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February 17, 2000
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Account No. 20.01402.761

U.S. Nuclear Regulatory Commission
ATTN: Mr. James Firth
Office of Nuclear Material Safety and Safeguards
Division of Waste Management
Performance Assessment and High-Level Waste Integration Branch
Mail Stop 7C–18
Washington, DC 20555

Subject: Transmittal of Report on External Peer Review of the Total-system Performance Assessment (TPA) Version 3.2 Code

Dear Mr. Firth:

The purpose of this letter is to transmit the revised version of Intermediate Milestone 01402.761.080, the External Peer Review of the Total-system Performance Assessment Version 3.2 Code. The report was revised in response to comments you forwarded in your acceptance letter of November 29, 1999.

If you have any questions, please feel free to contact me at 210.522.5082, Mr. James Weldy at 210.522.6800, or Dr. David Turner at 210.522.2139.

Sincerely yours,

Gordon Wittmeyer

Gordon W. Wittmeyer, Ph.D.
Manager, Performance Assessment

GWW/ls
enc.

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CNWRA 2000-01
Revision 1

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

Prepared for

Nuclear Regulatory Commission
Contract NRC–02–97–009

Prepared by

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

February 2000

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James R. Weldy
Gordon W. Wittmeyer
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Center for Nuclear Waste Regulatory Analyses
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ABSTRACT

The Nuclear Regulatory Commission (NRC) undertook a formal independent peer review of the Total System Performance Assessment (TSPA) methodology as embodied in the Total-system Performance Assessment (TPA) Version 3.2 code. This peer review, organized by the Center for Nuclear Waste Regulatory Analyses, 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 TSPA approach and evaluating the suitability of the TPA Version 3.2 code for use in reviewing the U.S. Department of Energy (DOE) License Application (LA) for the proposed Yucca Mountain repository. The external reviewers were generally quite positive about the quality of development of the TPA Version 3.2 code and were generally of the opinion that the code was suitable for reviewing the DOE LA. However, numerous suggestions were put forward by the reviewers for improving the technical bases for the model abstractions and 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. The results of the external review, as summarized in the report and documented in full in the appendixes, will be used to guide the development of future versions of the TPA code.

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ACKNOWLEDGMENTS

This report was prepared to document work performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA) for the Nuclear Regulatory Commission (NRC) under Contract No. NRC–02–97–009. The activities reported here were performed on behalf of the NRC Office of Nuclear Material Safety and Safeguards, Division of Waste Management. The report is an independent product of the CNWRA and does not necessarily reflect the views or regulatory position of the NRC.

The authors wish to thank S. Mohanty for his technical review and W. Patrick for his programmatic review of this report; their contributions led to significant improvements in the quality and readability of this report. Secretarial support provided by J. Wike is greatly appreciated as is the editorial review conducted by C. Gray.

In addition, the authors express their thanks to the many members of the staffs of the NRC and CNWRA who participated in the external review meeting in San Antonio, Texas, by making formal presentations on the technical bases for, and application of, the TPA Version 3.2 code.

QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

No analyses were conducted in the preparation of this report; therefore, no data or computer codes were used.

1 INTRODUCTION

The Nuclear Regulatory Commission (NRC), with assistance from the Center for Nuclear Waste Regulatory Analyses (CNWRA), has 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 radioactive waste (HLW) repository at Yucca Mountain (YM), 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 (TSPA) conducted by DOE [e.g., TSPA-95 (TRW Environmental Safety Systems, Inc., 1995)], and to investigate the safety case supporting the DOE Viability Assessment (VA) (U.S. Department of Energy, 1998). Ultimately, a version of the TPA code will be exercised by the NRC to aid in determining if the quantitative basis of the safety case for YM presented in the anticipated DOE License Application (LA) is sound.

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 TPA, 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. There are a number of peer-reviewed publications cited in the TPA Version 3.2 User's Guide (Mohanty and McCartin, 1998), that provide 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;[1] Mohanty et al.[2] Lu and Mohanty[3]; Jarzemba and Sagar, 1999[4]). 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 LA review in 2002.

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). Because the timing and execution of the peer review

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[1]Eisenberg, N., M. Lee, T. McCartin, K. McConnell, M. Thaggard, and A. Campbell. Development of a performance assessment capability in the Waste Management Program of the U.S. Nuclear Regulatory Commission. *Risk Analysis* 19(5). In press. 1999.

[2]Mohanty S., Y. Lu, and J.M. Menchaca. Screening of sensitive parameters for a complex geologic waste disposal system using Morris methods. *Risk Analysis*. Submitted for publication. 1999.

[3]Lu, Y., and S. Mohanty. Sensitivity analysis of a complex geologic waste disposal system using Fourier Amplitude Sensitivity Test (FAST) method. *Reliability Engineering & System Safety*. Submitted for publication. 1999.

[4]Jarzemba, M.S., and B. Sagar. A Parameter Tree approach to estimating system sensitivities to parameter sets. *Reliability Engineering & System Safety*. Accepted for publication. 1999.

process is largely controlled by the organizing body, organized peer reviews can be a very efficient procedure for vetting a research and development program and abbreviated timeframes, such as are typical of the HLW program, are more readily met. Moreover, by conducting the review in a group setting, the external reviewers are able to formulate more probing follow-up 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 (FACA) of 1972. The FACA 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, records of all working papers and reports used by the committee be available to the public, and 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 three years ago, the DOE established a Performance Assessment Peer Review Panel that was charged with providing an independent evaluation of the TSPA-VA and suggestions for improving the TSPA approach to be used to support the LA. The DOE Performance Assessment Peer Review Panel, which operated for approximately 2 ½ yr under FACA guidelines, produced three interim reports and one final report that reflected the consensus view of the panel.

The NRC instructed staff of the CNWRA to conduct an organized peer review of the TPA Version 3.2 code and the overall NRC TPA methodology. This review was not undertaken with the purpose of obtaining a consensus opinion from a panel and, therefore, was not subject to FACA 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 in this summary report. While reference is made within this summary report to the "external review group (ERG)," 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 the key results contained in section 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 appendixes, particularly if he or she wishes to examine in detail strengths and weaknesses of the TPA Version 3.2 code.

