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A STRATEGIC PLAN FOR DEVELOPMENT AND DOCUMENTATION OF THE NUCLEAR REGULATORY COMMISSION TOTAL-SYSTEM PERFORMANCE ASSESSMENT METHOD

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ABSTRACT

The Nuclear Regulatory Commission (NRC) continues to develop its independent performance assessment (PA) capability to review the license application (LA) for a proposed repository at Yucca Mountain (YM), Nevada. According to the current plan, the U.S. Department of Energy (DOE) will submit an LA in the year 2002. DOE has sole responsibility for demonstrating the ability of the proposed repository at YM to meet the applicable standards. As the licensing authority, NRC will conduct its own independent analyses to probe the DOE safety case. To meet its review goals, NRC should be confident that its PA tools are technically sound and well documented so the review can be defended if subjected to a hearing. This report assesses the current status of NRC's ability to conduct a PA, identifies areas of weakness, and proposes a strategy to refine its PA capability and confidence building efforts to conduct the review of DOE's LA. The strategy prepared in this report charts the future course of Total-system Performance Assessment tool development and outlines the supporting documentation needed to demonstrate to the scientific community and stakeholders the NRC ability to conduct a credible and defensible quantitative assessment of the DOE safety case for YM.

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ACKNOWLEDGMENTS

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QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

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

1 INTRODUCTION

The Nuclear Regulatory Commission (NRC) will perform independent quantitative analyses as a part of its review of the license application (LA) for a proposed repository at Yucca Mountain (YM), Nevada. Analyses may range from simple "back of the envelope" calculations to check the reasonableness of the U.S. Department of Energy (DOE) findings to complex computer simulations needed to verify compliance with the overall risk standard. The lengthy regulatory compliance period and the enormous complexity of the natural and engineered systems that compose the repository, require using complex computer models except where simple, but demonstrably conservative, models provide reasonable assurance of compliance with the overall risk standard. The complex processes affecting the repository preclude determining whether or not a simple model is conservative without first constructing more complex models. Experience gained by NRC through the conduct of performance assessments (PAs) during the past 15 yr suggests that the nonlinearities of the underlying process models generally demand relatively sophisticated computational models.

In conducting the quantitative PA, the NRC will focus on aspects most important to safety and explore or review concerns that may be less fully described in the DOE's Total-system Performance Assessment (TSPA) and, consequently, are licensing vulnerabilities. Currently, NRC is developing or acquiring PA tools [i.e., the Total-system Performance Assessment (TPA) code, the sensitivity analysis techniques, and the visualization capabilities] for quantitative analyses and developing staff expertise in implementing these tools. It is, however, solely the responsibility of the DOE to produce a complete, quality-assured Total System Performance Assessment (TSPA)[1] (Johnson, 1994) as part of its LA. NRC may use the DOE assessment tools to probe the adequacy of the DOE safety case, or use its independently developed PA tools to perform calculations to assess DOE parameter values and conceptual models.

According to the current schedule, DOE will conduct two more TSPAs leading to the final LA—the TSPA-SR (site recommendation) and the TSPA-LA. The TSPA-SR will be issued in fiscal year 2001 (FY2001) and the TSPA-LA in 2002 (figure 1-1). It is anticipated that DOE may make several changes to the repository design during this 2-yr period. Consequently, NRC should be ready to modify its PA tools to accommodate both known and anticipated design changes, as well as new site characterization information. NRC should also assess its capabilities and identify and remedy weaknesses in its PA to assure NRC's readiness to review the DOE PAs in support of the SR, the LA, and performance confirmation.

The PA capability developed by the NRC during the past several years has been used to review several TSPAs conducted by DOE. The PA capability has also proved useful in evaluating the completeness and sufficiency of current regulations and developing a draft site-specific rule that considers the integrated effects of the physical aspects of the repository system that affect the radiological safety of the proposed repository at YM. Currently, the PA capability is used to develop and test appropriate review methods and the acceptance criteria in the YM Review Plan. There is a need for continued development of the PA capability so the NRC staff can

- Prepare for the review by enhancing its own understanding of technical issues potentially most important to safety

