk were to be examined to find the associated parameter subranges and important subsystems. Then the calibration/derivation or, in NRC terminology, 'abstraction' of the PA submodels concerned were re-examined to see if they were satisfactory. If not, recalibration would be carried out and those realisations recalculated. If substantial differences in results were found the entire simulation should be repeated.

Critical review of the arguments in TPA documents and supporting literature may reveal shortcomings in simplified models, but the ultimate judgement must result from quantitative reanalysis, as above. Such 'error' or 'bias' analysis should be documented to provide confidence in the modules of TPA and hence give a better idea of their domain of applicability.

3.3 The NRC Reference Dataset

Appendix A of the TPA 3.2 User Guide comprises an admirably comprehensive and explicit tabulation of the input values and probability density functions (pdf's) that can be used as a starting point for PA simulations and as a basis for training material for new users of the code. For a real application to licensing, however, the extensive and honest comments show that at least 230 of the approximately 830 items listed seem not to be justified by a clear, traceable, record back to reliable sources.

Many observations may be made on this Appendix, such as:

(1) The need to distinguish clearly where proponent's data and assumptions are adopted and if these have been done only after independent review? Data from design studies and site specific investigations, including the ESF, should be highlighted, as opposed to information from other sites or of a general nature.

(2) When data or judgements are 'expected' or are to be further 'evaluated', the references to explicit work packages in NRC or DOE(YM) forward programmes should be given.

(3) Have the items 'assumed' as quoted in the references been independently reviewed and justified or are they open to further challenge because they may not be traceable to relevant sources?

(4) Many 'constants' could misrepresent the true level of uncertainty. Elicitation of Maximum Entropy pdf's over ranges bounded by physical fundamentals (say) would be much better.

(5) Unbounded Gaussian pdf's are unjustified surely as the truncation is open to endless discussion.

(6) Many references to Appendix A could also be in the main list as surely the decisions and justification for the models and dataset go together?

(7) Some confusion over terms e.g. how can a 'best estimate' also be a 'conservative' value?

(8) Biosphere data could not be found for any climate state applicable to the critical group behaviour for the groundwater pathways compatible with the extensive (e.g. soil) data listed for the volcanic pathway.

(9) Much is made of correlations - but in hardly anywhere are they to be found or elicited (especially if not multivariate Normal?) Comments, elsewhere, indicate they may not matter, anyway?

3.4 Uncertainty

3.4.1 Model uncertainty

There are within TPA 3.2 several excellent examples of the employment of different interpretations of the same underlying information. These interpretations are called 'alternative' (or, incorrectly, 'alternate') conceptual models' and are used to explore uncertainty about the physical understanding of processes. In NUREG 1668 and in the presentations during the Review Meeting, results from many PA simulations or single realisations were used to examine the implications of this current uncertainty. Results should, however, **not** be combined using 'degree of belief' probability weights on these models, and this temptation largely seems to be avoided in the NRC programme.

3.4.2 Parameter uncertainty

For each such simulation system representation, the essence of TPA is to reveal uncertainty about possible performance, radiologically, that results from uncertainty over the appropriate values to use for the large number of independent variables defining the problem. The Monte Carlo method is, at present, the only satisfactory means of tackling this problem and is applied to a very high standard in the NRC/CNWRA programme. Nevertheless, a few comments are appropriate:

(1) Uncertainty is not well expressed by point estimators such as means, medians, etc... but rather by showing how the percentiles of dose, and other output of interest, vary over time and depend upon assumptions. Comparisons of design options (as in NUREG 1668) could be compromised by not showing (say) the 95 to 5 percentile range as well as sample estimates of the mean.

(2) Displaying only indications of high doses does not give a balanced 'reasonable' account of estimated behaviour when a large proportion of realisations show values that are much lower than regulatory limits and may satisfy targets for acceptable or negligible levels of risk.

(3) Uncertainty needs to be logically and defensibly determined at the level of basic information from site studies, design and research in terms of scales appropriate to the quantities concerned. Then it needs to be translated into estimates for the various modelling levels of detail, used as the assessment proceeds, ending in the pdf's and bias evaluation for the aggregated quantities used in TPA models. This reasoning, including questions posed to elicitation groups operating at a system or at a process level, was not readily apparent from information supplied.

(4) The range of pdf's given in TPA 3.2 Section 3 looks admirably comprehensive and the inclusion of triangular and log triangular shapes is a good feature.

3.4.3 Statistical sampling

Before attending the ERG Meeting at CNWRA, this reviewer had many doubts over the use of Latin Hypercube Sampling (LHS) and the apparent lack of attention throughout the NRC programme to establishing statistical convergence and showing explicit confidence limits on their results. Much work was published under the UK regulatory research programme between 1984 and 1993 regarding the use of Importance Sampling and the estimation of sample precision. This was followed up in the Nirex work related to the Sellafield site. Doubts were expressed, for instance by Sinclair and Robinson (1990), about the inability to estimate sample precision when using LHS and to combine LHS samples, for instance. However, further reading reveals that the WIPP CCA analyses overcame these limitations, Helton (1998), as also apparently did an aborted CNWRA study in 1995? Importance Sampling was clearly shown to have considerably greater efficiency than either random or LHS sampling and should be considered seriously for the NRC programme in future developments of TPA. The ERG Meeting was reassured by accounts, not yet published, of the influence of sample size upon TPA results. Without confidence intervals on results, such as those in NUREG 1668, however, the conclusions from sensitivity analysis, and the comparison of different PA, cannot be entirely credible.

3.5 Understanding the results from TPA - Sensitivity analysis

There is considerable emphasis in the Yucca Mountain programme upon the use both by NRC and by DOE of sensitivity analysis to:

(1) understand and reduce uncertainty and,
(2) to find out what determines the estimated performance of the repository system

This, in turn, is expected to guide further research, site investigation and design changes in a cost efficient manner and to provide a basis, through the issue resolution process, for NRC to probe DOE's arguments in preparation for the LA Review, for example.

The studies reported in NUREG 1668, using TPA versions 3.1.3 and 3.1.4 and in the subsequent analyses of TPA 3.2 results described by Codell during the Review Meeting, demonstrate the application of an impressive range of techniques including new ones developed recently by CNWRA. This NRC work appears to be considerably more comprehensive than that in the TSPA-VA.

Such techniques have not been used directly by this reviewer but the following comments seem appropriate:

(1) Comparing overall performance from full simulations each with different engineering (controllable) design decisions (backfill, cladding, choice of alloys etc...) is very informative (see Fig 3.2 NUREG 1668). The results purport to show directly that risk levels of about 2×10^{-5} p.a. from the base case or up to 7×10^{-5} p.a. from degraded cases (no retardation) can be reduced to between 10^{-6} p.a. and 10^{-5} p.a. This is a very neat demonstration of the approach to satisfy 'best practical means' requirements and the 'Tolerability of Risk' principles widely adopted in the regulation of UK industry as well as in radioactive waste management and, although expressed differently, seems implied in 10CFR63 Statement of Consideration III(4) and 63.21(c)(7) but without economic considerations.

(2) As presented, the use of different code versions and calculations for different possible regulatory decision variables (mean peak dose over time in NUREG 1668 and peak mean dose at time, using TPA 3.2) makes the practical implications of the results difficult to understand at short acquaintance, as does the overwhelming use of YM programme specific acronyms, jargon and TPA specific variable identifiers, instead of plain English descriptions.

(3) Sophisticated statistical methods appear broadly to support the general conclusions reached in this study but they appear to this reviewer to rely upon non-intuitive assumptions of monotonicity and Normality. They seem to have been overruled by engineering *ceteris paribus* methods when planning future DOE work, see page 6.13, Vol.3, TSPA-VA, for instance They seem to obscure physical interpretation especially if applied to all variables of the problem at once. For example, may it not be better to consider one nuclide chain at a time except where elemental solubility (say) determines behaviour? Very few nuclides seem significant for the groundwater exposure pathway

from Figs 4.13, 4.14 in NUREG 1668, for instance. Smith (1993) recommended the HMIP regulatory assessments programme turn to interactive graphical methods of directly exploring multi-dimensional scattered data.

(4) The use of non-distributional techniques such as Kolmogorov-Smirnoff or the Sign Test may be more robust in practice. Seigel (1956), however, states the latter is for 'related samples' whilst K-S is for 'independent samples'. Does this affect applicability of either to the present problem?

(5) The 'process level' studies outlined in Appendix A of NUREG 1668 are interesting but not, it appears, reported yet in sufficient detail for real understanding by independent readers. It is frequently difficult to see how the models used differ from those in TPA systems studies themselves.

(6) Elicitation of pdf ranges and shapes may not achieve confident consensus. The implications of differing opinions about inputs to PA should be explored.

3.6 Conservatism and risk 'dilution'

Appeal to 'conservative' assumptions and approximations is made frequently in the TPA 3.2 User Guide and, indeed, throughout the Yucca Mountain literature both in the NRC and the DOE programmes. If, indeed, this bias can be evaluated to confirm that all such assumptions are consistently pessimistic on overall performance then, from the results shown to date, there seems little need for much further development of TPA if the time of interest remains as proposed in 10CFR63. Should, however, the period be extended substantially, this conclusion may not be true and is in any case subject to the detailed opinions of others in the Expert Review Group.

Overuse of bounding or conservative reasoning can be a serious concern if it leads to estimates for mean values that are so biased that they nullify the entire logic of a risk-informed simulation approach using Monte Carlo sampling to account for uncertainty. 'Worst cases' have been shown many years ago, as explained in Thompson and Sagar (1993), to lie typically orders of magnitude above the expected performance.

If applied inconsistently, 'conservatism' could significantly change the results of comparisons between different PA that might be related, for instance, to different engineering options.

3.6.1 Risk 'dilution'

Concern is often expressed over possible underestimation of risk if the range of uncertainty is increased due, for example, to cautious judgements by experts in the absence of desired levels of information. However, it can be readily shown for uniform pdf's with the same arithmetic mean values of dose (H), that, if $H \alpha x^n$, the increase in uncertainty (range of x) causes a **rise** in estimated mean risk, if $n > 1$. Only if $0 < n < 1$ does risk fall and, for linear dependency, the risk does not change.

Hence, judgements during probability elicitations should **not** be swayed by concerns over so-called 'dilution' effects on risk. Consistently conservative assumptions can only be achieved, if that is what is desired (see, for instance, page 2.39, Vol.3, TPSA-VA DOE (1998)), if the response of dose to variations in the value of each parameter is understood.

3.7 Computer software issues and Quality Assurance

No formal scrutiny of QA or of software standards was intended during this Review, but the initial concerns of this reviewer were allayed in a satisfactory manner during the ERG Meeting and from an initial examination of the TOP-18 document, CNWRA (1998). Quality procedures appear to be of a high standard and applied properly in the development and use of PA software. This message does not come across from the TPA 3.2 User Guide, however.

The assessment 'Toolkit' needs to be explained clearly and not only from the analyst point of view, but also from a software engineering standpoint. A full structured documentation system seems invisible as yet (from the material supplied) and should be stated well in advance of licensing reviews.

The TPA design seems to enable ready changes/additions of submodels and different loop structures, nesting etc...? This is essential if the desired **flexibility** of operation is to be achieved.

The TPA manual and all related documents should show the document structure and give references to standards etc. separately from general scientific references. Data flows could be illustrated graphically and could, in principle, be obtained from CASE tools. Configuration management is understood to apply to everything consistently, including:

- Program versions
- Simulation cases
- Data sets,
- Control files, and
- Output files and post processing results, all co-ordinated and recorded to avoid mismatches etc... and, of course, all
- Related documentation.

During a stage of rapid product development it is difficult to ensure consistent documentation of all aspects but it is somewhat disturbing that no documentation was referenced for the following TPA Modules:

UZFLOW, NFENV, EBSFAIL, EBSREL (are these in EBSPAC?), UZFT, SEISMO, VOLCANO, ASHPLUMO, ASHRMOVO (are these in ASHPLUME?), DCAGW, DCAGS.

4. STRENGTHS OF TPA

S.1 The approach by NRC to develop and apply the TPA total system modelling, with variants, and employing Monte Carlo simulation to account for uncertainty, is entirely **appropriate** to their requirements for LA review of Yucca Mountain.

S.2 TPA capability seems shrewdly matched to the NRC proposed regulations, expressed in 10CFR63, in practice.

S.3 Since the implementation of the EXEC framework code, application of TPA versions 3.1.3, 3.1.4, in NUREG 1668, and 3.2 in the Codell ERG presentation, show that TPA is extremely **flexible** in enabling NRC staff to incorporate different hypotheses about thermal reflux, waste dissolution, etc..., and also to analyse and compare the effects of different design options from DOE.

S.4 TPA is an assessment tool that acts as a successful focus for multidisciplinary teamwork by NRC and CNWRA personnel and is an excellent basis for probing DOE's arguments through the support to the various KTI's that it provides. Indeed, in the absence of well established process level detailed models, it has been found possible to innovate within TPA directly, according to remarks at the ERG Meeting.

S.5 The active participation by **NRC staff** at all stages of design, development and application of TPA, is strong proof of their professional competence in the regulatory application of PA and, if maintained, should enable them to be entirely **credible** as witnesses at the LA Review Hearings and in prior 'discovery' sessions.

S.6 The TPA User Guide is well written for NRC staff and its contractors; especially good is the clear statement of assumptions and limitations for the component models and the clear tabulation of the NRC Reference Dataset in Appendix A.

S.7 NRC/CNWRA are to be congratulated upon the application, explained in NUREG 1668, Vol.II and further by Codell at the ERG, of a range of sensitivity analysis techniques that is much wider than in TSPA-VA. These methods should be incorporated into a suite of post-processing tools for TPA and their application exposed to open literature review within a specialist applied statistics journal.

S.8 As presented at the Review Meeting (but not in the TPA documentation) the treatment of infrequent random events, such as volcanic eruptions, appears to be an ingenious means of overcoming problems with sampling convergence that would otherwise be encountered by LHS or random sampling methods. This approach works well for the 10,000 years time period of interest.

S.9 The range of pdf's offered to the TPA user is extensive and the inclusion of triangular and log-triangular forms as well as Maximum Entropy distributions is admirable.

S.10 The processes and subsystems comprising the TPA 3.2 system model seem broadly appropriate to10CFR63 requirements except for future human intrusion which has not yet been included.

S.11 The User Guide provides a very clear and comprehensive account of the many input and output files required to perform a full performance assessment.

5. WEAKNESSES OF TPA (for each strength S(n) listed above)

W.1 The approach is documented inadequately for those outside the long established Yucca Mountain programme that inevitably has acquired its own language. The TPA User Guide is only one of a structured set of documents that are required to perform this function if NRC are to obtain full acknowledgement for their efforts and be credible in public.

W.2 EPA may decide to introduce standards that require substantial changes to 10CFR63. The present simplifications in TPA 3.2 might no longer be adequate for much longer time periods of interest, or for different treatments of critical group behaviour and/or for different definitions of risk (say).

W.3 There is no clear reference to EXEC in the User Guide and there appears to be no separate document showing how best to design and implement new modules for incorporation into TPA. It is not clear if EXEC permits loops in the call sequence of modules.

W.4 The KTI for TSPAI makes strength S.4 clear but the details of how much of this promise will be fulfilled are not obvious because no procedure is set out yet by NRC for the use of one performance assessment to review another performance assessment. See the proposed method of 'compatible bias evaluation' in Thompson (1999), to be published.

W.5 This is fragile as it depends upon experienced staff still being available in 2005! NRC need to give priority to fully documenting their entire assessment toolkit, how it will be used and how it is justified under uncertainty, etc. ... as recommended below.

W.6 However, the justification quantitatively for these model abstractions and the reference data is not clear as written and requires the new documents to provide traceable, transparent and defensible support for each module, as recommended below. This should be done in combination with the aggregation of data and compatible accounting of uncertainty.

W.7 As NRC are most interested in parameter subspaces yielding the high dose realisations, analysis should be more focussed there, if necessary ensuring statistical convergence of PA by using Importance Sampling. NUREG 1668 needs rewriting **in plain language** for deserved recognition in the wider literature, and TPA 3.2 results could beneficially replace those concerned with mean peak doses.
No attempt seems to have been made to explore the sensitivity of the results to the shape and range of parameter pdf's. This can be done, in principle, by reweighting realisations without repeating the simulation.

