BUILDING CONFIDENCE IN U.S. NUCLEAR REGULATORY COMMISSION QUANTITATIVE SAFETY ASSESSMENT METHODS: EXTERNAL PEER REVIEW OF THE TOTAL-SYSTEM PERFORMANCE ASSESSMENT VERSION 3.2 CODE [a]

by
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ABSTRACT

To build confidence in its readiness to review the U.S. Department of Energy (DOE) post closure safety case for the proposed Yucca Mountain (YM) repository, the Nuclear Regulatory Commission (NRC) undertook an independent peer review of its 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 and DOE 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 DOE safety case for the proposed YM 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 safety case. 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 the level of documentation used to support the TPA Version 3.2 code. The results of this peer review will be used to guide the development of future versions of the TPA code.

INTRODUCTION

The Nuclear Regulatory Commission (NRC), with technical 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 (PA) (1), to evaluate preliminary Total System Performance Assessments (TSPA) conducted by the DOE [e.g., TSPA-95 (2)], and to investigate the safety case supporting the DOE Viability Assessment (VA) (3). 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.

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 (4), that provides 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[b]; Mohanty et al., 1999[c]; Lu and Mohanty, 1999[d]; and Jarzemba and Sagar, 1999[e]). Development of an extensive body of peer-reviewed literature needed to support the TPA code is a time-consuming process and will continue in the future.

Conducting organized peer reviews by external experts to establish the technical or scientific merit of research and development programs are a well-established practice among federal agencies (5). Because the timing and execution of the peer-review process is largely controlled by the organizing body, an organized peer review can be an efficient procedure for vetting a research and development program, and assure that abbreviated timeframes, 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 reviews 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. FACA requires that advisory committees conduct open meetings, publish timely meeting notices in the Federal Register, record detailed meeting minutes, make available to the public all records of working papers and reports used by the committee, and have in attendance at each advisory committee meeting a designated officer of the Federal Government.

Approximately 3 years ago, the DOE established a Performance Assessment Peer-Review Panel 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 of the panel.

The NRC instructed CNWRA staff to conduct an organized peer review of the TPA Version 3.2 code and the overall NRC TPA methodology. This review was not undertaken to obtain 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. A summary of the key results is provided in this paper; however, the reader is referred to Weldy (6) to examine in detail the specific strengths and weaknesses of the TPA Version 3.2 code identified by the ERG.

THE EXTERNAL REVIEW GROUP

The members of the ERG were selected using a peer nomination process. One hundred twenty letters were sent to members of the international PA community soliciting nominations for experts in eight general areas of technical expertise which were identified as geochemistry, hydrology, material sciences and corrosion engineering, rock mechanics and mining engineering, health physics, volcanology, overall PA, and features, events, and processes analysis.

Fifty responses were received. Based on the number of nominations received, experts were identified by peer acclamation (largest number of recommendations) 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.

Selected nominees were contacted regarding availability and willingness to participate in the external review of the TPA Version 3.2 code. Nominees were asked to provide information to assess any conflict-of-interest (COI). Eight participants in the identified technical areas were selected based on availability and freedom from COI (Table I).

Table I. Members of the external review group for the Total-system Performance Assessment code

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

Because of the uniqueness of the proposed repository at YM, technical expertise in the different components of the repository was considered more relevant than familiarity with the DOE HLW disposal program.

Each member of the ERG was provided with the TPA 3.2 User's Guide (4) and the TPA 3.1 Sensitivity Analysis Report, NUREG–1668(7), for their initial independent evaluation of the TPA Version 3.2 code.

In addition, references cited in the reports were provided to the reviewers upon request. The materials for review were provided to the members of the 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 weeks were available to review the material prior to meeting with CNWRA and NRC staffs in San Antonio, Texas. Final comments were provided by the reviewers approximately 3–4 weeks after the meeting.