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 development of the TPA Version 3.2 code and concluded that the code was suited for use in reviewing the DOE LA. 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. In particular, one reviewer had serious concerns about the technical bases supporting the saturated zone flow and transport (SZFT) module. An over-arching 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 code could be enhanced by preparing documents that explain how features, events, and processes (FEP) were included or excluded.

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 TPA Version 3.2 code, identifies materials provided to the reviewers in advance of a meeting, outlines the primary goals of the review and 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 ERG 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 (PA)
- FEP Analysis

More than 50 responses were received. Based on the number of nominations received, clear experts were identified by peer acclamation in hydrology, geochemistry, overall PA, and FEP analysis. Insufficient responses were received to provide a clear-cut preference in the remaining technical areas. Consequently, technical staff at the CNWRA and NRC were asked to nominate reviewers to fill the remaining positions on the ERG. A final short list of reviewers was identified for the eight positions on the ERG.

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

Eight participants in the above technical areas were selected based on availability and freedom from COI (table 2-1). Because of COI restrictions, five of the eight reviewers were from outside the United States. Because of the uniqueness of the proposed repository at YM, technical expertise in the different components of the repository was considered to be more critical than familiarity with the DOE HLW disposal program.

Table 2-1. Members of the external review group for the Total-system Performance Assessment 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 Consultant 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

2.2 MATERIALS PROVIDED TO THE EXTERNAL REVIEW GROUP

For their initial independent evaluation of the TPA Version 3.2 code, the TPA 3.2 User's Guide (Mohanty and McCartin, 1998) and the TPA 3.1 Sensitivity Analysis Report, NUREG–1668 (Nuclear Regulatory Commission, 1999) were provided to each member of the ERG.

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 ERG 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 wk were available to review the material prior to meeting with CNWRA and NRC staff in San Antonio, Texas. Final comments (appendices A–H) were provided by the reviewers about 3–4 wk after the meeting.

2.3 PRIMARY GOALS OF THE REVIEW

The overall goal of conducting the external review of the TPA Version 3.2 code is to receive an independent critical evaluation of the NRC approach to TPA from recognized authorities in different fields of research. The scope of the review covered the TPA Version 3.2 code and associated documentation, but not the NRC HLW program or the regulations associated with the YM repository. More specifically, the members of the ERG 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 TPA studies as implemented in the TPA Version 3.2 code
- Recommend improvements that could be made in subsequent revisions, modifications, and updates of the TPA code
- Evaluate implementation of conceptual models, including parameter choices
- Determine whether the NRC approach to TPA is suitable for achieving its objectives of reviewing the DOE LA and associated TSPA

In addition to these general goals, the members of the ERG were provided with a number of specific questions to consider in evaluating the TPA Version 3.2 code.

- Is the TPA Version 3.2 code sufficiently complete?
    - Are the included FEPs sufficient to provide credible results and meaningful insights? If the included FEPs 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 a 3-day meeting held 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 wk earlier on July 13–14, 1999. During the meetings, the reviewers were provided with additional information on the regulatory framework for HLW disposal in the United States, the role of the TPA Version 3.2 code in the licensing process, site characteristics at YM, conceptual models used in the NRC TPA, the basis for model parameters and parameter uncertainty, TPA Version 3.2 code results, sensitivity analyses with the TPA Version 3.2 code, and quality assurance (QA). Reviewers were provided copies of all presentation materials, and encouraged to ask questions for clarification 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, each member of the ERG was asked to independently prepare a brief report evaluating their general area 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 the 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 RESULTS OF THE EXTERNAL REVIEW

This chapter provides a summary of the significant comments made by the external reviewers. It is noted that this summary does not include all the results and comments made by the external reviewers. To get the full context of the comments, the reader is encouraged to read the full reports provided by the reviewers of the 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. This report does not attempt to rebut any of the technical comments of the external review group, as it is simply a summary of their findings. However, in cases where the reviewers have misinterpreted the abilities of the TPA Version 3.2 code in their comments, a clarification of the capability of the code has been included.

The detailed technical presentations made by CNWRA and NRC staff during the formal meeting relieved the initial concerns of a number of the external reviewers regarding the technical bases for the code. Additionally, many reviewers had concerns about the QA Program under which the code was developed prior to the formal meeting, which were mostly eased by the formal and informal briefings on the CNWRA configuration control procedures. This indicates that the currently available background material supporting the TPA Version 3.2 code, which was given to the reviewers prior to the formal meeting, did not provide sufficient information about the sound technical underpinnings for the model abstractions, input data, and probabilistic approaches embodied in the code.

3.1 OVERALL IMPRESSION

There was general agreement among the reviewers that the TPA Version 3.2 code is well-developed and that the experience and qualifications of the NRC and CNWRA staff are appropriate for developing the code. There was general agreement that the code, with some improvements, is sufficient in technical quality and in flexibility to be used in the evaluation of the DOE LA as long as the repository design is similar to that described in TSPA-VA (U.S. Department of Energy, 1998). Despite this general appreciation for the technical content of the code, most of the reviewers commented that there were some areas of the code that still require additional work, particularly for analyses that extend beyond 10,000 yr.

The documentation of the code received mixed reviews from the group. Several of the reviewers concluded that the overall documentation was adequate to support the models used by the code, but improved traceability is needed for reviewers to find information in different documents. Additionally, several reviewers remarked that the transparency of the code was impressive, and documentation of the code and ability to view intermediate outputs from the code prevented the code from being a "black box." However, other reviewers felt the documentation of the TPA Version 3.2 code and supporting models was inadequate and felt that more documentation was necessary to define the TPA Version 3.2 code role within the NRC HLW program and provide information on how the code was developed. This will improve the understanding of how the code will be used by NRC staff in the review of the anticipated DOE LA and provide confidence to people outside the HLW program that the code results are reasonable.

In general, the individual experts indicated that the QA Program under which the code was developed seemed appropriate for the purpose for which the code will be used, though this was based on a very brief review of the program. Several reviewers stated that the QA Program should be clearly described in the documentation for the code for easy reference for users and reviewers of the code. Additionally, one reviewer questioned why the QA Program under which the TPA Version 3.2 code was developed was not as stringent as the QA Program required of the DOE TSPA code.