W.8 Substantially longer time periods of interest will require consideration of futures with two or more volcanic events and somewhat larger seismic magnitudes. The complexity of the sampling scheme explained during the ERG Meeting may then approach that of the WIPP CCA, Helton (1998).

W.9 At present the emphasis on Latin Hypercube Sampling overlooks much useful work on sampling convergence and the estimation of sample precision in the United Kingdom programme. LHS is not seen as an **independent** approach to that used by DOE. There seems to be some dispute in the literature concerning the ability to combine samples using LHS, and to provide confidence bounds, although these limitations seem to have been successfully overcome in the WIPP CCA.

W.10 The TPA system representation is a subset of all possible processes and interactions etc... that might be considered at the conceptual level for Yucca Mountain. Nowhere is this process of conceptualisation and reduction described and justified, whether using FEP analysis or by some other method. There is no visualisation of the results of this process, for instance using influence diagrams as in the regulatory assessments undertaken in Sweden, SITE'94, SKI (1996), and in the UK, Dry Run 3, Thorne (1993) At present many potential interactions between subsystems are omitted from the TPA 3.2 system, without explicit justification, despite earlier reported studies within the NRC programme.

W.11 The present implementation of TPA seems somewhat dated and the user interface requires too much knowledge about and interest in FORTRAN and in file handling from the user, who should be allowed to concentrate upon the regulatory tasks without distraction of computing considerations. There is a confusion between 'Auxiliary Codes and 'Auxiliary Files', which are unrelated. There is no general purpose Post-Processing Module as seems standard for other PA codes. The sensitivity analysis techniques adopted by NRC could usefully be described in Chapter 8 of the TPA User Guide.

W.12 'Conservatism' is claimed but not demonstrated for the assumptions underlying many models, data values and distributions. No formal decision logic records seem to have been kept nor is the subsequent evaluation of cumulative bias undertaken as proposed under the HMIP programme, Thompson and Williams (1997) for instance.

6. RECOMMENDATIONS

R.1 **Appropriateness:** In order to achieve a fully appropriate TPA capability for NRC the weaknesses W.2, 4, 9, 10 and 11 must be overcome satisfactorily before the Licence Application is received.

R.2 **Flexibility:** TPA should be further developed to overcome weaknesses W.2, 3 and 8.

R.3 **Completeness:** Formal elicitation and documentation of all steps from raw data and FEP catalogues, for instance, to the conceptual model of the integrated system used in TPA is needed to resolve weakness W.10. Model + data + uncertainty must be handled at each stage in a comprehensive and compatible manner to overcome weakness W.6.

R.4 **Defensibility:** Similar concerns may be expressed as with recommendation R.3 in order to overcome weaknesses W.10 and W.6 but, also, **conservatism** needs to be evaluated by a **bias evaluation procedure** at all stages of model development to resolve W.12. If consistent levels of conservatism are not achieved, comparisons between performance assessments may be misleading and the present data and results using TPA 3.2 should be evaluated to see if significant further development is really necessary to meet 10CFR 63 requirements.

R.5 **Uncertainty:** Further examination of sampling methods and of statistical convergence is required to resolve W.8 and W.9. Fears of risk 'dilution' seem mistaken but could be re-examined in more detail by NRC if conservatism is an issue during elicitation and this should reduce concern W.12.
Further sensitivity studies might usefully explore the influence of uncertainty over such pdf elicitation to see if W.7 is a significant concern, in practice, for Yucca Mountain.

R.6 **Documentation:** Inadequate documentation results in the many weaknesses W.1, 3, 4, 5, 6 & 7 outlined above, and is a major impediment to wider NRC credibility in PA. Fundamental requirements of **traceability** and **transparency** must be met in all aspects of PA related work by the NRC and its contractors, as they themselves rightly insist upon when dealing with DOE.

An initial structure is suggested in the closing section, below, together with some thoughts on the provision of a computer-based knowledge management system to handle information relevant to performance assessment and to provide intelligent support for the production of documentation in different forms and levels of detail suited to the needs of a range of stakeholders concerned over that aspect of licensing at Yucca Mountain.

If such a system is not already being set up by NRC then the most important recommendation that results from the present review is that NRC management should have the courage to pause the apparently continual process of PA development and refinement in order to consolidate a well defined release of TPA and all related assessment tools, techniques and datasets. Then to spend substantial time and resources designing and implementing this support system and all the resulting linked documentation in order to reveal the strength of their achievements to the scientific and technical world beyond the Yucca Mountain programme.

Such work will take time to complete through prototyping with end users so, in the interim, the short term requirement is to complete the review of the Viability Assessment and at least to complete a clear documented release of TPA 4.0 with the corrections and improvements recommended by the Expert Review Group that are related to current scope and assumptions. Then the longer term developments of the full system should be completed at least 6 months before the LA arrives.

7. AN OUTLINE DOCUMENTATION SCHEME AND KNOWLEDGE MANAGEMENT SUPPORT SYSTEM FOR PA

Documentation related to integrated PA can be thought of as representing an **information matrix** that can be described in two principal ways; see Thompson, Wakerley and Sumerling (1993):

(1) **'longitudinal'** reporting that shows the sequence of events, decisions and associated evidence from initial data through to the end product as a model (say) of a particular part of the problem (repository system and its environmental setting). Hence traceability is achieved, in principle at least, for a given subproblem which, however, may in general involve more than one discipline.

(2) **'lateral'** documentation that shows how, at a particular stage of the above process, the different subsystems/subproblems areas were integrated together in a comprehensive, consistent and explicit way to describe to the extent practical the entire system at some level of interpretation. This encourages or even enforces true team collaboration and the coordination of related software developments (say) and gives readers a picture of the overall situation. This leads eventually to the fully integrated simulation the regulations require to estimate safety.

For NRC licensing a possible hybrid scheme is:

An **Overview** of the NRC performance related programme for Yucca Mountain giving background history[1] and good graphical explanations of the system and the main results of its use over time, with resources, etc ... The overall documentation schemes intended for analyst and for software engineers should be explained visually together with 'roadmaps' (as for instance in the Dry Run 3 Overview, Sumerling (1992)). These diagrams show which parts of what documents should be read in a particular sequence to understand fully the reasoning that led from fundamental information to a particular aspect of interest at TPA level. Bibliographies should be indexed in different ways according to assessment topics, not solely by first author name.

[1] Regrettably, the CNWRA Annual Report Sagar (1996) has not been followed up and the IRSR 'snapshots' do not explain the continuity of the NRC PA programme.

A **Worked Example** (lateral document) of TPA-application can be drawn initially at least from the material given by Dr. Mohanty during the ERG Meeting and also from the Sensitivity Analysis results described by Dr. Codell as an update of NUREG 1668. This volume should be related to an NRC Dataset which could be referenced in a separate volume or annexed here.

The **TPA 4.0 User Guide** (lateral document) should be developed with minimal changes from version 3.2 but probably excluding the Dataset and with a wider coverage of output analyses in a revised Chapter 8. Diagrams of the overall integrated system structure, showing all data flows between modules and different models within modules, must be given at both scientific and software levels.

The detailed account of the abstraction and quantitative justification of each module should be documented in separate **Technical Derivation Reports** (longitudinal documents). 'Roadmaps' will be essential in each of these documents.

Underpinning all this, but difficult to do in retrospect for version 3.2, should be a description of the **System Concept Model** development for the TPA system from basic information, FEP catalogues etc... showing what has been considered, screened out or retained and why this has been done, with full evidence referenced including all **Elicitation Sessions.** Comprehensive illustration through corresponding influence diagrams related to a underlying computer-based representation of this information, as in SITE'94, SKI (1996) is essential and provides a powerful, explicit base for future developments in response to design changes that may be received from DOE.

This together with the **Factual Database Document**, is the foundation of all performance assessment work. Both are lateral documents.

Standards and **quality assurance** aspects should be in supporting documents as at present.

TPA should be clearly related to the overall 'assessment toolkit' for licensing review that has been approved by NRC and each of these software items (detailed finite difference codes, say) should also have a clear structured documentation set that is fully explained in the Overview and the TPA User Guide.
The 'analyst' user documentation described should be paralleled by documents for use by software engineers, at least in principle. At present many modules in TPA 3.2 are not clearly documented in a consistent way.
The formal specification and design of documentation schemes for PA is well beyond the scope and time limitations of this review project but it is hoped these suggestions will prove useful to NRC and CNWRA.

The 'Knowledge Management'[2] system underlying all this must enable the coordinated storage and manipulation of information from site data, and from design information, elicitation records etc... through to TPA together with their use in performance assessment calculations of various kinds. Configuration control is essential throughout, and the tracking of all decisions, assumptions and omissions (DAO) through the assessment process is vital to enable observers, in principle at least, to be able to reproduce the entire process and its results independently. The system should also provide a basis for evaluation of bias as a possible means of reconciling the results obtained from independent performance assessments, if this is, indeed, part of the NRC licensing review process.

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[2] Reading recommended by J.H. Bair, Visiting Professor, School of Information Studies, Syracuse University includes:

- Bair, J.H. and O'Connor, E. The State of the Product in Knowledge Management, Journal of Knowledge Management, Vol.2, No.2, Dec 1998.
- Davenport, T.H. and Prusak, L. Working Knowledge: How Organizations Manage What They Know, Harvard Business School Press (1998).

No time was available, unfortunately, to find out if the currently planned information systems outlined in Sections 4.3 and 5.2 of Volume 4 of the Viability Assessment, DOE (1998) could fulfil these requirements. It is clear that any NRC system will need to access the technical databases and geological framework models, for example, of the DOE, but, overall, NRC should be perceived as **independent** of DOE in its manipulation of such information.

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   Volume 1: Introduction and Site Characteristics
   Volume 2: Preliminary Design Concept for the Repository and Waste Package (not read)
   Volume 3: Total System Performance Assessment
   Volume 4: License Application Plan and Costs (Chapters 1, 2 & 3 not read)
   Volume 5: Costs to Construct and Operate the Repository (not read)
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APPENDIX G

REPORT OF FRITS VAN DORP

External Review of

Total-system Performance Assessment (TPA) Version 3.2 Code: Module Descriptions and User's Guide CNWRA San Antonio Texas Predecisional - September 1998

Draft, 24 August 1999

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0 Summary

The Total-system Performance Assessment (TPA) Version 3.2 Code is a flexible tool for NRC to use in the evaluation of DOE's licence application for a HLW repository at Yucca Mountain Nevada. NRC and CNWRA have a very competent and experienced team for such an evaluation. Scenario development techniques can help demonstrating in a traceable manner comprehensiveness of the Total-system Performance Assessment. The definition of a documentation system can help to put the TPA Version 3.2 Code in a framework consisting of past and future project phases and the documents produced in these phases.

1 Preface and Summary of Conclusions

1.1 Preface, Areas reviewed

I have experience in (1) overall "performance assessments" or "safety analyses", (2) "scenario development", (3) "biosphere (or surface environment) modelling" and (4) "radiation protection" (legal & regulatory aspects and operational radiation protection).

I have reviewed the report mainly in view of scenario development, i.e. completeness or comprehensiveness of the features, events and processes considered, logical structure, clarity of presentation and the documentation of these aspects.

The Review included an External Review Meeting from 27 - 29 July 1999 at the CNWRA Office. NRC and CNWRA presented background and details of the Yucca Mountain Project and the TPA Version 3.2 Code developed for NRC. These presentations provided a wealth of detailed information, which the Document does not and can not provide.

Basis for the evaluation of compliance of DOE's applications will probably be the proposed regulation: 10 CFR PART 63-- DISPOSAL OF HIGH-LEVEL RADIOACTIVE WASTE IN A GEOLOGIC REPOSITORY AT YUCCA MOUNTAIN, NEVADA ; [Federal Register: February 22, 1999 (Volume 64, Number 34)][Proposed Rules] [Page 8630-8679] / [FR Doc. **99-4022 Filed** 2-19-**99**; 8:45 am] BILLING CODE 7590-01-P

This note contains my personal view, and does not necessarily reflects Nagra's opinion.

1.2 Weaknesses

The Document "Total-System Performance Assessment (TPA) Version 3.2 Code: Module Description and User's Guide" describes, as the title indicates, a computer code. It includes short descriptions of the system and the conceptual models and of the assumptions made for defining the conceptual models. Whether a computer code appropriately represents the conceptual models and whether the conceptual models are appropriate to the assessment context (including aims and purposes of the assessment) can only be judged when information about the assessment context is available. The assessment context includes site, waste and repository design information as well as information on the purpose and phase of the assessment. Experience (BIOMOVS II Reference Biospheres Working Group, NEA Working Group on an International FEP Database) shows that without detailed knowledge of this assessment context, an assessment (the conceptual model, the computer codes and the parameter values) cannot sensibly be reviewed or compared. The Document contains some, but not enough, information about the assessment context. However, the External Review Meeting (27 - 29 July 1999) provided the required information.

Detailed documentation can show whether the developed code fulfils the requirements implied by the assessment context. The Document does not contain sufficient information. Scenario development can be a tool to demonstrate, in a structured manner, sufficient completeness or comprehensiveness of an assessment. It can be used to identify interactions between different features, events and processes (FEPs).

It is not clear what the position of this Document is within a documentation system. Such a documentation system could show the past and future phases and the different tasks and results of a series of performance assessments.

1.3 Strengths

The description of the code and its modules is detailed and should enable its application, which, of course, can only be tested by applying the code.

Information on input and output of the modules is described clearly and in much detail.

Sources of information and of (default) input data are given.

The modular structure of the code assures flexibility. It should be easy to adapt the code by exchange of modules to include alternative or new conceptual process models. This is particularly important as the understanding of the repository system at Yucca Mountain is developing.

The structure of the Document is clear.

The presentations and discussions at the External Review Meeting (27 - 29 July 1999) showed (1) that the NRC and CNWRA team is competent and (2) that the code as a whole and its modules are based on good system understanding, detailed process-level models and a wealth of data and information. A chain of information exists from field and laboratory observations, measurements, and experiments, their interpretation, conceptual models, process models to the Total-system Performance Assessment code.

1.4 Recommendations

How all potential relevant "features, events and processes" (FEPs) and in particular the Key Technical Issues (KTIs) have been selected, including detailed reasons for this selection and for the omission of others should be documented. This should include all potential interactions between FEPs (e.g., coupled processes) and the reasons why they are in- or excluded. How the included FEPs and their interactions are treated in the different scenarios as well as in the different process level models and in the modules of the Total-system Performance Assessment Code should be documented. This process is often called scenario development and assists in the demonstration of completeness or comprehensiveness in view of the assessment context. The results of the scenario development do not necessarily have to be contained in one document, part may even be available only in electronic form. However, structure and location of the information should be clearly presented.

A structured system of documents should be designed which shows the position of the Document on the TPA Version 3.2 Code in the series of studies and phases of the performance assessments.

The flow of information from field and laboratory observations, measurements, and experiments, through system understanding, the development of conceptual models, the development of process level models, to the development of the Total-system Performance Assessment code should be documented. This should include the source of the information, e.g. general, DOE, or NRC/CNWRA. In addition it should show which information has been used for the development if the models and codes and which for validation or confidence building and benchmarking (benchmarking can be both verification (check on correctness of the calculations) and validation (check on "fit for purpose")).

2 General Comments

2.1 Comprehensiveness and scenario development

The use of a Total-system Performance Assessment (TPA) approach is consistent with, but not equal to the proposed 10 CFR 63 (sec. 63.102 Concepts, (j)). The sections in the proposed 10 CFR 63 dealing with "performance after permanent closure" require more than just the application of a TPA code. In particular: " Performance Assessment. Demonstrating compliance with the postclosure performance objective specified at Sec. 63.113(b) requires a performance assessment to quantitatively estimate the expected annual dose, over the compliance period, to the average member of the critical group. The performance assessment is a systematic analysis that identifies the features, events, and processes (...) that might affect performance of the geologic repository; examines their effects on performance; and estimates the expected annual dose." In addition: "The expected annual dose to the average member of the critical group is estimated, using the selected features, events, and processes, and incorporating the probability that the estimated dose will occur."