SCOPE OF THE EXTERNAL REVIEW

The overall goal of conducting the external review of the TPA Version 3.2 code was to receive an independent critical evaluation of the NRC approach to PA from recognized authorities in fields of research that span the technical issues considered in the TPA Version 3.2 code. The review included the TPA Version 3.2 code and associated documentation, but not the NRC HLW program nor the regulations associated with the YM repository. Specifically, the ERG was provided a list of primary goals for the review of the TPA Version 3.2 code. The reviewers were asked to (i) examine the methods and assumptions of the NRC TPA studies as implemented in the TPA Version 3.2 code; (ii) recommend improvements that could be made in subsequent revisions, modifications, and updates of the TPA code; (iii) evaluate implementation of conceptual models, including parameter choices; and (iv) determine whether the NRC approach to PA is suitable for achieving its objectives of reviewing the DOE safety case.

In addition to these primary goals, the members of the ERG were given 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 regulatory 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 considering the intended application of the code to support the NRC licensing decision?

The reviewers were also requested to provide questions and discussion points for the staff prior to the 3-day meeting in San Antonio, Texas.

RESULTS OF THE EXTERNAL REVIEW

This section provides a summary of the significant comments made by the external reviewers. For the full context of the comments, refer to Weldy et al. (6), which include as appendices the reports prepared by each member of the ERG, this paper makes no attempt to rebut any of the technical comments of the ERG—it is simply a summary of the findings. In cases where the reviewers have misinterpretation of the abilities of the TPA Version 3.2 code in the reviewers comments, however, a clarification of the capability of the code has been included.

The detailed technical presentations made by CNWRA and NRC staffs during the formal meeting relieved the initial concerns of several external reviewers regarding the technical bases for the code. Additionally, many reviewers had concerns about the quality assurance (QA) program under which the code was developed. These concerns were eased by formal and informal briefings on the CNWRA software configuration control procedures. The need for briefing indicates that the currently available background material on the TPA Version 3.2 code given to the reviewers prior to

the formal meeting did not provide sufficient information about the technical underpinnings for the model abstractions, input data, and probabilistic approaches embodied in the code.

Overall Impressions

General agreement among the reviewers was that the TPA Version 3.2 code is well developed and the developers of the code are well qualified. There was general agreement that the code, with some improvements, is sufficient in technical quality and flexibility to be used in the evaluation of the DOE safety case as long as the repository design is similar to that described in the TSPA-VA (3). Despite this general appreciation for the technical content of the code, most reviewers commented there were areas of the code that require additional research, particularly analyses that extend beyond 10,000 yr.

Code documentation received mixed reviews from the group. Several reviewers concluded that the overall documentation was adequate to support the models used by the code, but improved traceability is needed to locate information in other documents. Additionally, the transparency of the code was impressive, and documentation of the code and the ability to view intermediate outputs from the code prevented the code from being a "black box." Other reviewers felt the documentation of the code and supporting models was inadequate and more documentation was necessary to define the TPA Version 3.2 code role within the NRC HLW program and to provide information on how the code was developed.

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. Several reviewers stated that for easy reference the QA program should be clearly described in the code documentation. Additionally, one reviewer questioned why this QA program, was not as stringent as the QA program required of the DOE TSPA code.

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 it did not appear that any FEPs 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 the probabilistic nature of the code was appropriate for the evaluation of the DOE safety case against the proposed regulations for the repository. Specific compliments were given to the method 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 possible to conduct a large number of PA calculations in a timely way and thus reduced statistical uncertainty in the results by improving the convergence of the results to a stable mean dose history. 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, and the modular structure of the code to allow process-level models to be easily incorporated into the code. Several reviewers, however, noted that the flexibility of the code could be improved.

Documentation was cited by most reviewers as a strength of the TPA Version 3.2 code. Code documentation would be particularly useful for users of the code familiar with the YM program. Specific aspects of the User's Guide noted by several reviewers as useful include clear description of the model abstractions and data, identification of assumptions and weaknesses for each of the modules of the code, and inclusion of the reference data set, which contained 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, noting the information in input and output files from modules was clearly described in the documentation.

Finally, the extensive use of sensitivity analyses was cited as a strength of the code. Many 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."

The reviewers 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 potentially could have a significant effect on the performance of the system. The user interface of the code is poor and 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 involved code documentation. Several reviewers stated that the TPA Version 3.2 code needs a more complete system of documentation for people outside the HLW program to understand fully the capabilities of the code and the technical work that supports the model abstractions in the code. It was recommended that the documentation for the code should contain a better description of the NRC HLW program and how 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 documentation 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 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 back more easily to technical documents. The level of QA, verification, and validation in the code needed more visibility in the documentation. Reviewers 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.