3.2 STRENGTHS AND WEAKNESSES OF THE TOTAL-SYSTEM PERFORMANCE ASSESSMENT VERSION 3.2 CODE

The reviewers identified many strengths of the TPA Version 3.2 code. There was general agreement that most of the modules in the code had strong technical bases, including field and laboratory data and detailed process modeling. Several reviewers stated that the model abstractions and data in the code captured the important aspects of the physical processes occurring at the YM site, and that it did not appear that any FEPs that were likely to be important to performance of the system had been omitted from the analyses. The reviewers noted that the disruptive scenarios modeled in the code were appropriate for the YM site, except for human intrusion, which is not modeled in the TPA Version 3.2 code.

The structure and flexibility of the code were consistently cited as strengths of the code. Many reviewers noted that the probabilistic nature of the code, using Monte Carlo sampling to account for parameter uncertainty, was appropriate for the evaluation of the DOE LA against the proposed regulations for the repository in draft 10 CFR Part 63. Specific compliments were given to the method that is used to treat the probability of disruptive events and the large variety of input parameter distributions available within the code. Several reviewers commented that the simple, clear structure of the code helped people understand the functioning of the TPA Version 3.2 code. One reviewer noted that the simplicity of the abstractions made it is possible to conduct a large number of PA calculations in a timely way and thus reduce statistical uncertainty in the results by improving the convergence of the results to a mean dose history that does not significantly change with an increased number of realizations. However, another reviewer commented that the NRC staff did not seem to place an appropriate level of attention on demonstrating that the results of the code did converge. The flexibility of the code was noted by several reviewers as a strength, based on both the ability of the code to model many different hypotheses and different design options, as well as the modular structure of the code allowing process-level models to be easily incorporated into the code. However, several reviewers noted that the flexibility of the code could be improved. They mentioned that although the code provides a very useful tool for evaluation of the current repository design under existing NRC regulatory requirements, if there is a substantial change in the design of the repository or the regulations imposed on the repository by the U.S. Environmental Protection Agency, the code may not be able to be modified easily to account for these changes.

Documentation was cited by most reviewers as a strength of the TPA Version 3.2 code. It was noted that the documentation would be particularly useful for users of the code who are familiar with the YM program. Specific aspects of the User's Guide that were noted by several reviewers as being useful include the clear description of the model abstractions and data, the identification of assumptions and weaknesses for each of the modules of the code, and the inclusion of the reference data set, which included references and justification for many of the values and distributions used to define input parameters. The transparency of the code was also cited as a strength by several reviewers, who noted that the information included in input and output files from modules was clearly described in the documentation.

Finally, the extensive use of sensitivity analyses was cited by many reviewers as a strength of the code. The reviewers commented that the use of these analyses provided significant insights into the workings of the code and should be viewed as a "notable achievement" (appendix A).

The reviewers also noted many weaknesses associated with the TPA Version 3.2 code and its documentation. Several reviewers cited problems in the conceptual models, which will be detailed in the next section. Many reviewers observed that the code did not account for various couplings among FEPs, which could potentially have a significant affect on the performance of the system. Several reviewers commented that the user interface of the code is poor and that the code could be made much easier to use and understand with a pre-processor to create input files and a post-processor to display code output and perform statistical and sensitivity analyses.

The majority of the weaknesses identified by the reviewers involved code documentation. Several of the reviewers stated that the TPA Version 3.2 code needs a more complete system of documentation in order for people outside the HLW program to understand fully the capabilities of the code and the technical work that has been completed that supports the model abstractions in the code. It was recommended that the documentation for the code contain a better description of the NRC HLW program and where the TPA Version 3.2 code fits within the program. Several reviewers stated that the method used to determine whether to include or exclude FEPs and interactions among FEPs in the TPA Version 3.2 code should be documented. This document could also track how FEPs are treated in different scenarios, different process level models, and different code modules. Additionally, several reviewers thought that the basis for selecting the radionuclides that are tracked in the TPA Version 3.2 code should be clearly identified and consistently followed. Other reviewers felt that additional documentation was needed for assumptions made in modules and data and that the documentation for these assumptions should be traced more easily back to technical documents. Some reviewers also thought that the level of QA, verification, and validation in the code needed to be more visible in the documentation. Several reviewers mentioned that some of the modules needed clearer presentation, including the EXEC module and several of the utility modules. There were also reviewers who thought that the lack of a document describing how to design and implement new modules was a weakness of the code. One reviewer commented that a logical flow chart illustrating the links between modules would improve the transparency of the code.

One reviewer mentioned that the results of the code should be studied by focusing on those realizations that lead to high doses. Also, it was commented that the sensitivity studies should evaluate the sensitivity of the code results to the distribution shapes selected for uncertain parameters.

3.3 SPECIFIC TECHNICAL COMMENTS

3.3.1 Comments Relevant to the Entire Code

Several external reviewer comments were relevant to the entire code. Thompson suggested that the code maintain an overall mass balance for the entire repository system in order to ensure that material is not inadvertently lost or double counted during the execution of the code. Ouzounian and van Dorp both indicated that the code needs a better basis for the selection of radionuclides to consider in the analysis.

Thompson commented that the excessive use of constants in the input data set could lead to an underestimation of the uncertainty in the system and that the use of unbounded Gaussian distributions is unwarranted as the truncation of the distribution could be questioned. Thompson and van Dorp noted that parameter uncertainty may dilute the calculated risk from the repository system while Thompson indicated that as long as the mean of the distribution was the best estimate for the parameter value, this may not be a concern. Van Dorp also recommended that the uncertainty in knowledge of processes should be evaluated and documented. Thompson recommended the evaluation of the implications of differing opinions when using expert elicitation to determine input parameter ranges and shapes. Thompson also recommended reanalyzing the parameter subranges and important subsystems of those realizations that contribute most of the overall risk in order to ensure that the modeling is appropriate for these higher risk realizations.

Thompson stated that Latin Hypercube Sampling may not be the most efficient type of random sampling that could be used, and suggested consideration of Importance Sampling instead. Van Dorp cautioned against imposing too many simplifications into the TPA Version 3.2 code to improve the efficiency of the code unless these simplifications are justified by more detailed considerations, as this can reduce transparency and lead to unexplainable results.