Thus, according to the proposed 10 CFR 63 and to international experience a review of a performance assessment involves the following items:

(1) "Completeness" or "comprehensiveness": Although completeness never can be proven, several approaches are possible to achieve a reasonable sufficient level of completeness or comprehensiveness (see work on Scenario Development by the OECD/NEA). These involve:

(1.1) Identification of all relevant Features, Events and Processes (FEPs) and their interactions.

(1.2) Comprehensiveness of the FEPs can be achieved by

(1.2.1) comparison of the FEPs with other FEP-lists (e.g. the International NEA FEP Database, or other project specific FEP-lists)

(1.2.2) the use of a logical structure of the FEP-list

(1.2.3) the use of experts

(1.3) Screening of the FEPs against a set of criteria which is specific for the project (Assessment Context) => a list of relevant FEPs

(1.4) Checking, whether all relevant FEPs are included in the assessment models

(2) Assuring that the assessment models are appropriate in view of the assessment context ("validation") and represent a sufficient level of the state-of-the-art.

(3) Assuring that the models are numerically correct ("verification"), e.g. by benchmarking.

(4) Assuring that the parameter values used for the assessment are appropriate in view of the assessment context, the used models and the state-of-the-art.

(5) A review of the uncertainties involved in system understanding (including future evolution and effects of external processes), models and data (see e.g. chapter 1 in CNWRA 94-002)

Several additional methods are being used within the framework of scenario development: e.g. process influence diagrams, interaction matrices etc.. These can help to identify interactions and to assure comprehensiveness.

These Features, Events, and Processes (FEPs) can be combined into scenarios. A common categorisation of scenarios is into scenarios caused by "external FEPs" (NUREG-1464) and the "normal evolution" scenario. For both categories it is necessary to demonstrate the level of "comprehensiveness".

Although scenario development techniques are being applied, they seem not to be used for demonstrating "comprehensiveness".

Scenario development techniques can provide traceability and documentation of decisions made about the treatment of FEPs in process level models and in the (alternative) modules of the TPA. This might be of particular importance in view of the frequent design changes by DOE. Also scenario development techniques can document, which of the processes described in words, are actually included in calculation codes. At the External Review Meeting (27 - 29 July 1999), several processes have been presented which are not included in the TPA Code. It was not always clear whether they are included in process level codes (e.g. shedding of infiltration = concentration of flow between the drifts because of higher temperatures around the drifts).

Scenario development techniques can provide a framework into which the results of expert elicitation and expert judgement can be documented.

2.2 Use of the TPA code

The Document gives little information about the NRC's approach for reviewing the DOE proposals in prelicensing and licensing phases. What is the position of the TPA code within this review? More information was presented at the External Review Meeting (27 - 29 July 1999): Key technical questions identify the most important features providing safety and the most important processes jeopardising this safety. Several process level models and codes are being, and will be, used and the TPA would be a central code. Also different code modules can be used within the TPA code for testing different hypotheses (flexibility).

The Document concentrates, as the title suggests, on the description of the code. However, in a review, the evaluation and assessment of the actual system understanding and the conceptual models behind the codes is more important.

Advantages and disadvantages of using a total system simulation model against individual sub-system or process models should be discussed. The conclusion would be that both are required. Actually, the correlations derived in detailed process models and used as modules in the TPA code demonstrate this. At the External Review Meeting (27 -29 July 1999) many examples have been presented.

Imposing too many restrictions and/or simplifications, to assure short runtimes for inclusion into a probabilistic code, can reduce transparency and the code might, under certain conditions, not behave as expected. An example of such modification is given in Section 4.6.3.3 on Page 4-80, although these might be totally justified and correct.

Warning: uncertainty in parameters might dilute the calculated risk (as discussed at the External Review Meeting of 27 - 29 July 1999)(D. Hodgkinson in "D. Savage (editor) The scientific and regulatory basis for the geological disposal of radioactive waste, Wiley and Sons Chichester 1995", Section 10.1.6 Risk dilution in PSA, page 364).

2.3 Documentation

The Document is part of a series of documents and the work documented is part of a sequence of studies. The relationships to other documents and other studies are indicated only to a very limited extent. This is a common feature of performance assessment documents produced in other countries and organisations. However, as external reviewer, I would appreciate to see the context of this Document. The External Review Meeting (27 -29 July 1999), however, clarified most of the context of the Document.

2.4 Flow of information and data

The transition from field and laboratory observations, measurements, experiments and general knowledge through conceptual models to computer code or modules should be demonstrated, otherwise how is it assured that a consistent "picture" or system understanding is the basis for the different assumptions? Examples of where detailed information would be required to review the code and data is:

(1) understanding of the properties of the geological unit, leading to

(1.1) a frequency of fractures, joints etc.

(1.2) thermal, hydraulic and mechanical properties

(2) which will be used in

(2.1) two phase flow models (unsaturated flow in a temperature field changing with time)

(2.2) temperature calculations

(2.3) estimates or models of rock mechanical processes.

What will be the effects of uncertainty in knowledge of processes, in conceptual models etc. on the application of the code? Some of these effects were presented at the External Review Meeting (27 - 29 July 1999) and I assume that more will be documented as result of the sensitivity and uncertainty analyses presently being carried out. Has the influence of the choice of parameter distribution function on the result been evaluated?

Which information and data have been used for the development of the models and codes and which for validation or confidence building? Validation should be discussed mainly in relation with the conceptual models and verification in relation with the codes. Have Codes been benchmarked against independent data?

Although the Document deals with a code, a major part is devoted to input data. In general both the code or modules of the code and the input data are insufficiently justified.

It might be useful to document the source of the data and information: e.g. (1) generic literature, NRC/CNWRA, DOE, (2) site specific, generic, (3) peer reviewed, other quality assurance, no quality assurance.

2.5 Coupling of processes, interactions of FEPs

As mentioned under 2.1 scenario development techniques can help to identify, screen, and document decisions and the reasons for in- or excluding interactions between FEPs in the assessment. Many examples of such couplings and interactions were presented and discussed at the External Review Meeting (27 - 29 July 1999). Those which I have noted are listed here:

Increased ventilation will increase salt content of solution which might enter drift during or after ventilation => increased corrosion.

Correlation of dripping model (EBSREL) and corrosion model; reflux would cause dripping => increased corrosion although relative humidity is still low.

Correlation of corrosion and mechanical failure model.

Effect of climate on water table, exfiltration of water and biosphere.

Faulting, seismicity and igneous activity are treated as not correlated.

Faulting, seismicity, igneous activity and hydrogeological processes are treated as not correlated.

Reactivation of faults by thermal stresses.

Correlation of water fluxes with thermal, chemical and mechanical processes.

Correlation of seismicity and rockfall.

Interaction between materials on corrosion potentials, (re)passivation potentials and localised corrosion.

Correlation of Kd's in the different environments (engineered barrier system, unsaturated zone, saturated fractured zone, saturated alluvium, biosphere), because of the chemical properties of elements in chemically different environments.

Igneous release: correlation of the assumption that ash might be transported in different directions (not only towards the critical group as is assumed at present) and that the waste might not be homogeneously distributed in the ash (giving thinner layers with higher concentrations).

2.6 FEPs

During the review and the External Review Meeting (27 - 29 July 1999), FEPs were identified, for which it was not immediately clear whether, or how, they are included in the assessment:

Transport of colloids formed when radionuclides are released form the waste or during radionuclide transport in the engineered barrier system, through the unsaturated zone and through the saturated zone.

Effects of collapsed drifts on the infiltration into the drifts and into the waste packages.

Effects of welds in waste packages on corrosion and mechanical stability.

2.7 Regulations

Two aspects in the proposed 10 CFR 63 need particular comments: (1) the time period of compliance of 10'000 years and (2) the definition of the critical group and reference biosphere.

The present design of the waste package, as presented at the External Review Meeting (27-29 July 1999) makes is very probable that radionuclide releases through groundwater will have their maximum long after the time of compliance of 10'000 years. I recommend, even if the regulations do not require this, to evaluate the consequences of the maximum radionuclide release by groundwater. The code should be able to do this. In most performance assessments in other countries this is common practice.

Section 63.115 of the proposed 10 CFR PART 63 defines the reference biosphere and the critical group to be used for the calculation of the TEDE. In addition to what is (expected to be) required by the Regulations, I would recommend to calculate also consequences of other release scenarios, both natural and "human induced", e.g. (1) for a release by groundwater in Death Valley, which is the location for release if the water is not abstracted by wells, and (2) for a release by free flowing wells in Amargosa Valley, if the groundwater table is higher than at present due to a climate with more rainfall. See also the discussions within Theme 1 of the international exercise BIOMASS as well as in the ICRP (Section 4.2 Paragraphs 38-40 of a draft report by ICRP Committee 4, Task Group on Radiation Protection Recommendations as applied to the disposal of long-lived solid radioactive waste, TG46d9, 1999-02-24, http://www.icrp.org/Solwaste.PDF) on the definition of critical groups for radioactive waste disposal.

3 Review Comments

3.1 TPA Version 3.2 Code, Module Description and User's Guide

CONTENTS, ETC.

List of Contents: Provide all titles with some meaning instead of e.g. just "UZFLOW". Better is the title of section 4.8. But what is the difference between Section 4.8 and 4.14?

INTRODUCTION

Page 1-2 to 1-4, Section 1.1: This section discusses the new knowledge which became available and which was used for the new version of the code. However, some of the new/improved knowledge would have been used for code improvement and some (perhaps the larger part) for data improvement. The text, except the last paragraph, does not distinguish code and data.

Page 1-2, Section 1.1, 1st Paragraph: This paragraph describes an approach, which is one of several possible approaches. It has its advantages and disadvantages as the other. The final result does probably depend less on the chosen approach than on the availability and quality of data and knowledge and other factors. (i) "the key factors controlling the degradation ..", I would prefer the term evolution in stead of degradation, some degradation might also have positive effects. Under (iii) and (iv) I miss the evolution of the site, its geology and topography. I do not agree with the statement of the last sentence: both probabilistic and deterministic approaches have advantages and disadvantages; the present state of the art shows that scenario-based assessments do not have more and other problems than the alternative, if there is an alternative.

Page 1-6, last Paragraph of Section 1.2: What is assumed for the conceptual models: backfilled or open drifts?. If the drifts are backfilled, what material is assumed? Further information was provided at the External Review Meeting (27 - 29 July 1999).

Page 1-7, Section 1.4, 3rd Paragraph and 2nd footnote: There seems to be an inconsistency between "system level ...Version 3.1.4 code" and footnote 2 "....within the TPA Version 3.2 code". This Paragraph shows the importance of Scenario Development, even if it is not named Scenario Development.

Page 1-9. Section 1.4, 2nd last bullet: Are not probabilistic processes (events) replaced by deterministic events?

OVERVIEW OF THE TPA CONCEPTUAL MODELS

General 1: "Completeness" Where is it shown that the processes considered in this Chapter are all possible processes? This Chapter describes what other assessments call the expected evolution scenario.

General 2: A system description from engineering and geologists view points would be useful, before the conceptualisation in view of the modelling. This Chapter gives little justification for the simplifications (e.g. why they are pessimistic).

Page 2-1, 1st Paragraph: The content of this paragraph demonstrates the limits of the probabilistic total system simulation approach. Because of the required simplifications the differences between this approach and the other partly deterministic approaches are, in practice, smaller than one would think on theoretical deliberations.

Page 2-1, Section 2.1., 1st Paragraph: It seems to be necessary to demonstrate in some way that and to give reasons why these assumptions are justified and would not lead to higher doses. Does the assumption of homogeneity mean that preferential flow paths or fracture flow are not modelled?

Page 2-3, Section 2.1, 2nd last Paragraph of the Section: How are "streamtubes" defined? What is a "production zone"? (Explanations later??)

Page 2-5, Section 2.2, 2nd last Paragraph before section 2.2.1: Often different conceptual models are used also to evaluate the consequences of alternative model conceptualisations.

Top of Page 2-7, Section 2.2.2, 2nd last Paragraph: The sentence "In general, the user selects code options by changing flag and variable values in the input file .." shows how difficult it is the develop a pure probabilistic total system simulation model.

Page 2-9, Section 2.2.4, 1st Paragraph: how have the 43 nuclides been selected? It is important to have rigorous and documented criteria for the selection of radionuclides to be included in an assessment.

Page 2-9, Section 2.2.4, 2nd Paragraph, last sentence: This is the first time conservatism is mentioned.

TPA CODE STRUCTURE AND MODULES

Page 3-1, Chapter 3, 2nd Paragraph, 3rd bullet: "scenario classes" !!

Page 3-1, Chapter 3, 3rd Paragraph: Discussion of scenarios, but very short !!

Page 3-4, Section 3.1, top of page 3-4: On what arguments are radionuclides selected for computation?

Page 3-9, Section 3.2.1, last Paragraph before 3.2.2: What does the RAN utility module do? RAN is not included in the Index

Page 3-15, Section 3.3.2: How are the 43 radionuclides determined (the Nagra inventory contains 117 radionuclides)? A basic problem is not addressed: The specific features of the site and repository concept may determine which radionuclides might contribute to the doses. It has to be shown that the preliminary choice of radionuclides is a sensible one in view of the results.

Page 3-22, Fig. 3-8: Why does the Cm-244 chain stop at Th-232?

Page 3-23, Fig. 3-9: What is the system of distribution of radionuclides over the 4 sub-figures?

CONSEQUENCE MODULES

Chapter 4. Generic: Although it is recognised that the code will almost only be used by NRC and CNWRA, it would still be useful, as the code is, in theory, openly available, for potential other users to indicate the limitations and boundaries for the use of the TPA Version 3.2 Code and in particular its modules.

Page 4-1 and following, Chapter 4: Structure of the consequence modules: A change in the order to (i) Conceptual Model, (ii) Assumptions, (iii) Information Flow and (iv) Intermediate Results, would be easier for the reader.

Chapter 4, Generic: The conservative and non-conservative assumptions documented in this Chapter and those presented at the External Review Meeting (27 - 29 July 1999) were not always identical. At the Meeting in general more details were presented.

Page 4-2 ff., Section 4.1: The USFLOW model description gives, as the title says, a description of the model, but offers no justification why this conceptualisation has been chosen and not another one. E.g., Page 4-4, Figure 4-1 is a reasonable conceptual model, however, why has this been chosen and not one of many others, some of the answers are given in section 4.1.4 "Assumptions and Conservatism ...", but only concerning some of the details. At the External Review Meeting (27 - 29 July 1999) several observations were mentioned which might confirm the assumptions made, e.g. from tracers (Cl-36, heat, chloride, C-14), fracture infillings. These should be documented, or reference should be made to available documents.

Page 4-12, Section 4.1.4, last Paragraph of the page: Runoff might tend to reduce infiltration if the water leaves the considered area. However local runoff might concentrate the water in small depressions where it then might infiltrate into a fracture; evapotranspiration might in such a case be less than expected.

Page 4-13, 2nd Paragraph of the page: Several geological units are discussed. To judge the whether the assumptions for deeper infiltration are justified, one needs more information about these geological units than is given in the geological description of the site.

Page 4-13, Section 4.2: The conceptual model assumes no backfill? The Introduction Section 1.2 states that the decision to backfill drifts is still open. On page 4-25, 2nd last Paragraph of the page, the possibility of backfill is mentioned again. A clear concept or alternative concepts would be required.

Page 4-26, Section 4.2.3.2: What would be the effect of backfill? This conceptual model differs considerably from the conceptual model(s) in section 4.2.3.1; has it been shown that these differences do not cause inconsistencies?

Page 4-39, Section 4.3: "Other degradation modes that may become important under certain conditions" are mentioned. More discussion is required, about why these are not included in the models. It is not quite clear whether initial failure (Type 1) and disruptive failure (Type 2) are included in EBSFAIL. They are discussed rather in detail in Section 4.3.3, but I still assume that they are not included. Further information was presented at the External Review Meeting (27 - 29 July 1999).

Page 4-42, Section 4.3.3.3: Is atmospheric corrosion the same as dry air corrosion?