Technical 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 to ensure that material is not inadvertently lost or double counted during the execution of the code. Ouzounian and van Dorp 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 uncertainty may not be a concern. Van Dorp also recommended that the uncertainty in knowledge of processes should be evaluated and documented. Thompson recommended 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 to the overall risk to ensure 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. Van Dorp cautioned against imposing too many simplifications into the TPA Version 3.2 code to improve the efficiency of the code because these simplifications 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.

Unsaturated Zone Flow Above the Repository Module

Although de Marsily indicated he believed the infiltration rates calculated by the unsaturated zone flow module for both the present and future climates are reasonable, he had concerns that the climate cycle used in the code is too simple and may not adequately represent the Milankovitch cycle, which may impact timing of the infiltration increase. Additionally, de Marsily suggested the TPA code should consider that the distribution of rain throughout the year may change with the climate. Both de Marsily and van Dorp had concerns about the assumption that neglecting runoff was conservative because 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 this assumption needs to be investigated because the presence of biota on the ground surface can significantly increase the permeability of the soil. Finally, de Marsily expressed concern that the code did not consider the potential that fault movement, or widening fractures caused by the thermal load, might increase infiltration into the mountain.

Near-Field Environment Module

Several experts had concerns about the assumptions and data associated with the near-field environment module. De Marsily recommended performing the thermal calculations with a three-dimensional (3D) model to produce more accurate estimates of the temperature profiles within the drift. A 3D model 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. A 3D model would also enable calculation of the temperature variation from canister to canister because of differences in waste characteristics. These temperature differences may have a significant effect when the temperature at the canister surface drops below the boiling point.

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 well water was necessarily representative of water that would be found in the unsaturated zone at the repository horizon. He and Kelly noted that minimal data are available to determine evaporation and condensation effects associated with the reflux process on water chemistry and more experimental data were needed to define this process. Both reviewers indicated that additional detailed modeling of thermal effects on chemical composition of water contacting the WP was necessary.

De Marsily and Kelly had concerns about the justification for the factors sampled in the TPA Version 3.2 code to determine the quantity of water dripping onto and into the WP. Both reviewers 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 praised the analyses performed to determine these parameters. However, he questioned the assumption that dripping would occur only when infiltration exceeds the hydraulic conductivity of the rock. Ouzounian also commented that keeping the F_{ow} factor constant through time was not conservative because the fraction of water that enters the WP will increase as the WP degrades. He recommended tracking the size of pits in the WP surface 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 suggested that the dripping abstraction should consider the effects of collapsed drifts on infiltration rates.

Finally, van Dorp, Brady, and de Marsily indicated that the TPA Version 3.2 code should consider the effects of 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 stated thermal stresses caused by temperature increases could reactivate faults in the repository area.

Failure of the Engineered Barrier System Due to Corrosion Module

Kelly declared development of the EBSFAIL module was "one of the most noteworthy achievements in corrosion engineering in the last 50 years." Despite this praise, concerns were raised with the WP corrosion modeling. Ouzounian and Kelly 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 suggested further research 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 if water-saturated rocks contacting the WP could influence the WP degradation rate because of crevice corrosion. Kelly indicated that the code should be able to model peroxide production on the WP surface caused by radiolysis, if a WP with thinner walls allowing higher surface radiation fluxes is used, Kelly also recommended that the effects of sulfur be modeled because sulfur is 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 as rockfall-induced 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, which would influence the corrosion rate. Kelly stated the corrosion model should be able to determine the pit density on the WP through time to calculate the amount of water that can enter the WP, which is likely to increase through time.