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[1] Browning, R.E. *Revised Modeling Strategy Document for HLW Performance Assessment.* Memorandum (July 23) to J.G. Davis, Nuclear Regulatory Commission. Washington, DC: Nuclear Regulatory Commission. 1984

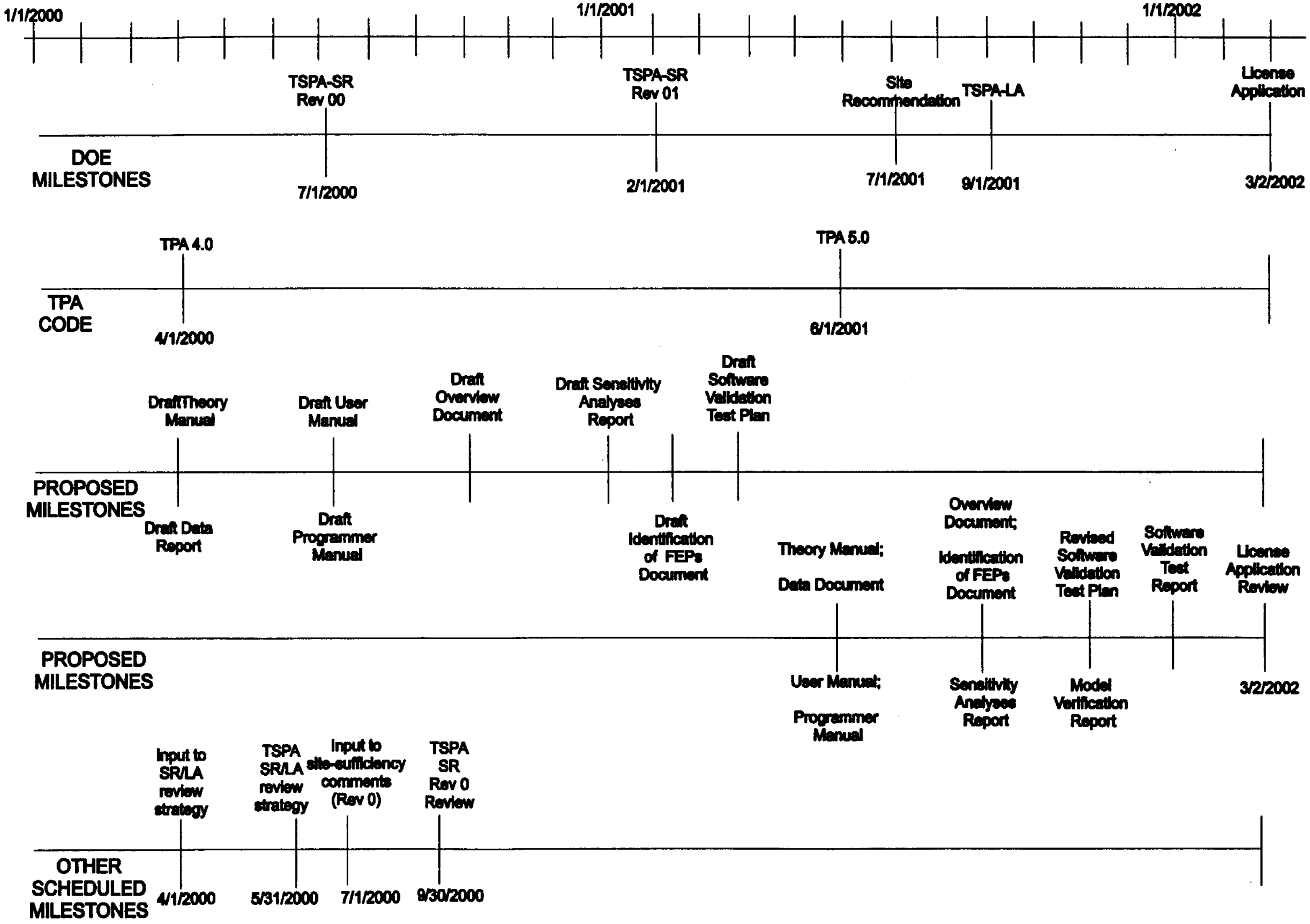

Figure 1-1. The U.S. Department of Energy and the Nuclear Regulatory Commission current and proposed milestone schedules