Page 4-48, 1st Paragraph of the page: The statements about conservatism are important, although not totally consistent with a probabilistic total system simulation approach.

Page 4-48 and 49: Bullet points: other approaches might be possible: e.g. (1) determine a minimal thickness required for mechanical stability or integrity of the canister, (2) calculate corrosion rates, (3) assume that a canister fails if the minimal thickness required for mechanical integrity is reached

Page 4-53, Failure Criterion: A combination of container thickness reduced by corrosion and rockfall has not been considered?

Page 4-55, Seismic Hazard Parameters, 1st Paragraph: The assumption that the seismic acceleration at the repository level is half that at ground surface seems, for non specialists, a rough assumption in view of the many other seemingly more refined assumptions. This item was discussed in detail at the External Review Meeting (27 - 29 July 1999).

Page 4-63, Section 4.5.3.4: An increased release rate for the "gap inventory" is not mentioned. At the External Review Meeting (27 - 29 July 1999) this item has been discussed in detail.

Page 4-70, Section 4.5.3.9: I may have missed the explanation of "Invert", it does not appear in the Index; reference to Figure 4-14 would be useful (afterwards, I learned that it is a technical term). Backfill is mentioned again.

Page 4-72, Section 4.5.4, 1st Paragraph: What about the "gap inventory"?

Page 4-74, Section 4.5.4, 2nd bullet on this page: The statement that doses form gaseous releases are negligible should be documented here or in a reference.

Page 4-74, Section 4.5.4, last bullet of the Section: That chain decay can be neglected should be demonstrated and documented.

Page 4-74, Section 4.6: Has the fracture flow model been benchmarked against other fracture flow models (with and without matrix diffusion)?

Page 4-76, Section 4.6.3.1, 1st Paragraph: The reasons given at the end of the Paragraph between brackets are a good example for why not considering certain processes. This should be applied everywhere in the Document.

Page 4-76, Section 4.6.3.1, 2nd Paragraph: It is very important that reasons and evidence for the choice of the conceptual model described in this Paragraph are given.

Page 4-78, Section 4.6.3.2: This is one possible conceptual model. Fractures with infill might exist, radionuclides could sorb on the infill material. Radionuclides could move by diffusion between the solute flowing through the fracture and the more or less stagnant flow in the matrix ("matrix diffusion"), (see also section on NEFTRAN II). The flow through the fractures might be so fast that matrix diffusion would be negligible.

Page 4-82, 2nd Paragraph on this page: Here the reasons are given for not including matrix diffusion in the conceptual model. See remark about page 4-78.

Page 4-83, bullet points: If no retardation is assumed in the fracture flow systems, colloids would not enhance the radionuclide transport. This could be mentioned.

Page 4-83; Section 4.7: Porosity and travel times: although the determination of porosity seems to be straight forward, the determination of the relevant flow porosity is very uncertain, and may depend on the water velocity. Therefore the calculation of travel times is subject to large uncertainties.

Page 4-83, Section 4.7: Have fracture flow models been considered for the flow path before the alluvium?

Page 4-87; Paragraph beginning with NEFTRAN II: If matrix diffusion is taken into account, the choice of parameters need to be carefully discussed and justified based on the/a conceptual model of the aquifer or stream tube. Has the model been validated or benchmarked, for matrix diffusion.

Page 4-89 Section 4.8 and Page 4-97 Section 4.9: These sections describe the models for two "critical" or "exposure" groups. Other exposure groups or "designated receptor groups" (Page 2-10) would also be possible, e.g. (i) natural exfiltration and accumulation of radionuclides in Death Valley an inhalation + external exposure of persons being in Death Valley for a short period of time, (ii) a totally self-sufficient agricultural society. I found no discussion on the aims of defining a "designated receptor group" or groups. Also the size of the population has not been discussed. However, these are defined in the proposed 10 CFR PART 63.

Page 4-89, Section 4.8: I did not find the definition of TEDE's, it is not included in the list of Acronyms. I found the definition on Page 2-10.

Page 4-90, Section 4.8.3, 1st Paragraph: Dilution of the radionuclide concentration as well as the fraction of the total radioactivity in the groundwater extracted by the wells depends strongly on the definition of the critical group, which is given by the proposed 10 CFR PART 63. Has a sensitivity analysis been carried out, although given 10 CFR PART 63 this would not be required?

Page 4-92, Section 4.8.3.2, 1st Paragraph: "A farming receptor group is reasonable" discusses why this group has been chosen, other possible groups, however, are not discussed. However, these are defined in the proposed 10 CFR PART 63.

Page 4-92, Section 4.8.4. What period is assumed for accumulation of radionuclides in soil by irrigation? One of the aims of irrigation, besides providing sufficient water for crop growth, is to enable long-term irrigation without the accumulation of salts in the root zone in a sustainable agricultural system.

Page 4-93, Figure 4-17: The left-hand box contains "Groundwater concentration", would "Well water concentration" not be better? Correctly speaking the Water Consumption of Livestock Uptake would not be derived from Irrigation Water but form Watering Cattle. The Inhalation Dose might also depend on the Duration.

Page 4-94, 4th Paragraph, last sentence " These assumptions may change when additional information on local consumption patterns is made available": Why so much weight on the present situation, whereas radionuclides will be released after a long period of time when habits will certainly have changed. I agree that the calculations should be carried out as they are, however, some reasons would be required and other calculations should at least be discussed, even if not carried out. Reason: these are defined in the proposed 10 CFR PART 63.

Page 4-95, 6th Paragraph: The amount of water extracted is larger than the amount of water delivered by the aquifer with the radionuclides. However, on page 4-91, Section 4.8.3.1 1st Paragraph and 1st sentence the greatest of the two can be chosen.

Page 4-96, 1st bullet on this page: Why so much weight on the present situation? Reason: these are defined in the proposed 10 CFR PART 63.

Page 4-96, 2nd bullet on this page: Children and infants are not considered. I agree because uncertainties are larger than the effect of including children and infants, however, reasons should be given in the report.

Page 4-96, 3rd bullet on this page: Why so much weight on what is permitted by local authorities. These rules might change, people might not obey the rules, and anyhow releases would take place, when the rules will have been forgotten.

Page 4-96, 4th bullet on the page: Another reason for using the highest DCFs would be that the environmental concentrations are expected to be low to very low and chemical form at such low concentrations is uncertain.

Page 4-96, 5th bullet: Why so much weight on the present situation? Reason: these are defined in the proposed 10 CFR PART 63.

Page 4-97, 2nd bullet on this page: This is the first time (?) that the term "critical group" appears.

Page 4-102, bullets: see comments on Page 4-96, 2nd bullet and 4th bullet.

Page 4-111, Section 4.11.4: Could volcanic eruptions and igneous intrusions change the hydrogeological and geochemical properties of the rock?

Page 4-130/131, bullet points, see comments on page 496, 2nd bullet and 4th bullet.

Page 4-133, Section 4.15.3: Ingestion of soil or dust is neglected?

INPUT DATA

Page 5-18: I do not understand the structure of the tables of radionuclides provided and the distinction between Nuclides and Radionuclide Chains.

OUTPUT FILES

PROGRAM INSTALLATION AND EXECUTION

Page 7-7, Section 7.5: How is Quality Assurance documented? This item has been discussed in detail at the External Review Meeting (27 - 29 July 1999).

AUXILIARY CODES

FUTURE DEVELOPMENT OF THE TPA 3.1.4

Page 9-1: What are the reasons for the planned improvements?

APPENDICES A, B, C, D, E,

not studied in detail

APPENDIX F

Why is this information in an Appendix and not in the main text?

OK.

3.2 NUREG-1668 NRC Sensitivity and Uncertainty Analyses ... Volume II: Results And Conclusions

Generic Comment: This type of study provides reasons for the selection of FEPs, modules and parameter values in the TPA Version 3.2 Code.

Page 3-1, Section 3, 1st Paragraph: This is a useful Paragraph about the relations, disadvantages and advantages of process models and total system simulation models.

Page 4-8 and following, Section 4.2: use of parameter descriptions in stead of abbreviations would help understanding. A table of abbreviations and descriptions might also be useful. Reference to Appendix C should be included in the headings of the tables.

Chapters 5 and 6: Many of the results depend strongly on the time of interest. Regulators and regulations in other countries require that consequences are calculated until the peak(s) have been reached. Experience shows that peaks often appear long after 50'000 years, in particular in the more realistic scenarios and calculations.

Page 5-1 last bullet point: "Different parameters may be important for different inner overpack materials. These important parameters are delineated by TPI (???) in chapter 4 of this report.

Page A-1, Section A1.1: How is assured that the interaction of the TKIs and the TPA does not cause potentially relevant Features, Events and Processes to be omitted or forgotten.

Page A-3, Section A1.1.8: Is "Total System Performance Assessment an Integration (TSPAI)" more than the TPA Code and is the TPA Code part of this TSPAI? If yes, where can I find a more detailed description? **This issue is very important to put the TPA Code description and development in the right framework!**

Page A-17, Section A2.3.3.1: The study of the parameter "Resuspension" in this release scenario is inconstant with not studying the effect at a similar level in the groundwater release scenarios. At this level of sensitivity studies one should stop at the same endpoint, e.g. concentrations in the environment and use a standard conversion factor to calculate doses from environmental concentrations.

4 CONSULTED DOCUMENTS

CNWRA, 1994: Background report on the use and elicitation of expert judgement; Center for Nuclear Waste Regulatory Analyses, San Antonio, TX, USA, CNWRA 94-019 *for* Nuclear Regulatory Commission Contract NRC-02-93-005

CNWRA, 1994: Review of scenario selection approaches for performance assessment of high-level waste repositories and related issues; Center for Nuclear Waste Regulatory Analyses, San Antonio, TX, USA, CNWRA 94-002 *for* Nuclear Regulatory Commission Contract NRC-02-93-005

CNWRA, 1995: Iterative performance assessment phase 3 ? Status of activities; Center for Nuclear Waste Regulatory Analyses, San Antonio, TX, USA, CNWRA 95-007 *for* Nuclear Regulatory Commission Contract NRC-02-93-005

CNWRA, 1997: Information and analyses to support selection of critical groups and reference biospheres for Yucca Mountain exposure scenarios; Center for Nuclear Waste Regulatory Analyses, CNWRA 97-009, San Antonio, TX, USA *for* Nuclear Regulatory Commission Contract NRC-02-93-005

CNWRA, 1997: NRC high-level radioactive waste program annual progress report ? Fiscal Year 1996; Center for Nuclear Waste Regulatory Analyses, Southwest Research Institute, NUREG/CR-6513, No. 1, CNWRA 96-OIA *for* Nuclear Regulatory Commission

Codell, R., Eisenberg, N., Fehringer D., Ford, W., Margulies, T., McCartin, T., Park, J., Randall, J., 1992: Initial demonstration of the NRC's capability to conduct a performance assessment for a high-level waste repository; U.S. Nuclear Regulatory Commission report, NUREG-1327, Washington D.C., USA

DOE, 1999: Yucca Mountain Project, Total System Performance Assessment ? Final Report; Peer Review Panel, U.S. Department of Energy report, Washington, D.C., USA

DOE-OCRWM, 1999: Viability assessment of a repository at Yucca Mountain ? Overview; U.S. Department of Energy report, US-DOE/RW 0508, Washington D.C., USA

EPRI, 1998: Alternative approaches to assessing the performance and suitability of Yucca Mountain for spent fuel disposal; US-EPRI report EPRI/TR 108732

Hanks, T.C., Winograd, I.J., Anderson, R.E., Reilly, T.E., Weeks, E.P., 1999: Yucca Mountain as a radioactive waste repository; U.S. Geological Survey Circular 1184

Kessler, J.H. 1998: Study of unsaturated zone flow and transport models of fractured tuff ? Final report; US-EPRI report EPRI /TR 108536

NRC, 1999: Disposal of high-level radioactive wastes in a proposed geological repository at Yucca Mountain, Nevada ? Proposed Rules, 10CFR, Parts 2, 19, 20, 21, 30, 40, 50, 60, 61, 63.; U.S. Nuclear Regulatory Commission, Washington D.C., USA

NWTRB, 1999: Moving beyond the Yucca Mountain viability assessment; U.S. Nuclear Waste Technical Review Board *for* the U.S. Congress and the Secretary of Energy

Stothoff, S.A., Castellaw, H.M., Bagtzoglou, A.C., 1999: Simulating the spatial distribution of infiltration at Yucca Mountain, Nevada; Center for Nuclear Waste Regulatory Analyses, San Antonio, TX, USA

Wescott, R.G., 1995: NRC iterative performance assessment Phase 2 ? Development of capabilities for review of a performance assessment for a high-level waste repository; U.S. Nuclear Regulatory Commission report, NUREG-1464, Washington D.C., USA

APPENDIX H

REPORT OF F. WARD WHICKER

EXTERNAL REVIEW OF THE TOTAL SYSTEM PERFORMANCE ASSESSMENT VERSION 3.2 CODE

For

Center for Nuclear Waste Regulatory Analysis
Southwest Research Institute
San Antonio, TX

Review meeting held
July 27-29, 1999

By

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August 31, 1999

INTRODUCTION

This document is focused on the biospheric transport portion of the Yucca Mountain performance assessment which in being conducted by the Nuclear Regulatory Commission and the Center for Nuclear Waste Regulatory Analysis. The primary biospheric transport pathways envisioned that could ultimately expose human receptors to radioactive materials stored in Yucca Mountain are the use of contaminated well water and the deposition of contaminated ash resulting from a volcanic event within the waste repository. The irrigation scenario for a resident farmer requires groundwater transport of radionuclides from the waste repository to a well at hypothetical farm in the Amargosa Valley located 20 km away, and the use of that well water for drinking and/or irrigation of land to produce agricultural products. The contaminated ash scenario requires the occurrence of a volcanic intrusion of the waste repository, followed by a surface eruption, deposition of contaminated ash on the landscape, and subsequent exposure of people through inhalation, ingestion, and external pathways. A non-farmer receptor group located between 5 and 20 km south of the repository is also considered. In the latter case, use of contaminated well water for drinking only is evaluated for the groundwater pathway, but external exposure is added for the hypothetical volcanic event. The current as well as a future pluvial (cooler and wetter) climate were both considered in the biospheric analysis.

The biospheric transport portion of the TPA 3.2 Code is handled with "site-specific dose conversion factors" or DCF values, which when multiplied by well water or surface soil concentrations of specific radionuclides, provide estimates of "total effective dose equivalents" or TEDE values. The TEDE values represent the 50 year committed total effective dose to an individual which results from a single year of exposure from all pathways and all radionuclides coming from the repository. The TEDE mean values, contained in files within the TPA 3.2 Code, were derived from runs of the GENII-S Code. The GENII-S Code was developed at Pacific Northwest Laboratories, and is generally considered one of the "mainstream" codes for estimating human dose from radionuclides in the environment.

Among the key questions to ask regarding the DCF values are:

1. Are the values used appropriately in the overall code?

2. How accurate are the values likely to be?

3. How uncertain are the values?

4. Are the reference biospheres and exposure scenarios reasonable?

5. Can the choice of parameter values be justified in relation to site-specific conditions?

6. Can use of the GENII-S Code be justified for this performance assessment?

AREAS REVIEWED

This review was restricted primarily to the portions of the code which deal with biospheric modeling. This is because my experience and expertise lie in understanding and modeling the transport of radionuclides in the surface environment and estimating dose and risk to plants, animals, and human beings from environmental radioactivity. Because of this restriction, my document review was focused primarily on:

- CNWRA (1998). *Total-System Performance Assessment (TPA) Version 3.2 Code: Module Descriptions and User's Guide* (Predecisional Draft dated September 1998). Center for Nuclear Waste Regulatory Analysis, San Antonio, TX. (Sections 2, 3 and 4, especially 4.8, 4.9, 4.13 and 4.14).

- CNWRA (1997). *Information and Analyses to Support Selection of Critical Groups and Reference Biospheres for Yucca Mountain Exposure Scenarios.* CNWRA 97-009. Center for Nuclear Waste Regulatory Analysis, San Antonio, TX.

In addition to these documents, my review was based on notes taken from formal presentations in San Antonio and informal discussions with CNWRA staff.