Release From the Engineered Barrier System Module

The primary concern about the models in EBSREL was that the chemistry of the water within the WP is not well understood. As indicated earlier, Ouzounian did not believe that J–13 well 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 because reactions between the water and the materials in the WP may lead to elevation of solution pH within the package. This elevation may affect the dissolution rate and nature of the spent nuclear fuel (SNF) reaction products. Kelly recommended investigating if 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 current modeling of the SNF dissolution rate may be overly conservative because 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 research is needed to reduce uncertainty in the model. He also commented that the mineral phases in the SNF need to be well characterized because the dissolution rate of SNF typically is approximately 100 times that of fresh fuel. Ouzounian recommended providing the rationale for excluding radiolytic effects on SNF dissolution rates.

Ouzounian indicated that the inventory of radionuclides in the gap and grain boundaries seemed reasonable, but more justification was needed for these values. 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 the code documentation does not indicate that the gap inventory is properly accounted for, but following discussions during the formal meeting, he asserted that the gap inventory is appropriately considered in the code.

For the bathtub model of water contacting the SNF, Kelly commented that radionuclides could be released from fuel above the waterline by water dripping on and running down the fuel or by humid air corrosion. He 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 which limited credit is taken for the cladding.

Unsaturated Zone Flow and Transport Below the Repository Module

De Marsily indicated that the model used for unsaturated zone flow and transport (UZFT) is generally adequate and consistent with available ^{36}Cl data for YM. De Marsily did not agree, however, 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 it was likely that the fracture would continue through all layers below it until the radionuclides reached the saturated zone. He recommended that in simulating the transport of radionuclides, those radionuclides that have already entered the fractures be forced to remain in the fractures until reaching the water table, unless they are removed by matrix diffusion.

Several reviewers commented that the groundwater flow modeling was not flexible enough to consider some potentially significant processes. De Marsily commented that assuming the thermal pulse had no effect on the groundwater hydrology below the repository 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.

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 all chemically similar elements, not just a few actinides, should be correlated because these values will tend to have comparable behavior under similar chemical conditions. Van Dorp and Whicker both noted that the code should account for colloid transport; although van Dorp indicated that zero retardation in fractures can adequately, though conservatively, model colloidal transport. Whicker also commented that the K_d value for plutonium seemed low.

Saturated Zone Flow and Transport Module

The basis for the saturated zone flow and transport (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 indicated that the U.S. Geological Survey data on which the SZFT model is based provide insufficient information to develop a suitable transport model. 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 occur only if the receptor was located less than 10 km from the repository). He commented that layering of the alluvium must be characterized to perform defensible dilution calculations and modeling of matrix diffusion using a linear exchange coefficient in the transport model is crude and should be modified. Based on this lack of data, he recommended replacing the SZFT model with a simple conservative model that transports all the water and radionuclides that reach the saturated zone to a community well with little or no retardation.

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 more investigation of 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.

Dose Conversion of Radionuclides in Groundwater Module

Overall, reviewers seemed to agree with the use of dose conversion factors (DCFs) in the dose conversion of radionuclides in groundwater module. 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 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 irrigation with contaminated water and reincorporation of contaminated plant and animal wastes. Whicker recommended conducting a study to determine site-specific, plant-to-soil concentration ratios and feed transfer coefficients because 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 that 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.

Failure of the Engineered Barrier System Due to Seismic Events Module

The experts who reviewed the SEISMO module indicated that the model was implemented correctly, and the assumption of no backfill was conservative, yet improvements could be made to the model. Brady indicated this could be accomplished by using a 3D finite element analysis to evaluate interactions between the rock and WP when both are in motion and between 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 longer than 10,000 yr, larger seismic events than are currently possible may need to be modeled in the code.

Failure of the Engineered Barrier System Due to Faulting Events 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 suggested more research to determine the threshold fault displacement that will cause rupture of the WP. He 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 because of 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 repository heating of the rock. Finally, he indicated the assumption 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 (3) and backfill is actually used.

Failure of the Engineered Barrier System Due to Igneous Activity Module

Delaney indicated that the probability of volcanism within the repository area is well determined, and modeling release with the VOLCANO module is acceptable. Thompson commented that, for time periods of interest longer than 10,000 yr, the code may need to model multiple volcanic events impinging on the repository. Kelly indicated that the

assumption that all WPs contacted by magma fail may be overly conservative, because ^{22}C is unlikely to melt at a magma temperature of 1,100 °C. He acknowledged, however, that the containers could experience creep, leading to failure, and the interplay between the stresses in the WP caused by the eruption and the creep rates is unknown. De Marsily suggested that the code should consider other effects of volcanism besides direct release, including failure of WPs 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.