Thompson had several suggestions about using the TPA Version 3.2 code to compare design options or conceptual models. He was concerned that the excessive use of conservative assumptions in the modeling may lead to unrealistic estimates of the mean, which could affect comparisons between different design options. Additionally, he recommended that comparisons between alternative conceptual models and design options should include the uncertainty in the results, as opposed to simply comparing the mean dose curves.

3.3.2 Unsaturated Zone Flow Above the Repository (UZFLOW) Module

Although de Marsily indicated that he believed that the infiltration rates calculated by the UZFLOW module for both the present and future climates are reasonable, he and the other experts identified several areas in which the code required additional justification or improvement. De Marsily had concerns that the climate cycle being used in the TPA Version 3.2 code may be too simple and may not adequately represent the Milankovitch cycle, which may impact the timing of the increase in infiltration. Additionally, de Marsily indicated that the distribution of rain throughout the year may change as the climate changes, but this possibility is not considered in the TPA Version 3.2 code. This omission may or may not be conservative. Both de Marsily and van Dorp had concerns about the assumption that neglecting runoff was conservative as water that runs off from one area may collect in small depressions or more permeable areas, which may reduce evaporation and increase total infiltration. The TPA Version 3.2 code assumes that plants growing on YM would decrease infiltration due to evapotranspiration and conservatively neglects these effects. However, de Marsily indicated that this assumption needs to be investigated because the presence of biota on the ground surface can significantly increase the permeability of the soil and thereby increase the infiltration. Finally, de Marsily expressed concern that the code did not consider the potential for physical processes, such as fault movement opening or widening fractures or dilation of the rock due to the thermal loading associated with the repository, to increase the infiltration into the mountain.

3.3.3 Near-Field Environment (NFENV) Module

Several experts had concerns about the assumptions and data associated with the NFENV module. De Marsily recommended performing the thermal calculations with a three-dimensional model in order to reduce the associated error. He indicated that this improvement likely would not add much calculational burden and would result in a more accurate calculation of the temperature profiles within the drift. This would eliminate several assumptions currently made in the thermal calculation, including the potential for underestimating the temperature of the waste package (WP) surface by assuming a uniform distribution in space of the heat flux and the use of an effective axial length of the WP to calculate the heat transfer from the WP to the drift wall. This would also enable the calculation of the temperature variation from canister to canister due to differences in waste characteristics. These temperature differences may have a significant effect when the temperature at the canister surface drops below the boiling point.

Both Kelly and Ouzounian expressed concern that the chemical composition of the water contacting the WPs was poorly understood. Ouzounian did not believe that the chemical composition of J-13 water was necessarily representative of water that would be found in the unsaturated zone at the repository horizon. Both he and Kelly indicated that very little data are available to determine the effects of evaporation and condensation associated with the reflux process on water chemistry and that more experimental data were needed to define this process. Both indicated that additional detailed modeling of the chemical composition of water contacting the WP was necessary, which should consider thermal effects and the effects of contacting repository materials. Ouzounian suggested separately modeling the thermal (repository temperature above boiling) and post-thermal (repository temperature below boiling) phases to appropriately incorporate all the processes associated with each phase.

De Marsily and Kelly had concerns about the justification behind the factors sampled in the TPA Version 3.2 code to determine the quantity of water dripping onto and into the WP. Both indicated that the current values for the F_{ow}, F_{mult}, and F_{wet} factors are not defensible in any scientific way and additional detailed modeling to provide an acceptable range of uncertainty for these parameters is needed. In contrast, Ouzounian indicated that the conceptual model used to represent dripping on WPs is attractive and complimented the analyses that have been performed to determine these parameters. However, he questioned the assumption that dripping would only occur when infiltration is greater that the hydraulic conductivity of the rock, as this is only true for homogeneous systems in which there are no rough patches on the wall and no additional interactions between wall materials and water. Ouzounian also commented that keeping the F_{ow} factor constant through time was not a very good model for the process, as the fraction of water that enters the WP will increase as the WP increasingly degrades. He recommended tracking the size of pits in the WP surface in order to improve the estimate of the quantity of water entering the WP. Several experts indicated that additional couplings between the dripping model and other FEPs should be considered. Kelly recommended that the dripping abstraction should be coupled to fracture flow, and he and van Dorp suggested that the dripping abstraction should consider the effects of collapsed drifts on infiltration rates. Although the dripping abstraction in the TPA code considers fracture flow, this coupling clearly needs to be documented better in the TPA code documentation.

Finally, van Dorp, Brady, and de Marsily indicated that the TPA Version 3.2 code should consider the effects of the increased temperatures on the rock surrounding the repository. Brady indicated that thermal expansion of the rock between the drifts could cause a reduction in the vertical permeability in this rock and reduce the amount of refluxed water that drains between the drifts. De Marsily commented that the thermal stresses could affect the quantity of rock that could fall during a seismic event. Van Dorp indicated that the thermal stresses caused by these temperature increases could cause reactivation of faults in the repository area.

3.3.4 Failure of the Engineered Barrier System Due to Corrosion (EBSFAIL) Module

Kelly expressed his compliments on the EBSFAIL module by declaring that the work done in developing it was "one of the most noteworthy achievements in corrosion engineering in the last 50 years" (appendix D). Despite this general praise, several concerns were raised with the WP corrosion modeling.

Ouzounian and Kelly both indicated that a better understanding of the chemical environment on the surface of the WP was necessary to determine the corrosion potential that will develop. Kelly and de Marsily expressed concern about the use of only a few years of data to predict corrosion processes for tens to hundreds of thousands of years. Kelly also indicated that more work was needed to assess the effects of localized corrosion due to the importance of the long-lived WP, but added that the basic model was excellent.