GENERAL COMMENTS

1. With respect to the overall review and presentations, I was extremely impressed with the breadth and depth of the performance assessment process and with the experience and qualifications of the project staff from both NRC and CNWRA. I believe the effort reflected in the review is commensurate with the seriousness of the task of putting high level wastes into the ground. The review was very professional and yet open and enjoyable. I personally learned a great deal about several fields in which I have little or no experience. I was also very impressed with the skills and knowledge of the review team and I felt that their comments were taken seriously by the NRC/CNWRA staff.

2. It seems that NRC and DOE should agree on reference biospheres and human exposure scenarios up-front, so that cross-comparisons of performance assessment (PA) results can be directly compared at the appropriate time. However, I believe strongly that the conduct of the PAs by NRC and DOE should be quite independent from one another. Otherwise, it will be difficult to gain public credibility. This comment is not meant to preclude exchange of scientific and technical information of a factual nature.

3. On p. 2-11, it is implied that the mean values of the DCFs are used in the overall TPA 3.2 Code. Does this mean that they are used as single value parameters rather than being treated a distributions? If this is the case, then I think it would be more defendable, since the TPA 3.2 Code is billed as probabilistic, to treat the DCF values as distributions subject to Monte Carlo sampling. The report CNWRA 97-009 has summarized stochastic runs to show the uncertainties in the DCFs (e.g. Tables 3-1 and 3-2). The flow diagram on p. 3-3 certainly has the dose conversion steps in the correct sequence, but I'm bothered some if this step is no more than a single-value multiplication at the last step, which I think would lead to an overall underestimate of the uncertainty in the TPA 3.2 Code output.

4. Based strictly on the material in the CNWRA (1998) TPA 3.2 Code document, it is difficult to appreciate all the effort which has gone into the development of the DCFs. I was much more appreciative of this effort, however, after reading through CNWRA 97-009. One possible recommendation, however is to develop an appendix to the TPA 3.2 Code document which: a) provides a structural (box & arrow) diagram of the GENII-S Code which shows all compartments and pathways treated; b) provides the entire set of equations (differential and analytic); c) provides a table describing all equation parameters (names, symbols, units, and single or distributional values assumed for the TPA 3.2 application); and d) describes how the GENII-S Code works (e.g. algorithms used to solve differential equation sets, time steps used, how it performs uncertainty/sensitivity analyses, etc.). These things would make it much easier to review and evaluate the DCFs, than is the case at present.

5. Because of reliance on the GENII-S Code, I believe it would add credibility to the ultimate PA conducted by NRC/CNWRA to show some sort of results comparison for a given scenario between GENII-S and other "mainstream" codes such as RESRAD, DnD, ECOSYS etc., and even more importantly, blind comparisons with real data such as has been done in the BIOMOVS project using data sets from Chernobyl fallout. Maybe this has already been done to some extent by the developers of GENII-S, and if so, a summary of this effort would probably suffice. As things stand presently, one can evaluate the uncertainty in the DCF values (e.g. Tables 3-1 and 3-2 in CNWRA 97-009), but nowhere do I find anything to give me confidence in the accuracy of the DCF values. I did spend a little time doing simple hand-calculations to check the water pathway DCFs for ^{137}Cs and ^{239}Pu. Using 2 l/day and effective dose per unit intake from Federal Guidance Report 11, I was able to reproduce the value in Table E-2 (CNWRA 97-009) for ^{137}Cs, but I came nowhere close for ^{239}Pu (using an f_1 value of 10^{-3}).

6. I gained the impression at the review that build up of radionuclides in the soil after years of irrigation with contaminated ground water was not accounted for in the TEDE computations. This could be particularly troublesome for radionuclides that are in relatively soluble form in deep groundwater but which become much less so in the oxidizing surface soil environment. This potential decrease in solubility of course could reduce plant uptake, but the external gamma field could certainly increase over time as a result of radionuclide buildup in surface soil. In a similar vein, it would be important to account for return, year after year, of radionuclides in vegetation and animal wastes to the soil surface. I am not certain whether GENII-S keeps track of these sorts of phenomena. A detailed structural diagram as noted in general comment 3 should answer the latter question.

7. Overall, I was quite favorably impressed with the document "CNWRA (1997). *Information and Analyses to Support Selection of Critical Groups and Reference Biospheres for Yucca Mountain Exposure Scenarios.* CNWRA 97-009". It demonstrates excellent knowledge of the art of pathway analysis and reflects a great deal of effort. Two things which would have added to the value of the report are a listing of the equations used in GENII-S (and relevant to Fig. 3-2) and uncertainty expressions for the radionuclide-specific parameters in Table 2-5. I am not clear as to whether or not the concentration ratios and transfer coefficients were treated stochastically in the

runs used to generate Tables 3-1 and 3-2. I am also a bit puzzled by the revised DCF tables in Appendix E, in that single values rather than distributions are presented. Perhaps this relates to my concern noted in general comment 2 that the DCF values appear to be single multipliers at the end of the TPA 3.2 Code, so this source of uncertainty would not be propagated in the final results.

SPECIFIC COMMENTS ON THE CNWRA (1998) TPA 3.2 CODE DOCUMENT

1. It appears that retardation of radionuclides in fractures is not taken into account. While this is conservative, it would seem that at least some fine materials would be present in most of the fractures and that substantial retardation would occur there. Are there data or observations to justify the assumption of no retardation in fractures?

2. It is indicated on p. 2-9 that lateral dispersion from streamtubes is neglected. I would like to see more rationale for this assumption because at first glance, this seems counter-intuitive.

3. On p. 2-10, the residential community is indicated to be < 20 km from the repository. Is it possible to be more specific about the location?

4. Having a table of acronyms in the document is very helpful to its review.

5. On p. 2-10, last bullet, does “direct contact” mean external gamma exposure from radionuclides in the soil? This term could have other connotations.

6. On p. 2-10, the pathways for the farming community receptor group are listed, but the list does not seem complete. For example, what about soil ingestion by farm animals and people?

7. On p. 2-11, it is indicated that the residential receptor group is exposed only through drinking of contaminated well water and direct exposure from radionuclides in ash following igneous activity. It seems that this may not be conservative or realistic, because such people might purchase food products from farms in Amargosa Valley, or they may well have small vegetable gardens that are irrigated with contaminated well water. Furthermore, has anyone considered the buildup of solid deposits on swamp coolers or humidifiers?

8. On p. 4-95 it is noted that plant/soil concentration ratios used are generic. Given the extremely large variations with soil type and water chemistry, I am surprised that some of this sort of site-specific work has not been carried out. At the very least, I would expect that one could narrow the range of reasonable assumptions based on soil characteristics in Amargosa Valley.

9. In the second paragraph on p. 4-95, a resuspension model is referred to. It would help to describe the type of model, since many exist.

10. I would challenge, perhaps naively, that the entire radionuclide plume from the repository would be captured by wells (paragraph 5, p. 4-95). Is this a reasonable assumption?

11. The first bullet on p. 4-96 indicates that food consumption rates are based on national averages. The Desert Research Institute in Las Vegas did a very large survey for areas near the Nevada Test Site in the late '80s. I recall some rather large differences from national surveys. Maybe it would be worth trying to get some of this information.

12. Table 4-7, p. 4-123 lists a K_d of 550 for ^{241}Pu. I have never seen such a low value for Pu in a natural environment. Is this a typo?

13. Referring to Table 5-1, p. 5-7, the quantity and units for the EPA limit (last column heading) should be given.

14. I would strongly second the notion on p. 9-1 that colloid transport should be added to TPA 3.2.

15. In Appendix A, p. A-47, a matrix K_d for Cm of 0 is assumed. I would expect Cm to have a K_d similar to that of Am. This would also seem inconsistent with the matrix retardation factor for Cm of 1.8e4 on p. A-80.

16. The fourth column in Appendix A often gives two values. Do these represent the range, the 5th and 95th quantiles, or what? For lognormal distributions (e.g. p. A-48), why not give the GM and GSD? Also, many parameters in Appendix A appear to be treated as constants, yet many of these must be somewhat uncertain. Is it clear anywhere why these are treated as constants?

WHAT CAN BE CONCLUDED WITH RESPECT TO KEY QUESTIONS POSED IN THE INTRODUCTION?

Based on the information that I could glean from the review and from a limited amount of time to study the documents provided, I would offer the following answers to the questions posed:

1. Are the DCF values used appropriately in the overall TPA 3.2 Code? It is clear that the DCF values are used appropriately, however, I question why the values were not treated as stochastic variables. There may be a reasonable rationale for this, but I believe that the overall TPA 3.2 Code output uncertainty may be less that it would be if the considerable uncertainty in the DCF values were accounted for.

2. How accurate are the DCF values likely to be? I suspect that the values are generally reasonable, but I did not find specific evidence to make one feel entirely comfortable with them. The use of sensitivity analysis to focus effort on the most important parameters is certainly to be applauded, as is the philosophy of trying to make reasonable rather than worst-case assumptions. Clearly there is a lack of site-specificity in some of the model parameters, which could raise some doubts, but these are not likely to result in order-of-magnitude differences in the DCFs. I believe it would help if the GENII-S Code output could be compared with real data from various scenarios and with other commonly used codes. If this has already been done, then something could be said about the outcomes of such efforts.

3. How uncertain are the DCF values? Stochastic model runs of GENII-S summarized in CNWRA 97-009 indicated lognormally-distributed output with GSDs generally ranging from about 1.4 to 2.0. These results are generally comparable to those for other models similar to GENII-S, and I believe these are reasonable estimates, based on my own experience with the PATHWAY Code.

4. Are the reference biospheres and exposure scenarios reasonable? I believe that with two probably minor exceptions, the reference biospheres and exposure scenarios are reasonable, judging from current lifestyles, agricultural practices, climates, and the expected pluvial climate. The exceptions, mentioned earlier in this report, are the potential build-up of radionuclides in soil from prolonged irrigation, and the potential use of agricultural products from the Amargosa Valley and home gardening by the non-farmer resident.

5. Can the choice of parameter values be justified for site-specific conditions? I think in general, yes. However, I do not think there is sufficient justification for the radionuclide-specific parameters (plant/soil concentration ratios and feed transfer coefficients to animal products). These parameters can vary a lot, depending on soil characteristics and chemical forms of the radionuclides. To do better in this regard, it would require site-specific experiments, which would be fairly expensive, or at least a more in-depth analysis of soil properties and expected chemical forms. On the other hand, if the current code comes up with doses and risks that are many orders of magnitude below current limits, then this kind of improvement may not be warranted.

6. Can the use of the GENII-S code be justified for this performance assessment? I believe this code has a generally good reputation and the developers seem to be in tune with the state-of-the-art. I believe this code can be justified, but a little more rationale (see GENERAL COMMENT 5) might be offered in the final report.

APPENDIX I

SCREENING ARGUMENTS FOR RADIONUCLIDES NOT INCLUDED IN THE TOTAL-SYSTEM PERFORMANCE ASSESSMENT VERSION 4.1 CODE

SCREENING ARGUMENTS FOR RADIONUCLIDES NOT INCLUDED IN THE TPA VERSION 4.1 CODE

Methodology Used to Screen Radionuclides for the TPA Version 4.1 Code

In response to comments made by the external reviewers during the peer review of the TPA Version 3.2 Code (see Weldy, et al., 1999), formal screening arguments have been developed to explain why the set of radionuclides included in the code as the base set of radionuclides was selected. Several different considerations evolve in any effort to screen radionuclides completely from the total system performance assessment analysis. Radionuclides need to be screened not only for the base case, but also for possible disruptive events, such as volcanism or human intrusion. Additionally, due to the process of radioactive decay, radionuclides may become more important or less important throughout the time period of the analysis. Therefore, the screening analysis will be based on the following:

- Separate screening analyses will be performed for the groundwater transport scenario and the volcanism scenario because of the substantially different transport modes. The human intrusion scenario will be included in the groundwater transport scenario by not taking credit for retardation in the invert or the unsaturated zone for those radionuclides being screened.

- The earliest time considered in the analysis is 100 years, which is the estimated time of permanent closure. If there are any waste package failures prior to this time, the consequences will be assessed in the preclosure safety analysis, which is evaluated using a separate code from the TPA Code.

- For the groundwater scenario, biosphere dose conversion factors will be developed by the GENII code for all possible radionuclides. Radionuclides will only be screened if there is another radionuclide in the analysis for which the product of the biosphere dose conversion factor and the inventory of the radionuclide is greater than 100 times the radionuclide to be screened. Additionally, the radionuclide used for the screening must have a longer half-life than the screened radionuclide or not decay significantly in 10,000 years, have a lower retardation coefficient in the saturated zone than the screened radionuclide, and be more soluble than the screened radionuclide. For radionuclides not in the GENII library, the product of the inventory times the inhalation dose conversion factor, the inventory times the ingestion dose conversion factor, and the inventory times the external exposure dose conversion factor of the screened radionuclide must all be less than 1 percent of the corresponding value for the screening radionuclide.

- For the volcanism scenario, because transport to the receptor group location is independent of radionuclides, there are no solubility or retardation considerations in the screening analysis. Screening is performed based on the product of the dose conversion factor times the inventory (in Ci/MTU) at 100 years. If this product for a radionuclide is less than 1 percent of another radionuclide in the fuel for the inhalation, ingestion, and direct exposure pathways, the radionuclide may be screened from further analyses. Again, the radionuclide used for the screening must have a longer half-life than the screened radionuclide or not decay substantially in 10,000 years.

The following is a summary of the process used to identify the radionuclides that needed to be tracked in the TPA Version 4.1 Code.

First, the ORIGEN2 computer code (Oak Ridge National Laboratory, 1991) was used to calculate the inventory of all radionuclides for a medium enrichment (4.0 percent), high burnup pressurized water reactor fuel (70 GWd/MTU) at 100 years. Pressurized water reactor fuel was selected because it has a higher inventory of most radionuclides than boiling water reactor fuel and also has a higher range of burnups than boiling water reactor fuel. A high burnup fuel was selected to generate a large inventory of heavy actinides (Cm, Cf, Bk), to ensure that these radionuclides are not screened inappropriately by using a median burnup fuel, because these radionuclides increase in inventory significantly as burnup increases. The radionuclides used most often for comparison (Np-237, Am-241, and I-129) all increase approximately linearly with burnup. Therefore, the use of the high burnup will not excessively increase the inventory of these radionuclides. Note that the only radionuclides that significantly decrease with burnup are U-235 and its daughters, and a low burnup (10 GWd/MTU) was used for these radionuclides. A median enrichment fuel was used because inventory of most radionuclides is not a strong function of enrichment. The ORIGEN2 code outputs the inventories of about 1,000 radionuclides.

Immediately all radionuclides with an inventory of 0 Ci/MTU at 100 years were screened out. This eliminates approximately 850 radionuclides. Approximately 45 additional radionuclides have short half-lives (< 20 days), but have parents with longer half-lives and, as such, are still present in the fuel in 100 years. These radionuclides will be assumed to be in secular equilibrium with their parent radionuclides and will contribute to the dose from intakes of the parent radionuclides, but their transport does not need to be tracked separately in the TPA Code. These radionuclides are listed in Table I–1.

Table I–1. Radionuclides Not Tracked in the TPA Version 4.1 Code but Assumed to be in Secular Equilibrium with Their Parents for Dose Calculations

^{210}Bi	^{209}Pb	^{210}Po	^{219}Rn	^{206}Tl
^{211}Bi	^{211}Pb	^{211}Po	^{220}Rn	^{209}Tl
^{212}Bi	^{212}Pb	^{212}Po	^{222}Rn	^{208}Tl
^{213}Bi	^{214}Pb	^{213}Po	^{223}Ra	^{207}Tl
^{214}Bi	^{227}Th	^{214}Po	^{224}Ra	^{233}Pa
^{242}Am	^{231}Th	^{215}Po	^{225}Ra	^{234}Pa
^{225}Ac	^{234}Th	^{216}Po	^{221}Fr	^{234m}Pa
^{217}At	^{242}Cm	^{218}Po	^{223}Fr	^{239}Np
^{108}Ag	^{137m}Ba	^{126m}Sb	^{126}Sb	^{90}Y

At this point, about 105 radionuclides remained for consideration for inclusion in the code that could not be screened purely on a half-life argument. For these remaining radionuclides, screening arguments had to be developed for both the groundwater pathway and the direct release scenario.