Airborne Transport of Ash Module

Delaney's review of the ASHPLUMO module code concluded that, although the module is based on an empirical ash-dispersal model, improved models would improve the results only marginally. He recommended a research program to develop more sophisticated ash-dispersal models to compare with the results of the Suzuki model and to develop a better basis for 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 suggested that the assumption that waste is homogeneously distributed in the ash, and not concentrated in thin layers within the blanket, be reevaluated.

Removal of Radionuclides from an Ash Blanket Module

Delaney commented that the ASHRMOVO module handled well the travel of radionuclides after deposition on the ground caused by a volcanic event. He suggested determination of the dose effect of radioactive material deposited close to the volcanic event and later redistributed and redeposited at the critical group location by fluvial processes. Radionuclide is his primary concern with the TPA code.

Dose Conversion of Radionuclides on the Ground Surface Module

The experts who reviewed the dose conversion of radionuclides on the ground surface (DCAGS) module commented that the use of DCFs to convert soil concentrations to doses was reasonable. Whicker's comment 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.

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, but many felt the documentation was inadequate and had suggestions to improve it.

The most common criticism of the documentation was about inadequate description of the selection of the FEPs to be modeled in the code. Most reviewers commented that a systematic process should be developed to identify relevant FEPs and interactions between these FEPs. The documentation of the code should justify the inclusion and exclusion of FEPs so that reviewers of the code can assess the completeness of the code. 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.

Several reviewers felt that the User's Guide by itself was an inadequate document to provide a comprehensive review of the approach taken by NRC to analyze the DOE safety case. 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 code will be used by the NRC in evaluating the DOE safety case. 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 the development, and van Dorp commented this system should include the rationale for selecting the conceptualization used in the module. This chain of documentation 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 the domain of validity. Thompson and van Dorp commented that data should be traceable from laboratory or field testing through incorporation into the code via input parameters or model abstraction. Ouzounian, Thompson, and Kelly recommended providing road maps to trace particular issues through sets of related documents. Thompson recommended identifying site-specific data as opposed to data from the literature, and determining whether the DOE data and assumptions used in the TPA Version 3.2 code have undergone independent review by NRC staff prior to use in the code.

Several reviewers commented that the inclusion of the reference data set in the User's Guide was an effective way to summarize data and provide links to the source of the data. Van Dorp and Thompson both indicated, however, 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 is needed 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. Kelly and Thompson both precisely very detailed suggestions for developing documentation systems that could be used to support the TPA Version 3.2 code.

Most reviewers felt the level of QA for code development 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 "the code is developed in an environment of rigorous configuration management." 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 similar input data and scenarios. Whicker suggested verifying the results of the GENII-S code used to generate DCFs using another standard industry code or comparing the results to real data.

SUMMARY AND CONCLUSIONS

The external reviewers were generally positive about the quality in developing the TPA Version 3.2 code and considered the code suitable for reviewing the DOE TSPA in support of the LA. During the July 1999 meetings, a number of the external experts revealed their misgivings about the technical bases for the code which were largely allayed by the detailed technical presentations made by CNWRA and NRC staffs. The experts felt that the background reading material given to them prior to the 3-day 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 inadequately details 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 CNWRA configuration control QA procedures and a visit to the CNWRA QA records vault.

There was a general feeling that many of the initial concerns of the external reviewers would have been avoided 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, made by the majority of reviewers, was that the level of documentation is insufficient in the TPA Version 3.2 code. 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 the effort to trace the sources of the input data in the TPA User's Guide was commendable, others felt the effort fell short of that required for a 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 why the code did not include or explain 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 other technical improvements to the TPA modules not summarized in this paper. 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 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. Consideration may be given to developing a subset of the supporting documents recommended by Thompson and Kelly to facilitate use of the TPA code during the LA review and to build public confidence in the decision-making process.

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FOOTNOTES

[a] This paper is a condensed version of the report of Weldy (6).

[b] 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.

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

[e] 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.