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- Conduct TSPAs as learning exercises that build staff technical expertise in reviewing DOE documents and keep staff knowledge current [Insights gained by the NRC staff will allow continued development of meaningful regulatory guidance, assure effective review of pre-licensing submittals, and facilitate interaction with DOE and stakeholders (Johnson, 1994)]

- Provide a firm basis for staff comments on the DOE-SR, which are statutorily mandated

- Test the veracity and reproducibility of the DOE results during review of the LA

- Probe the analyses performed by DOE using other sets of parameter values and explore the implications of alternative conceptual models

- Minimize the number of requests for additional information and optimize the time required for review

- Provide support for the licensing decision

The NRC has made significant progress in developing its PA capability. The NRC program, however, warrants attention to building confidence in its tools to demonstrate to the stakeholders that it has the ability to make independent and technically defensible assessments of the DOE safety case. Considerable effort has already been made to bolster confidence in the TPA code through the conduct of an external peer review and the submission of papers to peer-reviewed journals as well as through presentations at conferences. However, greater effort is warranted. Although DOE is responsible for fully supporting its demonstration of compliance with the pertinent regulations, the NRC staff should be able to defend its findings regarding DOE's demonstration during the license review process. Such a defense will be based on the technical strength of the review methods, including independent quantitative analyses employed by the NRC. It is anticipated that its quantitative tools (i.e., the TPA code and the sensitivity analysis and visualization tools) may undergo close scrutiny by the stakeholders. Therefore, with the approach of the license review period, NRC should focus on finalizing modifications to its PA tools, building confidence in their application, and developing the required support documents.

NRC can build confidence in its PA tools by ensuring (i) the soundness of the model abstractions implemented in the TPA code, (ii) the robustness of its sensitivity analysis tools, and (iii) the thoroughness of the quality assurance (QA) processes followed in code development, with emphasis on transparency and traceability. This report identifies the progress made by the NRC in developing PA tools, assesses the existing weaknesses of the assessment approach, and proposes a strategy to refine the TPA code and sensitivity analysis tools and build confidence in the codes. The report also provides a brief history of the NRC PA activities (table 1-1), describing how the TPA codes were used to review the DOE TSPAs, and outlines the iterative nature of the confidence building process. The report then outlines a proposal for further development of PA tools (primarily the TPA code) and provides a time frame and rationale for developing support documents (figure 1-2 and table 1-2). While the documents proposed in this report will prepare NRC to defend its PA tools during the review of DOE's LA, it is unlikely that these documents can be completed before the scheduled submittal of the LA. Therefore, priorities are assigned (table 1-3) so the most important documents can be completed in the available time. Because NRC is currently consulting with the Office of the General Counsel (OGC) to determine the level of documentation needed to support its independent quantitative PA, final recommendations may be different from those presented here.

Table 1-1. History of Nuclear Regulatory Commission iterative performance assessment activities

U.S. Department of Energy Milestones	Year	Nuclear Regulatory Commission Milestones
TSPA-92	1992	Initial Demonstration of the NRC Capability to Conduct a Performance Assessment for a High-Level Waste Repository. NUREG–1327.
TSPA-95	1995	NRC Iterative Performance Assessment Phase 2. NUREG–1464.
TSPA-Viability Assessment	1998 1999	NRC Sensitivity and Uncertainty Analyses for a Proposed HLW Repository at Yucca Mountain, Nevada, Using TPA 3.1. Volume I: Conceptual Models and Data. NUREG–1668, Volume 1.
		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, Volume 2.
		Total-system Performance Assessment (TPA) Version 3.2 Code: Module Description and User's Guide. Center for Nuclear Waste Regulatory Analyses—Letter Report.
		System-Level Sensitivity Analyses Using TPA Version 3.2 Code. CNWRA 99-002.