For the direct release scenario, radionuclides will be released to the environment in the same relative concentrations as found in the fuel. The inhalation and ingestion dose conversion factors were taken from FGR 11 (Oak Ridge National Laboratory, 1988) and the direct exposure dose conversion factors were taken from FGR 12 for a 15-cm [5.9-in.] layer of uniform contamination. Screening is performed based on the product of the dose conversion factor times the inventory (in Ci/MTU) at 100 years for the inhalation, ingestion, and direct exposure pathways. Note that radionuclides that build up significantly through time (greater than a factor of 5 increase in inventory) were considered separately to ensure that they were not inappropriately screened based on their 100-year inventory. For radionuclides that build up significantly, the peak inventory of the radionuclide in 10,000 years was used instead of the 100-year inventory to determine whether the radionuclide can be screened. The rationale for screening for radionuclides that were screened in this manner is contained in Table I–2.

After this screening step was completed, only the following radionuclides remained that could not be screened: Am-241, Pu-240, Sr-90, Pu-239, Am-243, Pu-242, Cm-245, Np-237, Sn-126, Nb-94, Th-229, Pu-238, Cs-137, and Cm-244. These radionuclides are already considered in the direct release calculations for the TPA Version 4.1 Code, so no further steps are necessary to justify that the set of radionuclides considered in the calculation is sufficient.

For the groundwater scenario, it is better and more efficient to use the GENII code (Napier, et al., 1988) to develop dose conversion factors from the groundwater concentration of radionuclides for all the radionuclides included in the GENII library. Of the radionuclides remaining to be screened, the following radionuclides are not included in the GENII library: Si-32, K-42, Nb-93m, Tc-98, Rh-102, Ag-108m, Ag-109m, La-138, Ce-142, Nd-144, Pm-146, Sm-146, Eu-150, Tm-171, Hf-182, Ir-192m, Pt-193, Ir-194, Pb-205, Bi-208, Bi-210m, Np-236, Pu-236, Np-240m, Bk-250, Cf-249, Cf-250, and Cf-251. The radionuclides in the GENII library will be screened by comparing the GENII dose conversion factor to other radionuclides. However, for the groundwater pathway, transport parameters are significant and must be considered. Two key transport parameters of radionuclides are the solubility of the radionuclide and the retardation of the radionuclide in the alluvium. A radionuclide can only be screened if the product of its GENII dose conversion factor and its inventory at 100 years is less than 1 percent of another radionuclide, and it is not more soluble or less retarded than the radionuclide against which it is compared (both minimum and mean retardation values). Therefore, I-129, which is essentially completely soluble in groundwater and essentially unretarded in the alluvium, can be used to screen any radionuclide with a much smaller inventory times GENII dose conversion factor product. Np-237, however, can only be used to screen radionuclides that are less or equally soluble and more or equally retarded than neptunium. Also, a screening radionuclide has to have a half-life longer than the half-life of the radionuclide being screened or a half-life that is long compared to 10,000 years (e.g., I-129 and Np-237) to ensure that radioactive decay does not inappropriately influence the results. The rationale for screening for radionuclides screened in this manner is contained in Table I–3.

For the radionuclides not in the GENII library, a methodology similar to that for the direct release pathway will be used for screening. Screening is performed based on the product of the dose conversion factor times the inventory (in Ci/MTU) at 100 years. If this product for a radionuclide is less than 1 percent of another radionuclide in the fuel for the ingestion and direct exposure pathways, it may be screened from further analyses. Note that the inhalation pathway was not considered in the screening because LaPlante and Poor (1997) demonstrate that the inhalation pathway is not significant (~1 percent or less of total dose) for any radionuclide considered in

Table I–2. Radionuclide Screening Arguments for the Volcanism Scenario			
Cm	246	Exclude	Dose conversion factor* inventory less than 1% of Am-243 for Direct Exposure, Inhalation, and Ingestion; Half-life less than Am-243
U	234	Exclude	Dose conversion factor* inventory less than 1% of Am-243 for Direct Exposure, Inhalation, and Ingestion out to 10,000 years
U	238	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Tc	99	Exclude	Dose conversion factor* inventory less than 1% of Am-243 for Direct Exposure, Inhalation, and Ingestion out to 10,000 years
I	129	Exclude	Dose conversion factor* inventory less than 1% of Am-243 for Direct Exposure, Inhalation, and Ingestion out to 10,000 years
C	14	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Se	79	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion; Inventory corrected for half-life of 1.1×10^6 years
Cl	36	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Inhalation and Ingestion; Direct Exposure just exceeds 1% of Pu-239 after approximately 6,000 years due to decay of Pu-239; Peak risk from volcanism occurs before 6,000 years
Th	229	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Inhalation and Ingestion; Direct Exposure just exceeds 1% of Pu-239 after approximately 6,000 years due to decay of Pu-239; Peak risk from volcanism occurs before 6,000 years
Pa	231	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion out to 10,000 years
Th	230	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion out to 10,000 years
Ac	227	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion out to 10,000 years
U	233	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion out to 10,000 years
Pb	210	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion out to 10,000 years
Ra	226	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion out to 10,000 years.
U	237	Exclude	Dose conversion factor* inventory less than 1% of Pu-240 for Direct Exposure, Inhalation, and Ingestion; Half-life less than Pu-240
Cm	247	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Pu	244	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Np	236	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion

Table I–2. Radionuclide Screening Arguments for the Volcanism Scenario (continued)			
Pu	236	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
U	240	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Pu	243	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Bi	210M	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Np	240M	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Pb	205	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Cf	252	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Bk	250	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Pu	241	Exclude	Dose conversion factor* inventory less than 1% of Am-241 for Direct Exposure, Inhalation, and Ingestion; Half-life less than Am-241
Am	242M	Exclude	Dose conversion factor* inventory less than 1% of Am-241 for Direct Exposure, Inhalation, and Ingestion; Half-life less than Am-241
Cm	243	Exclude	Dose conversion factor* inventory less than 1% of Am-241 for Direct Exposure, Inhalation, and Ingestion; Half-life less than Am-241
Ni	63	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Cd	113M	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Sm	151	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
U	236	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Eu	154	Exclude	Dose conversion factor* inventory less than 1% of Am-241 for Inhalation and Ingestion; dose conversion factor* inventory less than 10% of Am-241 for Direct Exposure; Dose from direct exposure from Am-241 is small fraction of total dose from Am-241 (<1% in Laplante and Poor, 1997); Half-life less than Am-241
U	232	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
U	235	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Inhalation and Ingestion; Direct Exposure is less than 1% of Am-243 for 10,000 years
Cs	135	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion

Table I–2. Radionuclide Screening Arguments for the Volcanism Scenario (continued)			
Zr	93	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Cf	249	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Ni	59	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Cm	248	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Sn	121M	Exclude	Dose conversion factor* inventory less than 1% of Am-241 for Direct Exposure, Inhalation, and Ingestion; Half-life less than Am-241
Co	60	Exclude	Dose conversion factor* inventory less than 1% of Am-241 for Direct Exposure, Inhalation, and Ingestion; Half-life less than Am-241
Eu	152	Exclude	Dose conversion factor* inventory less than 1% of Am-241 for Direct Exposure, Inhalation, and Ingestion; Half-life less than Am-241
Cf	251	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
H	3	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Np	238	Exclude	Dose conversion factor* inventory less than 1% of Am-241 for Direct Exposure, Inhalation, and Ingestion; Half-life less than Am-241
Ho	166M	Exclude	Dose conversion factor* inventory less than 1% of Am-243 for Direct Exposure, Inhalation, and Ingestion; Half-life less than Am-243
Ag	108M	Exclude	Dose conversion factor* inventory less than 1% of Am-241 for Direct Exposure, Inhalation, and Ingestion; Half-life less than Am-241
Cf	250	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Mo	93	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Pd	107	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Eu	155	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Ag	108	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Ce	142	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Sm	147	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Ca	41	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Sm	146	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion

Table I–2. Radionuclide Screening Arguments for the Volcanism Scenario (continued)			
Rb	87	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Tc	98	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Pm	146	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Be	10	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Hf	182	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Eu	150	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Ta	182	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Bi	208	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion.
P	32	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Ir	192	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Si	32	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Sb	125	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Pt	193	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Pm	147	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Te	125M	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Ir	192M	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
K	40	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Cs	134	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
La	138	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Nd	144	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Fe	55	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion

Table I–2. Radionuclide Screening Arguments for the Volcanism Scenario (continued)			
Rh	102	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Re	187	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Ir	194	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
K	42	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Tm	171	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Cd	109	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Ag	109M	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion
Kr	85	Exclude	Gas—will not settle on ground
Ar	39	Exclude	Gas—will not settle on ground
Kr	81	Exclude	Gas—will not settle on ground

Table I–3. Screening Rationale for Groundwater Release for Screened Radionuclides in the GENII Library			
Pa	231	Exclude	GENII dose conversion factor* inventory less than 1% of Np-237; Lower Solubility and Higher Retardation in saturated zone than Np-237; remains less than 1% of Np-237 out to 10,000 years
U	233	Exclude	GENII dose conversion factor* inventory less than 1% of Np-237; Lower Solubility and Higher Retardation in saturated zone than Np-237; remains less than 1% of Np-237 out to 10,000 years
U	237	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Cm	247	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Pu	244	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
U	240	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Pu	243	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Cf	252	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Am	242M	Exclude	GENII dose conversion factor* inventory less than 1% of Am-241; Same Solubility and Retardation in saturated zone as Am-241; Shorter half-life than Am-241
U	235	Exclude	GENII dose conversion factor* inventory less than 1% of Np-237; Lower Solubility and Higher Retardation in saturated zone than Np-237
Zr	93	Exclude	GENII dose conversion factor* inventory less than 1% of Np-237; Lower Solubility and Higher Retardation in saturated zone than Np-237
Cm	248	Exclude	GENII dose conversion factor* inventory less than 1% of Np-237; Lower Solubility and Higher Retardation in saturated zone than Np-237
Sn	121M	Exclude	GENII dose conversion factor* inventory less than 1% of Np-237; Lower Solubility and Higher Retardation in saturated zone than Np-237
H	3	Exclude	GENII dose conversion factor* inventory less than 1% of I-129; If released as a gas, extremely conservative calculation shows that dose from releasing entire contents of all juvenile failure waste packages is less than 10^{-6} rem and the dose from releasing the entire contents of all waste packages failing at 1,000 years is less than 10^{-27} rem
Mo	93	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Eu	155	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Sm	147	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Ca	41	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Rb	87	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Be	10	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Ta	182	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
P	32	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Ir	192	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Sb	125	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Pm	147	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Te	125M	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
K	40	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Cs	134	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Fe	55	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Re	187	Exclude	GENII dose conversion factor* inventory less than 1% of I-129
Cd	109	Exclude	GENII dose conversion factor* inventory less than 1% of I-129

that report. Since that report was released, biosphere modeling has not changed significantly other than the inclusion of buildup of radionuclides in soil, which does not significantly change the results. Also note that for U-234, the ratio of the (inventory*inhalation dose conversion factor) to the (inventory*ingestion dose conversion factor) is almost 500, but in LaPlante and Poor (1997), inhalation contributes less than 1 percent of total dose. No other radionuclide has a ratio much higher than U-234. Therefore, the inhalation pathway is not considered in the groundwater screening. The rationale for screening for nuclides screened in this manner is contained in Table I–4.

After this screening step was completed, only the following radionuclides remained that could not be screened: Ac-227, Am-241, Pu-240, Sr-90, Pu-239, Am-243, Pu-242, Cm-245, Cm-246, Np-237, U-234, Ni-63, Cd-113m, U-236, U-238, Sn-126, Tc-99, Nb-94, I-129, Cs-135, C-14, Cf-249, Ni-59, Se-79, Cf-251, Ho-166m, Ag-108m, Cl-36, Th-230, Pb-210, Ra-226, Th-229, H-3, and Pa-231. There are three additional noble gas radionuclides (Kr-85, Kr-81, and Ar-39) that will be evaluated separately.

Most of the remaining radionuclides are available in the TPA Version 4.1 Code if solubilities, gap fractions, and retardation factors are entered into the *tpa.inp* file. Therefore, the next step is to run the TPA Version 4.1 Code with these additional nonscreened available radionuclides turned on and determine whether they affect the calculated dose. To ensure the analysis is sufficient for both the base case and a human intrusion analysis, the code is run both during nominal unsaturated zone conditions and with the unsaturated zone neutralized. The effect of early waste package failure is included through the use of juvenile failures of the waste package (an average of approximately 30 waste packages per realization) and early failure of the drip shield. No process has been proposed that bypasses the saturated zone except for the igneous scenario discussed previously, so the modeling of the saturated zone is unchanged in this analysis. Additional solubility data for some of these additional elements are taken from the CRWMS M&O (2000) and additional data for the alluvium matrix R_d are taken from Triay, et al. (1997). Additionally, for some radionuclides, Sheppard and Thibault (1990) were consulted. Sheppard and Thibault (1990) present retardation coefficients for many elements in different soil types. If a new element was more strongly retarded than neptunium for all soil types presented (sandy, clay, loam, and organic), it was assumed that the alluvium matrix R_d for that radionuclide was at least equivalent to the alluvium matrix R_d for neptunium. Where data were not available for the additional radionuclides, it was assumed that the radionuclide was essentially infinitely soluble and unretarded in the saturated zone. Additionally, it was assumed that 6 percent of all new fission product and activation product radionuclides was present in the gap, which is the maximum gap fraction in the code for any nonvolatile radionuclide. Actinides were still assumed to be contained in the structure of the fuel. Finally, it was assumed there was no retardation in the invert for these additional radionuclides for which data are not available.

The results of the mean value of the probabilistic screening runs are presented in the following figures. Figure I–1 shows the dose history of radionuclides for the first 10,000 years assuming nominal performance of the unsaturated zone. Figure I–2 shows the dose history of radionuclides for 100,000 years assuming nominal performance of the unsaturated zone. Figure I–3 shows the results for 10,000 years with the unsaturated zone neutralized, and Figure I–4 shows the results for 100,000 years with the unsaturated zone neutralized.

Table I–4. Screening Rationale for Groundwater Release for Screened Radionuclides not in the GENII Library			
Np	236	Exclude	Dose conversion factor* inventory less than 1% of Np-237 for Direct Exposure, Inhalation, and Ingestion; Same Solubility and Retardation in saturated zone as Np-237
Pu	236	Exclude	Dose conversion factor* inventory less than 1% of Pu-239 for Direct Exposure, Inhalation, and Ingestion; Same Solubility and Retardation in saturated zone as Pu-239
Bi	210M	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
Np	240M	Exclude	Dose conversion factor* inventory less than 1% of Np-237 for Direct Exposure, Inhalation, and Ingestion; Same Solubility and Retardation in saturated zone as Np-237
Pb	205	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
Bk	250	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
Nb	93M	Exclude	Dose conversion factor* inventory less than 1% of Np-237 for Inhalation and Ingestion; Lower Solubility and Higher Retardation in saturated zone than Np-237; Direct Exposure dose conversion factor less than 1% of Nb-94
Cf	250	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure and Ingestion
Ce	142	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Inhalation and Ingestion; External exposure is negligible because a curie of Ce-142 only emits 1.5e-3 photons/sec (from ORIGEN2 output file)
Tc	98	Exclude	Dose conversion factor* inventory less than 1% of Tc-99 for Inhalation and Ingestion; Dose conversion factor* Inventory for Direct Exposure is less than 10% of Tc-99; Direct Exposure pathway is a small component of total dose from Tc-99 (20.1 %)*
Sm	146	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
Pm	146	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
Hf	182	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
Eu	150	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
Bi	208	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion; dose conversion factor DE from Al-28 due to similar decay characteristics
Si	32	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
Pt	193	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion

Table I–4. Screening Rationale for Groundwater Release for Screened Radionuclides not in the GENII Library (continued)			
Ir	192M	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
La	138	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
Nd	144	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
Rh	102	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
Ir	194	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
K	42	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
Tm	171	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
Ag	190m	Exclude	Dose conversion factor* inventory less than 1% of I-129 for Direct Exposure, Inhalation, and Ingestion
*LaPlante, P.A. and K. Poor. "Information and Analyses to Support Selection of Critical Groups and Reference Biospheres for Yucca Mountain Exposure Scenarios." CNWRA 97-009. San Antonio, Texas: CNWRA. 1997.			