Several reviewers suggested that additional processes should be considered in the corrosion model. Kelly and de Marsily recommended determining whether water-saturated rocks contacting the WP could influence the WP degradation rate due to crevice corrosion. Kelly indicated that the code should have the ability to model the production of peroxide on the WP surface due to radiolysis, in case the DOE changes to a WP with thinner walls that result in higher radiation fluxes at the surface. Kelly also recommended that the effects of sulfur on the WP be modeled in the code because sulfur has been reported to be present in the drifts and is known to lead to faster uniform corrosion of nickel-based alloys. Both Kelly and van Dorp indicated that the code should be able to account for coupling between the corrosion and mechanical failure models, such that packages that are damaged by rockfall, but not failed can undergo accelerated stress-corrosion cracking. Kelly and van Dorp also indicated that the effects on the corrosion rate of welds and interactions between the dissimilar materials making up the WP should be evaluated. Kelly indicated that for some corrosion resistant alloys, it is worse for the material to be in contact with a less corrosion resistant material than a deformable crevice. Van Dorp also commented that increasing the ventilation in the repository could increase the salt content of solutions that enter the drift, and thereby increase the corrosion rate of the WP. De Marsily commented that WPs with relatively low activity waste could have an outer surface that is cooler than the drift wall and serve as a condensation surface. This could lead to significantly more moisture collecting on the surface of the WP, influencing the corrosion rate; this process is not captured in the TPA Version 3.2 code. Kelly also indicated that the corrosion model should be able to determine the pit density on the WP through time in order to calculate the amount of water that can enter the WP, which is likely to increase through time.

3.3.5 Release from the Engineered Barrier System (EBSREL) Module

The primary concern about the models in EBSREL was that the chemistry of the water within the WP is not well understood. Both Kelly and Ouzounian mentioned that a better understanding of the chemical composition of the water inside the WP is necessary to defend the models in the TPA Version 3.2 code. As indicated earlier, Ouzounian did not believe that J-13 water would be representative of water found in the unsaturated zone prior to entering the WP. Kelly commented that the code should evaluate the effect of constituents from the container materials on the water chemistry, and stated that reactions between the water and the materials in the WP may lead to elevation of solution pH within the package. Kelly added that this may affect the dissolution rate and nature of the spent nuclear fuel (SNF) reaction products and should be considered. Kelly recommended investigating whether equilibrium may be achieved for one component of the SNF that dominates the local pH, which may lead to incongruent dissolution of other fuel components.

Ouzounian indicated that the current modeling of SNF dissolution rate seemed reasonably conservative, but had concerns that it may be overly conservative as the consideration of secondary minerals may lower the dissolution rate by several orders of magnitude. He indicated that the three orders of magnitude difference in dissolution rates between the natural analog and base models shows that more work has to be done to reduce uncertainty in the model. He also commented that the mineral phases in the SNF need to be well-characterized, as the dissolution rate of SNF typically is about 100 times that of fresh fuel. Ouzounian had concerns that the radiolytic effects on the dissolution rate of fuel were not considered in the code and recommended considering these effects or providing rationale for excluding these effects from the modeling.

Ouzounian, de Marsily, and van Dorp commented on modeling radionuclide release from the gap and grain boundary. Ouzounian indicated that the inventory of radionuclides in the gap and grain boundary seemed reasonable, but more justification was needed for these values, whereas de Marsily stated that the early release of fission products located at fuel grain boundaries does not seem to be properly addressed. Van Dorp stated that the code documentation does not indicate that the gap inventory is properly accounted for, but stated that after discussions during the formal meeting, he believes that the gap inventory is appropriately considered in the code.

For the bathtub model in the code, Kelly commented that radionuclides could be released from fuel above the waterline by either water dripping on and running down the fuel or humid air corrosion and recommended consideration of these processes. Ouzounian indicated that the long-term behavior of fuel cladding was difficult to predict and agreed with the approach in the TPA Version 3.2 code of limiting credit for the cladding.

3.3.6 Unsaturated Zone Flow and Transport Below the Repository (UZFT) Module

De Marsily indicated that the model used for unsaturated zone flow and transport is generally adequate and consistent with available ^{36}Cl data for YM. However, several reviewers commented on the conceptual model. De Marsily did not agree that radionuclides in fractures in one unsaturated zone layer would reenter the matrix when they entered an unsaturated zone layer in which matrix flow dominated. Instead, he thought that it was likely that the fracture would continue through all layers below it until the radionuclides reached the saturated zone. He recommended that the code model radionuclides that enter fractures as remaining in fractures to the water table unless a process such as matrix diffusion removed them from the fracture.

Several reviewers commented that the groundwater flow modeling was not flexible enough to consider some potentially significant processes. De Marsily commented that assuming that the thermal pulse had no effect on the groundwater hydrology below the repository—because WPs do not fail due to corrosion until after the thermal phase—was not defensible. He indicated that juvenile failures could lead to early releases from the WP and the UZFT model would not appropriately model the transport of these radionuclides through the unsaturated zone. Thompson and van Dorp stated that the code should consider the effects of faulting, seismicity, and volcanism on the groundwater flow system.

The treatment of retardation in the unsaturated zone was commented on by several reviewers. Whicker commented that the assumption of no retardation in fractures seemed overly conservative because it is likely that some fine material would collect in the fractures and provide a surface for retardation of radionuclides. Van Dorp commented that sorption coefficient (K_d) values for chemically similar elements should be correlated because they will tend to have comparable behavior under similar chemical conditions. Currently, the code includes correlations in K_d values for only a few actinides in the saturated alluvium. Van Dorp and Whicker both noted that the TPA Version 3.2 code should account for colloid transport, although van Dorp indicated that zero retardation in fractures can adequately, though very conservatively, model colloidal transport. Whicker also commented that the K_d value for plutonium seemed very low.