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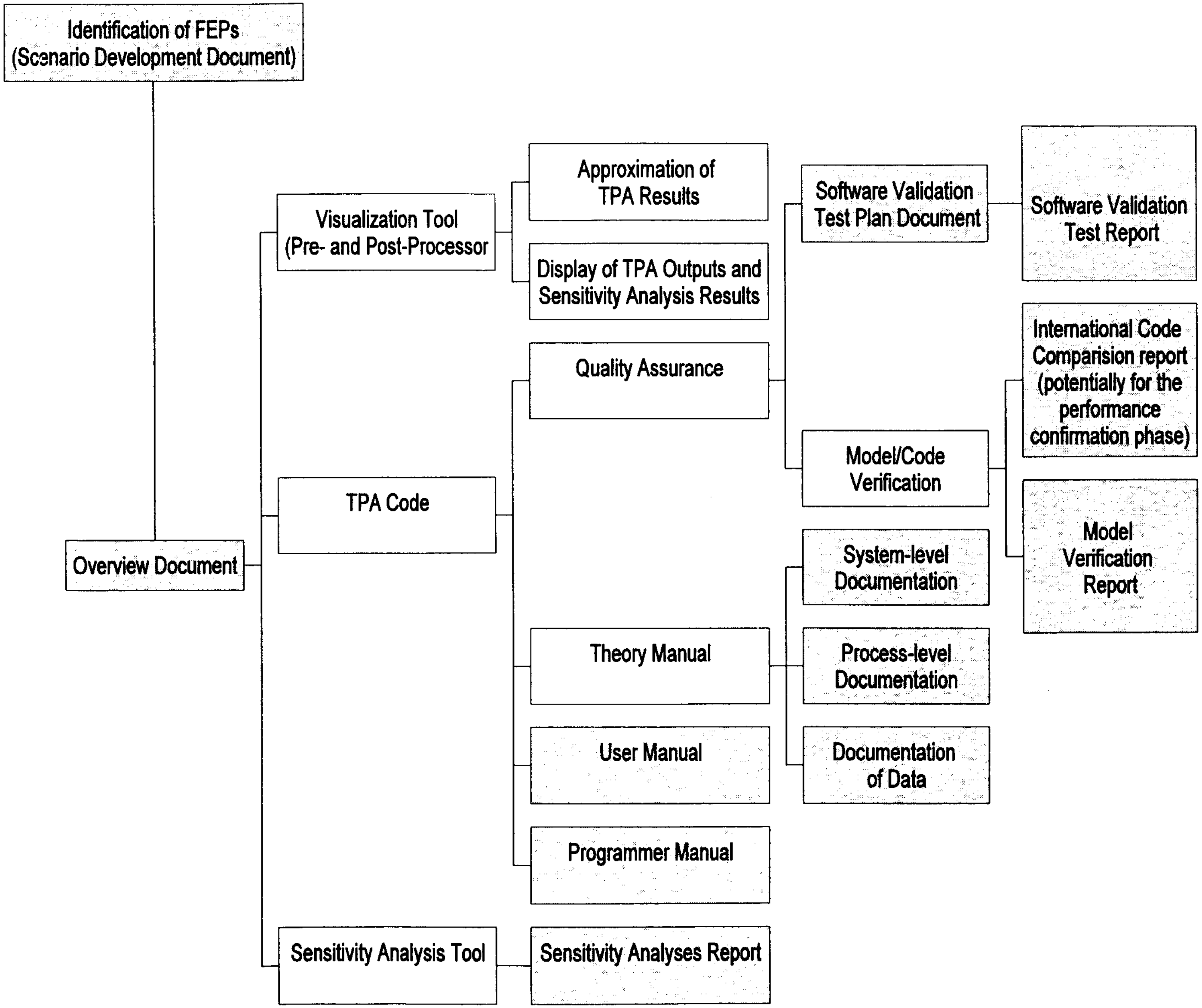

Figure 1-2. Hierarchy of proposed documents and performance assessment tools. Documents are indicated by the filled boxes.

Table 1-2. Proposed future Nuclear Regulatory Commission iterative performance assessment activities

U.S. Department of Energy Activity	Nuclear Regulatory Commission Performance Assessment Tools	Documents
TSPA-SR (Revision 0) (7/1/2000)	–TPA Version 4.0 code –Sensitivity analysis tools –Visualization tools	draft theory manual draft data document draft user manual draft programmer manual
TSPA-LA (9/1/2001)	–TPA Version 5.0 code –Updated sensitivity analysis tools –Updated visualization tools	draft overview document draft sensitivity analyses report draft identification of features, events, and processes document draft software validation test plan updated overview document updated theory manual updated data document updated user manual updated programmer manual updated identification of FEPs document updated sensitivity analyses report process-level documents final software validation test plan software validation test report
TSPA-XX	TPA Version 6.0 code for use during performance confirmation	