If a radionuclide does not reach at least 0.1 percent of the peak dose in 10,000 years (the time period specified in 10 CFR Part 63) or 1 percent of the peak dose in 100,000 years, the radionuclide may be excluded. The low threshold associated with the 10,000-year analysis provides confidence that even if new information leads to the reevaluation of input parameters associated with the excluded radionuclides, the peak dose in 10,000 years is unlikely to be substantially underestimated. The higher threshold associated with the longer analysis period is reasonable because this analysis is not associated with specific numerical limits in 10 CFR Part 63 or 40 CFR Part 197 and is conducted to gain information on how the system behaves during a long time frame. Tables I–5 and I–6 show the radionuclides that remain after this screening step.

All these radionuclides are included in the set of radionuclides tracked in the TPA Version 4.1 Code. It is recommended that in addition to these radionuclides, the most significant heavily sorbed radionuclides still be tracked for sensitivity analyses that evaluate the effect of colloids or limited retardation in the unsaturated and saturated zones. The most significant radionuclides considering both initial inventory and half-life include Am-241, Pu-240, Pu-239, and Am-243.

For the remaining radionuclides (Cd-113m, Cf-249m, Cf-251, Ho-166m, and Tc-98), the TPA Version 4.1 Code must be run a second time to evaluate their effects. The remaining radionuclides will be modeled in the TPA Version 4.1 Code by making changes to the input and data files to allow the physical and radiological characteristics of these radionuclides to be represented in the TPA Version 4.1 Code. These radionuclides were conservatively assumed to be soluble, have 6 percent of their inventory in the gap, and be unretarded in the invert, unsaturated zone, and saturated zone. All components in the code were set at their nominal performance, except for the drip shield, which was assumed to fail early. The results of these two runs are presented in the Figures I–5 and I–6 (for 10,000- and 100,000-year calculational periods).

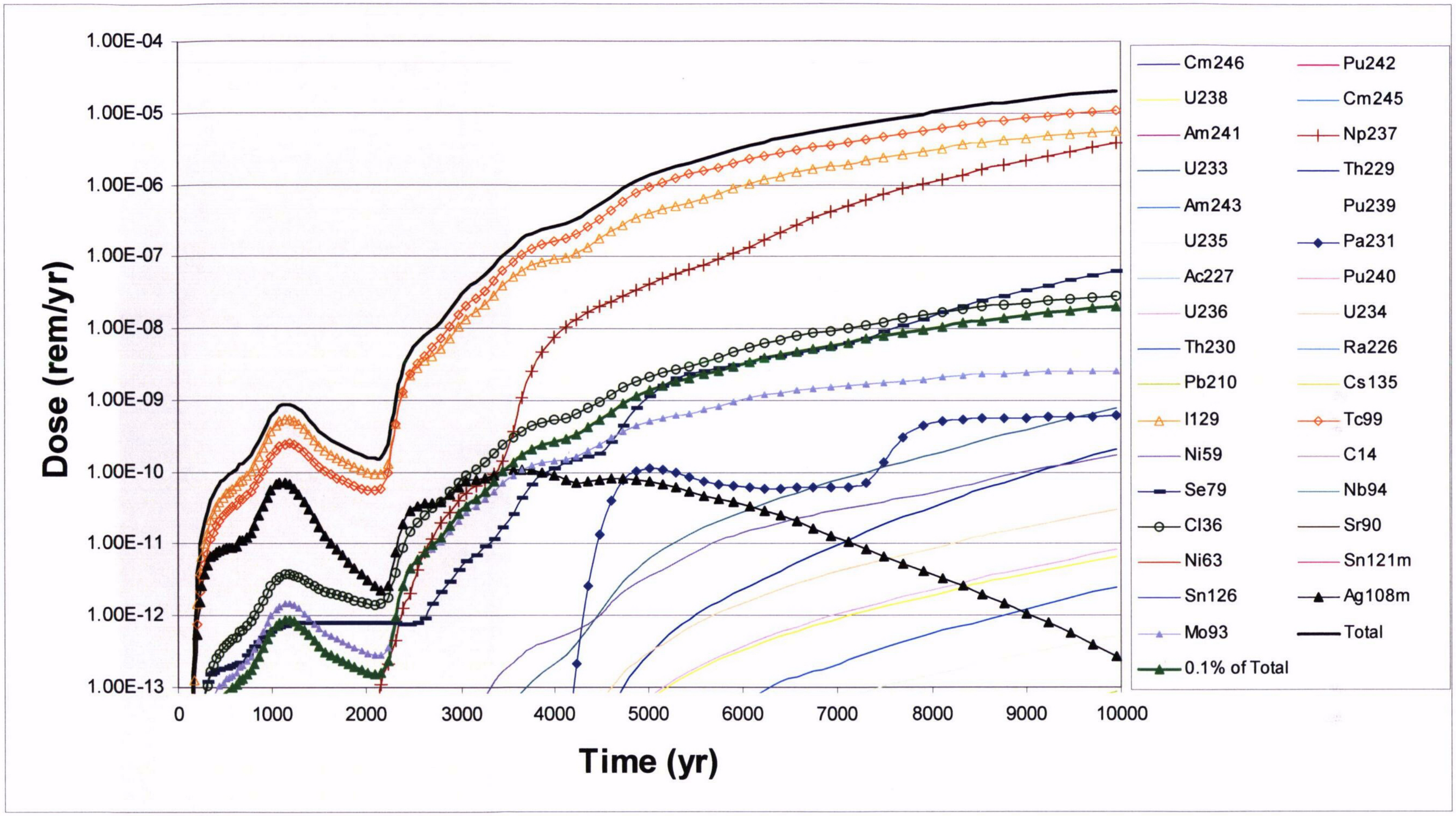

Figure I–1. Results of the TPA Version 4.1 Code under Nominal Conditions for 10,000 Years

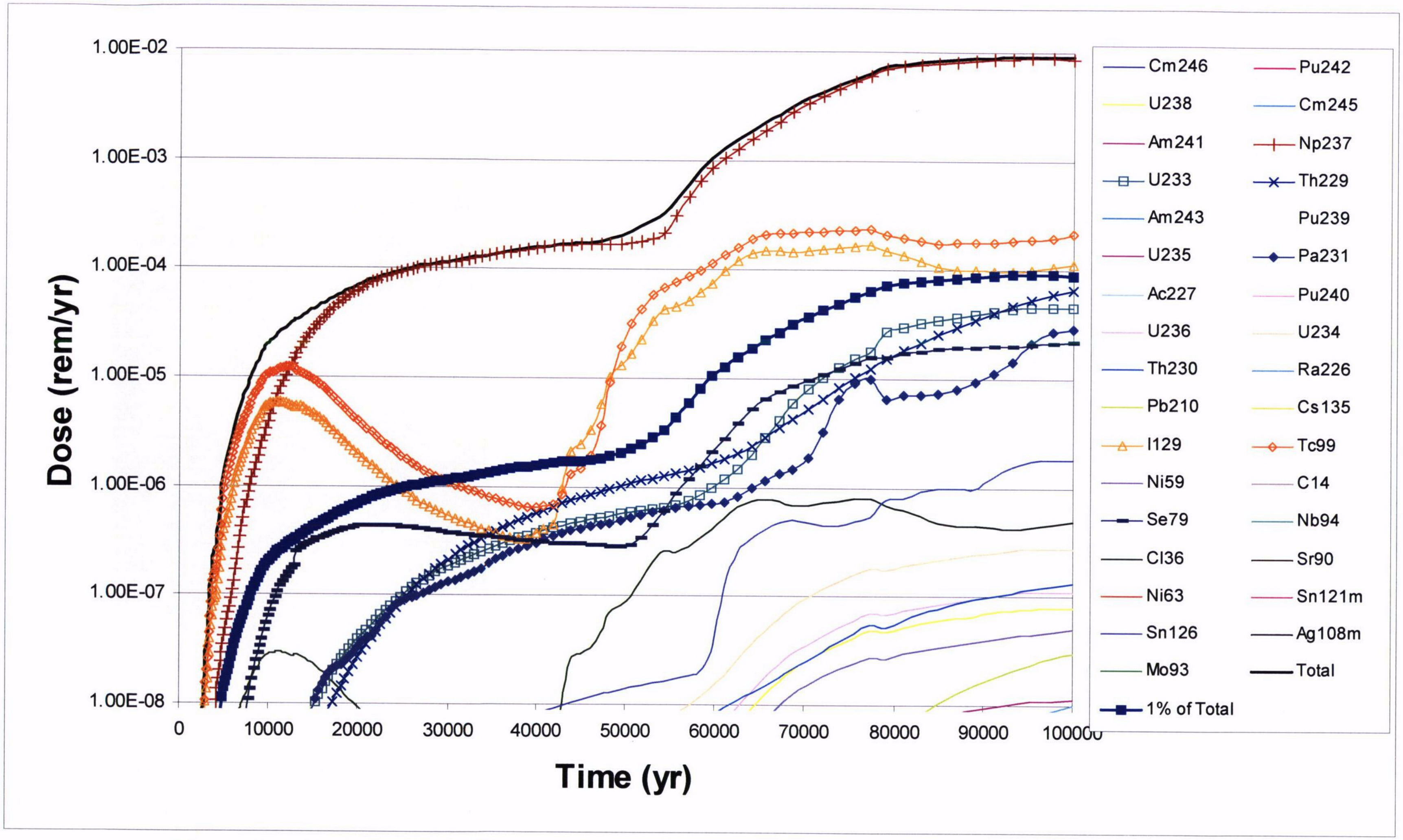

Figure I–2. Results of the TPA Version 4.1 Code under Nominal Conditions for 100,000 Years

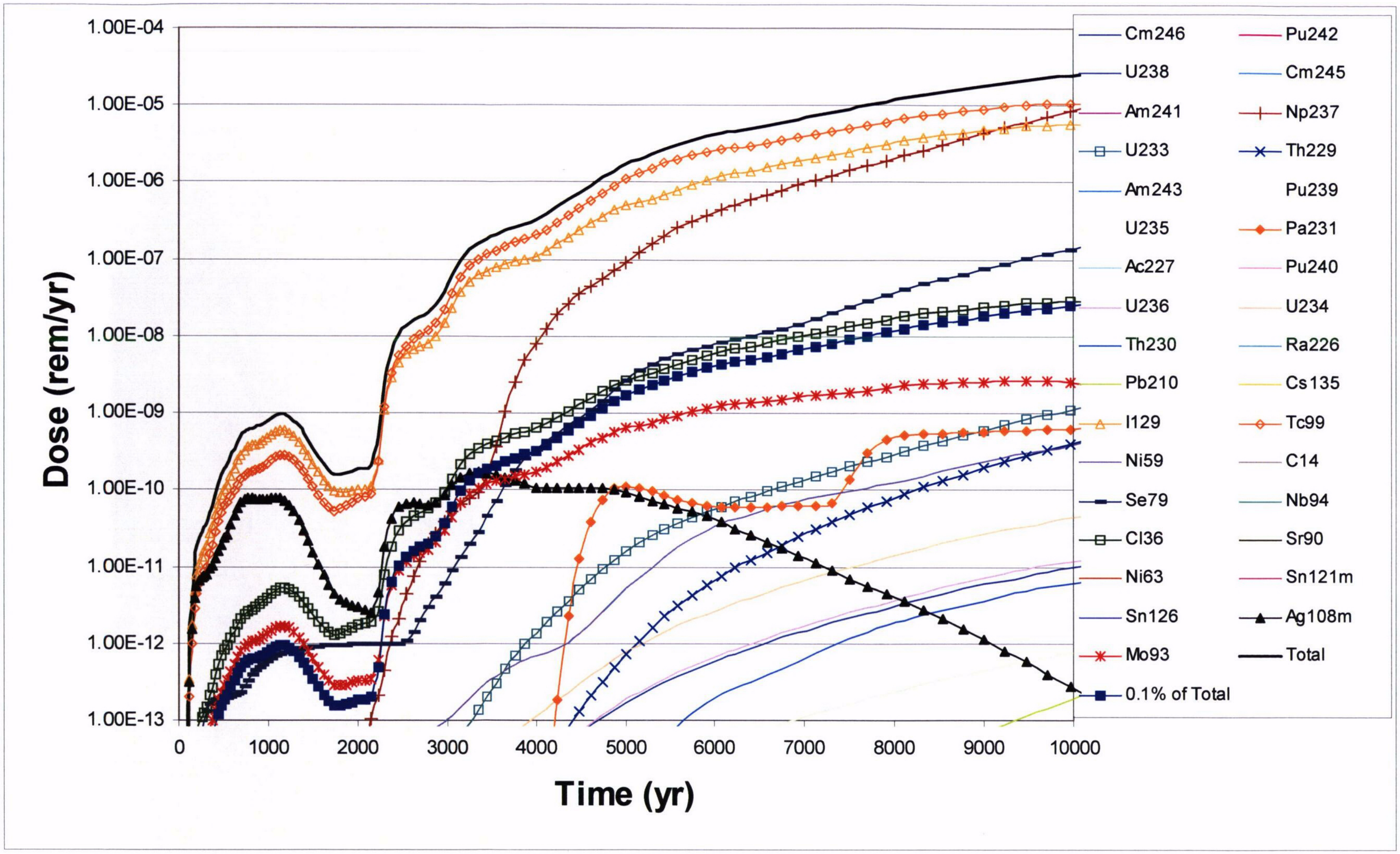

Figure I–3. Results of the TPA Version 4.1 Code with the Drip Shield and Unsaturated Zone Neutralized for 10,000 Years

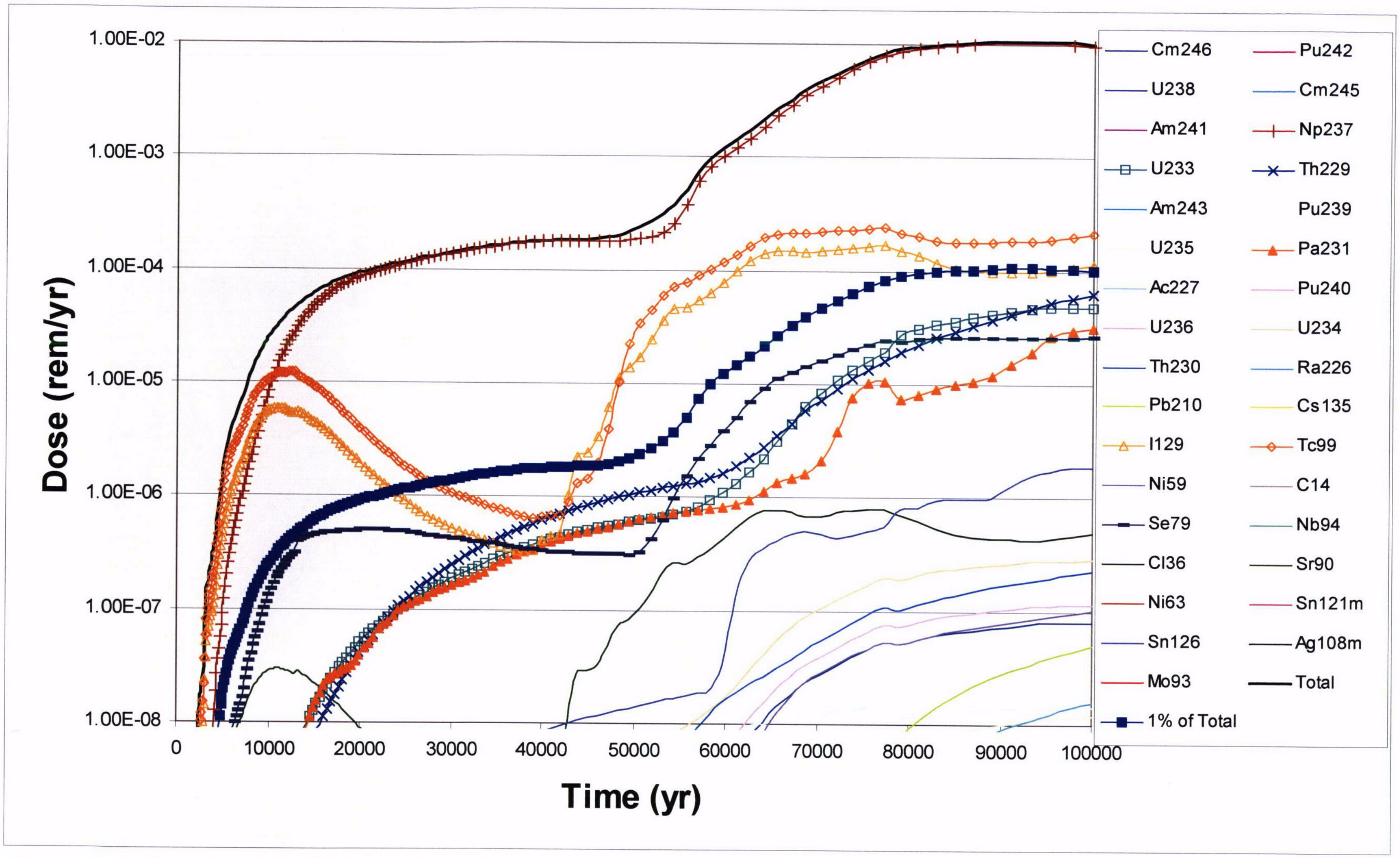

Figure I–4. Results of the TPA Version 4.1 Code with the Drip Shield and Unsaturated Zone Neutralized for 100,000 Years