3.3.7 Saturated Zone Flow and Transport (SZFT) Module

The basis for the SZFT module received numerous comments from the external reviewers. De Marsily in particular felt that the available hydrogeologic data were insufficient to justify the SZFT model. He stated the U.S. Geological Survey (USGS) data reports on which the SZFT model is based are inadequate. De Marsily's comments on the USGS data reports include the (i) role of the paleozoic carbonate aquifer is unclear as to whether water is flowing in or out of the carbonate, or both; (ii) horizontal anisotropy of the fractured volcanic tuff makes direction and velocity of flow difficult to determine; (iii) connectivity in the fracture network is not clear, so the level of mixing is difficult to determine; (iv) relationship between the volcanic tuff and alluvium is not clear so the level of vertical mixing in the alluvium is difficult to determine and the contact between the two rock types is poorly defined; and (v) geometry of the alluvium is not well-defined, and it is not clear where community wells will be drilled. As for the SZFT modeling itself, he questioned the use of streamtubes because the assumption of isotropic flow in the volcanic tuff is not defensible. He stated that the flow direction through the carbonate aquifer must be determined to define a recipient zone and that flow in the tuff cannot be modeled as an equivalent porous medium, especially if a well can be drilled in the tuff (which could only occur if the receptor was located less than 10 km from the repository). He commented that the layering of the alluvium must be characterized to perform defensible dilution calculations and that the modeling of matrix diffusion using a linear exchange coefficient in NEFTRAN is crude and should be modified to use half the distance between fractures, or another defined length, as the diffusion length. Based on this lack of data, he recommended replacing the SZFT model with a simple conservative model that, for each subarea, transports all the water and radionuclides that reach the saturated zone to a community well with little or no retardation. With this modeling, the water flowing from a single subarea (about 5,000 m^3/yr) can support a small community drinking well.

Other reviewers provided less extensive comments on the saturated zone flow and transport modeling in the TPA Version 3.2 code. Whicker questioned the assumption that there is no lateral dispersion in the streamtubes and whether the entire radionuclide plume will be captured by wells. De Marsily, Thompson, and van Dorp commented that climate change may alter the saturated zone flow pattern due to the rising water table. Thompson and van Dorp indicated that the saturated zone flow pattern could also be altered by disruptive events including seismicity, faulting, and volcanism, which should be considered. Ouzounian suggested that more work be done to investigate the spatial variability of geochemical properties of fracture surfaces and the rock matrix, and the heterogeneity of transport pathways at pore scale and formation scale, to determine if these variables could have a significant effect on performance.

3.3.8 Dose Conversion of Radionuclides in Groundwater (DCAGW) Module

Overall, reviewers seemed to agree with the use of dose conversion factors (DCFs) in the module DCAGW. Whicker indicated that the DCFs are used appropriately within the TPA Version 3.2 code and that not using worst-case assumptions when developing DCFs is reasonable.

Several recommendations were made by the reviewers to improve the modeling of DCFs. Whicker recommended using a range of DCF values instead of the mean values in the TPA Version 3.2 code in order to appropriately capture the uncertainty in the DCF values in the calculations. Whicker and van Dorp both commented that the code should model the buildup of radionuclides in the soil due to multiple years of irrigation with contaminated water and contaminated plant and animal wastes being returned to the soil. Whicker recommended conducting a study to determine site-specific plant-to-soil concentration ratios and feed transfer coefficients as these typically vary significantly from site to site. Whicker also commented that the consideration of only the drinking water pathway may be nonconservative for the receptor location less than 10 km from the repository if the residents at that location purchase food from Amargosa Valley or maintain a garden at this location. Whicker and de Marsily commented that the dose from water used in "swamp coolers" and humidifiers should be considered in the DCFs. De Marsily also stated that assuming a water consumption rate of 2 L/day may be nonconservative in an arid environment such as southern Nevada. Van Dorp suggested modeling a critical group at the release point of the groundwater in Death Valley if the radionuclides are not taken up by the wells, and considering doses from free-flowing wells in Amargosa Valley if the groundwater rises from its present depth during periods of cooler temperatures and increased rainfall.

3.3.9 Failure of the Engineered Barrier System Due to Seismic Events (SEISMO) Module

The experts who reviewed the SEISMO module indicated that the model was implemented correctly and the assumption of no backfill was conservative, but stated that improvements could be made to the model. Brady indicated that the modeling could be improved by using a three-dimensional finite element analysis to determine the behavior of the WP under dynamic loading. This would allow the evaluation of interactions between the rock and WP when both are in motion, as well as WP damage and rupture based on the principles of fracture mechanics. Brady and van Dorp indicated that the thermal stresses created by waste emplacement could cause rock slip on existing faults and increase the seismicity of the region. Thompson, van Dorp, and Brady stated that the occurrence of seismicity, faulting, and igneous activity should be correlated, whereas Delaney indicated that, because igneous activity initiates at depth, it may not be correlated to surface ground motion. Thompson commented that, for time periods of interest of longer than 10,000 yr, larger seismic events than are currently possible may need to be modeled in the code.

3.3.10 Failure of the Engineered Barrier System Due to Faulting Events (FAULTO) Module

Brady commented that the method used to calculate the recurrence rate of faulting in the repository region is scientifically sound, and provided several suggestions on improvements to modeling the consequences of the faulting event in the FAULTO module. Brady indicated that more research should be done to determine the threshold fault displacement that will cause rupture of the WP. Brady also commented that the code should be able to consider modes of damage other than complete rupture of the WP, such as an increase in corrosion rate due to the stresses placed on the WP during the event. Brady suggested that several processes may have the potential to initiate fault slip, including seismic events and the thermal stresses arising from temperature increase of the rock. Finally, Brady indicated that the assumption that there is no backfill in the repository would be nonconservative for the FAULTO module if the design of the repository changes from that specified in TSPA-VA (U.S. Department of Energy, 1998) and backfill is actually used. As mentioned above, several experts suggested that the correlations between the occurrence of faulting, seismicity, and igneous activity should be investigated.

3.3.11 Failure of the Engineered Barrier System Due to Igneous Activity (VOLCANO) Module

Delaney indicated that the probability of volcanism within the repository area is very well determined and modeling release with the VOLCANO module is acceptable. Thompson commented that, for time periods of interest of longer than 10,000 yr, the code may need to be able to model multiple volcanic events impinging on the repository, which complicates the scenarios that need to be analyzed. Kelly indicated that the assumption that all WPs contacted by magma fail may be overly conservative, as C-22 is unlikely to melt at a magma temperature of 1,100 °C. However, he acknowledged that the containers could experience creep, leading to failure, and that the interplay between the stresses in the WP due to the eruption and the creep rates are unknown. De Marsily suggested that the code should consider other effects of volcanism than direct release, including failure of WPs that are not directly exhumed and changes in groundwater flow patterns. The former effect is included in the TPA Version 3.2 code, but the documentation should be improved to make this clearer. Again, several experts suggested that the correlations between the occurrence of faulting, seismicity, and igneous activity should be investigated.