Table I–5. List of Significant Radionuclides for the Nominal Performance	
Radionuclides That Contribute to the Peak Dose in 10,000 Years—Nominal Unsaturated Zone Performance	**Radionuclides That Contribute to the Peak Dose in 100,000 Years—Nominal Unsaturated Zone Performance**
Tc-99	Np-237
I-129	Tc-99
Np-237	I-129
Se-79	
Cl-36	

Table I–6. List of Significant Radionuclides for the Human Intrusion Analysis	
Radionuclides That Contribute to the Peak Dose in 10,000 Years—Neutralized Unsaturated Zone Performance	**Radionuclides That Contribute to the Peak Dose in 100,000 Years—Neutralized Unsaturated Zone Performance**
Tc-99	Np-237
I-129	Tc-99
Np-237	I-129
Se-79	
Cl-36	

Results of the two runs show that although some of these additional radionuclides modeled using conservative assumptions may contribute (more than 0.1 percent) to the small total doses early in the analysis, even within 10,000 years, none of these additional radionuclides contribute to the peak dose. Therefore, these additional radionuclides can be screened from the analysis.

Finally, it is necessary to screen the gaseous radionuclides separately for the groundwater release scenario. These gaseous radionuclides could be released at the time of waste package failure and travel in gaseous form up through the mountain. They could then be released from the surface of the mountain and be transported by wind to the receptor group location.

Radionuclides that could be released from the repository in gaseous form include H-3, C-14, Ar-39, Kr-81, and Kr-85. A conservative calculation will be performed to model the potential dose from an airborne release of these radionuclides.

The calculation will postulate two release scenarios. First, it will be assumed that every initially defective waste package fails in a single year. Second, it will be assumed that every waste package in the repository fails in a single year at year 20,000. Current results from the TPA Version 4.1 Code indicate that corrosive failures of the waste package are not likely before year

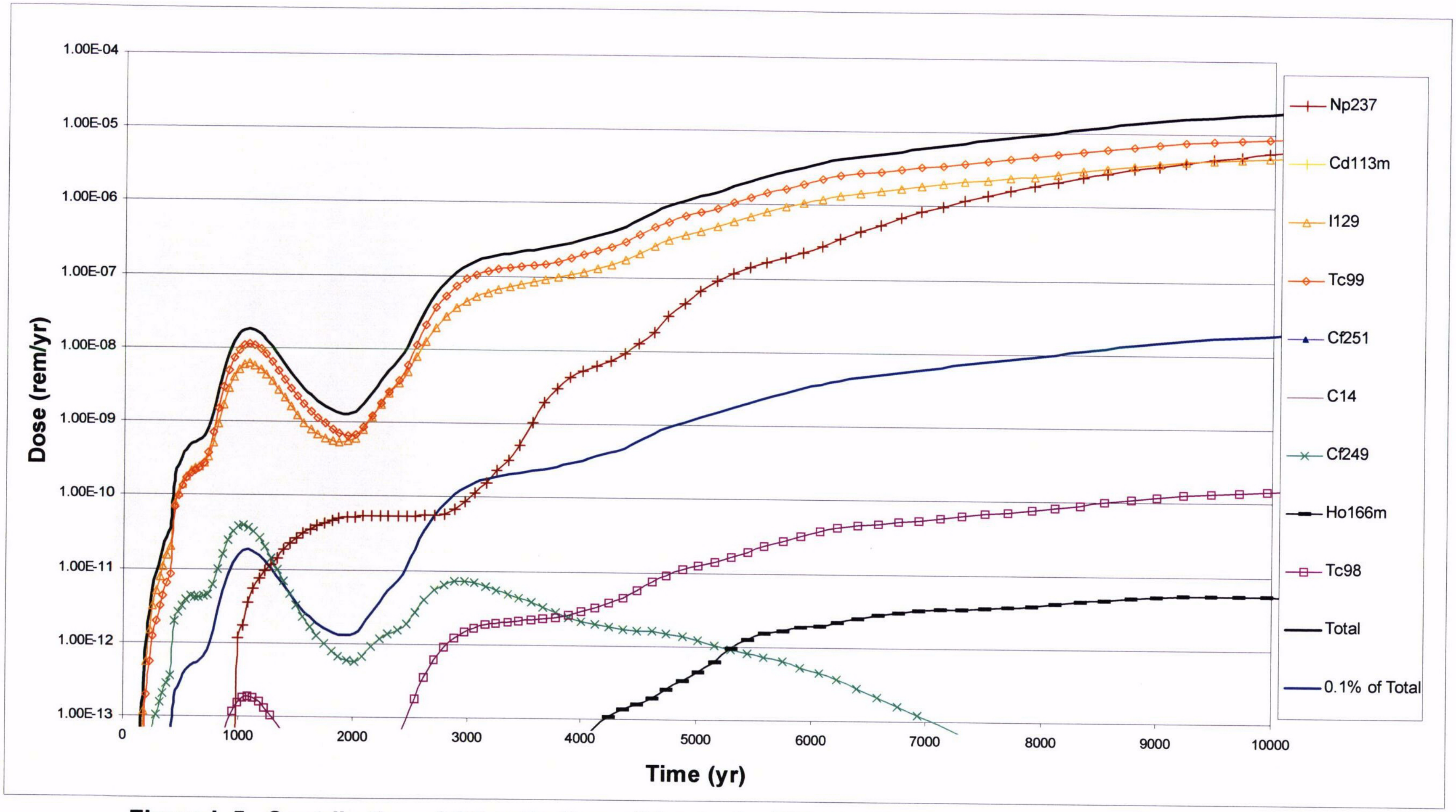

Figure I–5. Contribution of Other Radionuclides to the TPA Version 4.1 Code Results for 10,000 Years

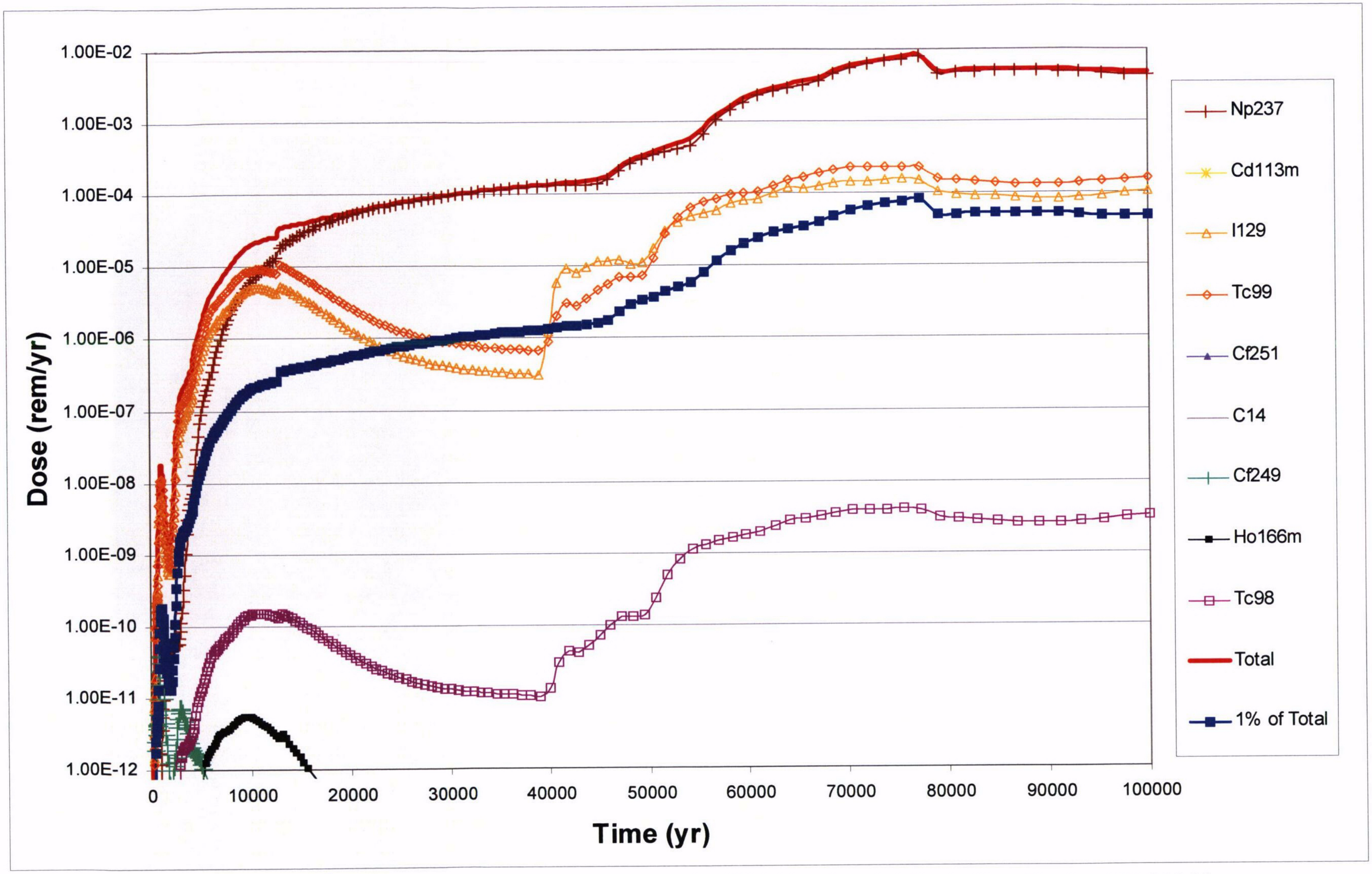

Figure I–6. Contribution of other Radionuclides to the TPA Version 4.1 Code Results for 100,000 Years

Table I–7. Inventories of Gaseous Radionuclides in the Repository at Different Times		
Radionuclide	**Inventory in Repository at Year 100 (Ci)**	**Inventory in Repository at Year 10,000 (Ci)**
H-3	3.59×10^5	0*
C-14	1.01×10^5	3.03×10^4
Ar-39	8.05	0*
Kr-81	0.14	0.14
Kr-85	1.66×10^6	0*
*Zero activities were reported for activities less than 10^{-20} Ci at 10,000 years.		

30,000 and may extend beyond 100,000 years, so this assumption of the failure time of the waste packages is conservative. From Mohanty and McCartin (1998), the mean value of the range of the sampled fraction of waste packages initially defective is 0.00505, and the average inventory of C-14 is 1.44 Ci/MTU. ORIGEN2 (Oak Ridge National Laboratory, 1991) was used to calculate the inventory of the remaining radionuclides for 4.0 percent enriched fuel with a burnup of 70 GWd/MTU at year 100, which is assumed to be the time of repository closure. These fuel characteristics would bound the inventory of these additional radionuclides at the time of repository closure. The calculated total inventories in the repository for the 70,000 MTU of fuel in the repository are listed in Table I–7. Only the fraction of C-14 in the gap and grain boundaries will be available to be released in the year of waste package failure. The C-14 in the cladding and fuel structure cannot be released until the fuel or cladding oxidizes, which is slow compared to the rate of release from the gap and grain boundaries. The fraction of the C-14 in the gap and grain boundaries is 10 percent (Mohanty and McCartin, 1998). It is assumed that 100 percent of the other gaseous radionuclides are released in the year of waste package failure.

Transport of these radionuclides to the critical group location was modeled using a Gaussian plume model described in Regulatory Guide 1.111 [Nuclear Regulatory Commission (NRC), 1977] as shown in Eq. (I–1) assuming a ground level release at a location 18-km [11.2-mi] south of the repository. The weather characteristics are taken from a DOE site characterization document (CRWMS M&O, 1999), from which the frequency of stability classes and the annual average wind speed can be calculated.

$$\frac{\overline{X}}{Q} = 2.032 \frac{n}{N x \bar{u} \sigma_z(x)} \qquad \text{(I-1)}$$

where

$\frac{\overline{X}}{Q}$ = Average annual effluent concentration normalized by source strength in a given direction from the source (s/m^3)
n = Number of hours that the wind is blowing in a given direction (h)
N = Total number of hours of data (h)
x = Distance downwind (m)
$\bar{u}$ = Average windspeed (m/sec)
$\sigma_z(x)$ = Vertical plume spread at a distance x (m)

From the Environmental Baseline File Meteorology and Air Quality document (CRWMS M&O, 1999), the fraction of the time that the wind blows from Yucca Mountain toward the critical group location, which is equivalent to n/N, is 18.2 percent. From Regulatory Guide 1.111 (NRC, 1977), the vertical plume spread at 18 km [11.2 mi] for Class F stability conditions is 58 m [190.3 ft]. These data were used with dose conversion factors for submersion and inhalation from Oak Ridge National Laboratory (1988), to calculate the doses shown in Table I–8 for the two release scenarios.

Table I–8. Results of Conservative Calculation of Dose from Gaseous Releases from the Repository

Radionuclide	Dose from Juvenile Failures (1 percent of Inventory at 100 Years) (mrem/yr)	Dose from Corrosion Failures (10 percent of Inventory at 10,000 Years) (mrem/yr)
H-3	2.61×10^{-3}	0
C-14	2.39×10^{-3}	4.23×10^{-2}
Ar-39	1.56×10^{-10}	0
Kr-81	5.26×10^{-11}	9.81×10^{-9}
Kr-85	2.74×10^{-7}	0
Total	5.27×10^{-3}	4.23×10^{-2}

The peak annual dose for aqueous releases in the nominal scenario in 10,000 years is 0.021 mrem and is 10.1 mrem in 100,000 years. Even these conservative calculations show that a large release of gaseous radionuclides from the repository would not lead to a dose that exceeds the dose from aqueous releases of radionuclides at the receptor location. Therefore, it is reasonable to screen the gaseous release of these radionuclides from further consideration in the TPA Code.

Conclusions

It is recommended that the radionuclides listed in Table I–9 continue to be tracked in the TPA Version 4.1 Code for the direct release and groundwater release scenarios.

Table I–9. Radionuclides That Should Be Included in the TPA Version 4.1 Code

Radionuclides to be Included in the Direct Release Scenario	Radionuclides to be Included in the Groundwater Release Scenario
Sr-90	Cl-36
Nb-94	Se-79
Sn-126	Tc-99
Cs-137	I-129
Th-229	Np-237
Np-237	Pu-239
Pu-238	Pu-240
Pu-239	Am-241
Pu-240	Am-243
Am-241	—
Pu-242	—
Am-243	—
Cm-244	—
Cm-245	—

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