3.3.12 Airborne Transport of Ash (ASHPLUMO) Module

Delaney's review of the ASHPLUMO code concluded that although the module is based on an empirical ash-dispersal model, improvements due to better modeling "would have a marginal effect, at best, on the total population of outcomes" (appendix B). He recommended the development of a research program to develop more sophisticated ash-dispersal models to compare to the results of the Suzuki model and to develop a better basis for the input parameters for the code. Delaney and van Dorp recommended additional consideration be given to transport of ash in directions other than toward the critical group during the eruption. Delaney suggested collecting data on the wind direction, speed, and atmospheric stability at the expected heights of the ash clouds and integrating the ash-fragment paths through changing wind conditions throughout transport. Van Dorp also mentioned that the assumption that waste is homogeneously distributed in the ash, and not concentrated in thin layers within the blanket, should be evaluated.

3.3.13 Removal of Radionuclides from an Ash Blanket (ASHRMOVO) Module

Delaney commented that the ASHRMOVO module handled the travel of radionuclides after deposition on the ground due to a volcanic event very well. However, he noted that an assessment should be performed to determine the dose effect of radioactive material that is deposited close to the volcanic event and later redistributed and redeposited at the critical group location by fluvial processes. He gave this as his primary concern with the TPA code.

3.3.14 Dose Conversion of Radionuclides on the Ground Surface (DCAGS) Module

The experts who reviewed the DCAGS module commented that the use of DCFs to convert soil concentrations to doses was reasonable. Whicker's comment on the DCAGW module that the DCFs should be assigned a range of values because of their uncertainty applies to the DCAGS module as well. Additionally, Thompson commented that the influence of volcanic deposits on soil characteristics should be considered in the derivation of DCFs in the code.

3.4 LEVEL OF DOCUMENTATION AND QUALITY ASSURANCE

Many comments were received from the experts concerning the level of documentation of the TPA Version 3.2 code. Some reviewers were impressed with the documentation available for the code, but many felt that the documentation was inadequate and had suggestions to improve it.

The most common criticism of the documentation was related to the selection of the FEPs to be modeled in the code. Most reviewers commented that a systematic process should be developed to identify all FEPs potentially present at the site and interactions between these FEPs. The documentation of the code should then provide justification for either modeling or excluding these FEPs and interactions among FEPs so that reviewers of the code can quickly determine which FEPs have been modeled in the code and which have been considered but not modeled. Additionally, van Dorp suggested that this documentation should indicate how the FEPs were modeled in different modules in the code and different process level models to help ensure the consistency of the code. Several reviewers suggested that this FEPs identification process be conducted independently by the NRC, without reliance on the current DOE list. Similarly, several reviewers suggested that the list of radionuclides to be considered in NRC models be developed independently of DOE.

Several reviewers felt that the User's Guide by itself was an inadequate document to provide a comprehensive review of the approach being taken by NRC to analyze the DOE LA. The reviewers indicated that a document was needed to explain the assessment context for which the TPA Version 3.2 code was being developed and how the TPA Version 3.2 code will be used by the NRC in evaluating the DOE LA. Van Dorp recommended including a discussion in the User's Guide of the advantages and disadvantages of using a total-system code instead of individual subsystem codes or process level models.

Reviewers indicated that the model development process should be made more traceable. Ouzounian suggested the addition of simple flow charts to the User's Guide to demonstrate how information is transferred between code modules. Thompson suggested each of the TPA modules should be documented, including the entire chain of reasoning that led to their development and van Dorp commented that this sort of documentation system should include the rationale for selecting the conceptualization that was used in the module as opposed to other apparently valid approaches. This would help put the TPA Version 3.2 code in a framework consisting of past and future project phases. Additionally, van Dorp and Ouzounian suggested that the description of modules should include a summary of limitations and boundaries of applicability of the modules and data to ensure that computation is not performed outside of the domain of validity. Thompson and van Dorp commented that data should be able to be traced from laboratory or field testing through incorporation in the code in input parameters or model abstraction. Ouzounian, Thompson, and Kelly recommended providing "road maps" to assist in the tracing of particular issues through sets of related documents. Thompson recommended identifying site-specific data as opposed to data from the literature and identifying whether the DOE data and assumptions used in the TPA Version 3.2 code have undergone independent review by NRC staff prior to their use in the code.

Several reviewers commented that the inclusion of the reference data set in the User's Guide was a very effective way to summarize data and provide links to the source of the data. However, van Dorp and Thompson both indicated that the current version of the reference data set provides insufficient justification for many parameters and needs further development to be useful. Delaney indicated that a strong body of fundamental scientific research was necessary to justify parameter values in the code.

Thompson recommended clearly explaining the assessment toolkit from a software engineering standpoint, including a description of the structure of the codes and how data are transferred between modules. Whicker suggested adding a more complete description of the GENII-S code and the parameters used to calculate DCFs in the User's Guide.

Thompson suggested rewriting documents, particularly NUREG–1668 (Nuclear Regulatory Commission, 1999), in plain language so they are more easily understood.

Kelly and Thompson both suggested documentation systems that could be used to support the TPA Version 3.2 code. Kelly's system consisted of the following features:

- An overview of the code that describes the approach taken and contains links to additional information on the consequence modules
- Consequence module descriptions that contain links to any external codes used as the basis for the model abstractions and the documents that provide the data used for the analyses
- Influence diagrams that clearly show which issues are modeled and are not modeled in the code

Thompson's system consists of the following:

- An overview document of the NRC program for YM, including information on the site and a description of the documentation system
- A document that contains a worked example of the TPA Version 3.2 code, which could include the Reference Data Set
- A User's Guide similar to the current version but containing a wider coverage of output analyses. This document should also contain diagrams of the overall integrated system structure, and showing the flow of all data within and between modules
- A Technical Derivation Report for each module that contains a detailed account of the derivation of the abstraction and quantitative justification of each module
- A system conceptual model detailing the FEPs that have been screened out or retained and justification for these decisions; this document should also describe all expert elicitation sessions conducted to support data or models in the code
- A factual database document

Most reviewers felt that the level of QA that the code was developed under was adequate for the planned use of the code and the QA Program provided confidence in the results of the models. In fact, Brady was particularly complimentary and noted that "the code is developed in an environment of rigorous configuration management" (appendix A). However, de Marsily questioned why the NRC TPA code was developed at a lower level of QA than the DOE TSPA code. Most reviewers mentioned that the QA Program and software standards under which the TPA Version 3.2 code was developed should be documented in the User's Guide.

Brady indicated that additional verification of the entire code should be attempted and suggested two possible methods. The first would be to construct a prototype to represent the entire repository system. The second would be to modify the TPA Version 3.2 code input data set to model a natural analog, such as the Peña Blanca uranium ore body and compare the TPA Version 3.2 code estimates of radionuclide transport to measured values. De Marsily recommended benchmarking the TPA Version 3.2 code by comparing its outcome with a similar calculation done on the DOE TSPA code, using as close as possible input data and scenarios. Whicker suggested verifying the results of the GENII-S code used to generate DCFs using another standard industry code such as RESRAD (Argonne National Laboratory, 1998), DandD (Sandia National Laboratories, 1998), ECOSYS (Müller and Pröhl, 1993), or comparing the results to real data.

4 SUMMARY AND CONCLUSIONS

The external reviewers were generally positive about the quality of work that has gone into developing the TPA Version 3.2 code and were of the opinion that the code was suitable for purposes of reviewing the DOE TSPA in support of the LA. During the July 1999 meetings, it was revealed that a number of the external experts had developed misgivings, about the technical bases for the code, that were largely allayed by the detailed technical presentations made by CNWRA and NRC staff. This underscores the widespread concern among the experts that the background reading material given to them prior to the meeting did not provide sufficient information. There was a sense among the experts that the lack of formal documentation associated with the TPA Version 3.2 code "sells short" the sound technical underpinnings for the model abstractions, input data, parameter values, and probabilistic approaches embodied in the code. Concerns by a number of the external reviewers regarding the rigor of the QA Program under which the TPA Version 3.2 code was developed were also eased by formal and informal briefings on the CNWRA configuration control procedures embodied in Technical Operating Procedure (TOP)–018, Development and Control of Scientific and Engineering Software, and by a visit to the CNWRA QA records vault.

There was a general feeling that many of the initial concerns voiced by the external reviewers would not have arisen had more effort been devoted to developing a system for tracking and identifying all of the documents that support the TPA Version 3.2 code. Indeed, a major criticism, which was made by a majority of the external reviewers, of the TPA Version 3.2 code, is that the level of documentation is insufficient. In particular, the experts suggested that the transparency of the processes and physical interactions in the TPA Version 3.2 code would be greatly enhanced by producing documentation detailing the methods used to screen FEPs. Such documentation should perhaps include FEPs interaction diagrams. Although several of the experts thought that appendix A of the TPA Version 3.2 code User's Guide was commendable in its effort to trace the sources of the input data used, others felt that the effort fell short of providing the level of data traceability required for thorough review of a safety assessment.

There was general agreement that the modules in the TPA Version 3.2 code had solid technical bases and that the model abstractions and data included in these modules captured the important physical processes occurring at YM. Nonetheless, the experts provided many suggestions for improving the technical bases of the code. An over-arching 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 of the 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. Some of the external reviewers also felt that the interdependence of seismicity, tectonism, and volcanism warranted greater consideration. The external reviewers proposed many other technical improvements to the TPA modules that are summarized in section 3.3. However, there was particular concern that the level of understanding of the saturated zone hydrogeology at YM is insufficient to support the development of a credible transport model.

Many of the technical improvements suggested by the external reviewers can and will be implemented in Versions 4.0 and 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 the effect that the suggested change has on reducing uncertainty in the performance calculation (i.e., dose to the critical group). Those improvements requiring additional site-specific data may not be implemented until new data are gathered by DOE during the performance confirmation period. Again, it must be stressed that gathering site data is solely the responsibility of the DOE. The recent strategic plan for the development of the TPA code (Mohanty and Wittmeyer, 1999) strongly recommends that future effort focuses on developing thorough documentation for the TPA code. A subset of the supporting documents recommended by Thompson and Kelly may be developed in order to facilitate the use of the TPA code during the LA review and to build public confidence in the decision-making process.

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APPENDIX A

External Review

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

Report by Barry H Brady

Final version, 25/8/1999

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Contents

The views expressed in this report are those of the author only and do not reflect those of The University of Western Australia or any other organization with which the author has been or is associated.

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

September 1999

Nuclear Regulatory Commission
Center for Nuclear Waste Regulatory Analyses
Southwest Research Institute
San Antonio, Texas

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

Comments by:

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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

Nuclear Regulatory Commission
Center for Nuclear Waste Regulatory Analyses
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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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University Paris VI

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

(ii) 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.

(iii) 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.

(iv) 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 :

(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 ?

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. <u>Comments on the hydrology of the unsaturated zone</u>

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.

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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) Review of Report USGS R96-4300

1. Boundaries. 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. Lithofacies. 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 :

(i) 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.

(ii) 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

External Review of

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

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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

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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ANDRA (France)

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:
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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

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:

(a) 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.

(b) 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.

(c) 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?

(d) 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.

(e) Unbounded Gaussian pdf's are unjustified surely as the truncation is open to endless discussion.

(f) 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?

(g) Some confusion over terms e.g. how can a 'best estimate' also be a 'conservative' value?

(h) 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.

(i) 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:

(a) 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.

(b) 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.

(c) 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.

(d) 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:

(a) understand and reduce uncertainty and,
(b) 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:

(a) 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 x 10^{-5} p.a. from the base case or up to 7 x 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.

(b) 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.

(c) 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.

(d) 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?

(e) 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.

(f) 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):

(a) **'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.

(b) **'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.

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.

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[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.

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.

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.

[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).

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3. US Department of Energy (DOE), Viability Assessment of a Repository at Yucca Mountain, Office of Civilian Radioactive Waste Management, Las Vegas, Nevada, DOE/RW-0508, 1998, in five volumes:
   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

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

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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?

APPENDIX G

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

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.