Table 1-3. Prioritization of proposed documents

Document	Purpose	Priority	Status and Comments
Identification of FEPs Document	To record the process by which FEPs were included or excluded from the TPA code and to provide guidance prior to the receipt of TSPA-LA if the NRC selection of FEPs is significantly different from the DOE.	H	New work should begin and a report should document contributions from all key technical issues.
Overview Document	To serve as a comprehensive reader's guide to the documents that support the NRC PA methodology. This overview document would also contain synopses of the TPA code structure, input and output, modeled processes, and simplifying assumptions.	M	Chapter 1, Total system performance assessment 3.2 user's guide gives limited overview of total system performance assessment code. New document should expand this chapter.
Theory Manual	To describe the theoretical basis for NRC PA models.	H	Document to include theory presented in total system performance assessment 3.2 user's guide. New materials added or revisions made only to support total system performance assessment code updates.
User Manual	To provide necessary information to the staff and other users for successfully operating the TPA code for PA calculations.	M	A brief description currently exists in the TPA 3.2 User's Guide. Current description will be updated and expanded into a full report.
Programmer Manual	To provide software development-related information for future code development.	M	This document will be developed by expanding the limited information provided in the TPA 3.2 User's Guide.
Data Document	To systematically record data used in the TPA code.	M	NRC data set is an appendix in the total system performance assessment 3.2 user's guide. Appendix should be expanded into a document with appropriate data tracking.

Table 1-3. Prioritization of proposed documents (cont'd)

Document	Purpose	Priority	Status and Comments
Sensitivity Analyses Report	To document those parameters in NRC's calculation that contribute most to uncertainties in estimated performance and NRC's approach for conducting the analyses.	H	Document to be updated to reflect two major changes to total system performance assessment code.
Process-level Documents	A series of reports to be developed documenting the detailed analyses by the subject-matter experts, in support of all abstracted models in the TPA code.	M	New documents to be prepared using KTI staff inputs (model and data) to total system performance assessment code.
Software Validation Test Plan	To document the test plan for evaluating correct implementation of mathematical formula and algorithms in the PA tools.	H (required)	Document to be prepared fulfilling requirements of Technical Operating Procedure (TOP)-018.
Software Validation Test Report	To document the results of tests for implementation of mathematical formulas and algorithms in the PA tools.	H (required)	Document to be prepared fulfilling requirements of TOP-018, including formal documentation of tests conducted on several versions of total system performance assessment code.
H—High M—Medium L—Low			

2 HISTORY OF THE NUCLEAR REGULATORY COMMISSION PERFORMANCE ASSESSMENT CAPABILITY

To date, the NRC and the Center for Nuclear Waste Regulatory Analyses (CNWRA) (table 1-1) have developed three major PA tools. The first TPA code was developed under the Iterative Performance Assessment (IPA) Phase 1 program (Codell et al., 1992) as part of the effort to demonstrate NRC's independent PA capability. The results from the IPA Phase 1 study were used to provide guidance to DOE on its site characterization program and led to the NRC's first formal technical exchange with DOE on PA (Johnson, 1994). The second TPA code, TPA Version 2.0 code, which was developed and used under IPA Phase 2 (Wescott et al., 1995), combined the knowledge of specialized technical disciplines (engineering and earth sciences) with those of system modelers, to produce an integrated PA. Special attention was directed toward improving methods for scenario identification; screening of features, events, and processes (FEPs); and implementing alternative sensitivity analysis methods. An equally important aspect of this effort was the evaluation of the relationship of the NRC subsystem requirements to the compliance with the U.S. Environmental Protection Agency Standard. The IPA Phase 2 analysis was used in the NRC review of DOE TSPA-95. The third NRC TSPA (Nuclear Regulatory Commission, 1999) developed and used the TPA Version 3.1 code to determine whether the NRC would be able to quantitatively evaluate the soundness of the conclusions reached by the DOE in its viability assessment (VA). Subsequent to developing and testing the TPA Version 3.1 code, detailed sensitivity and uncertainty analyses were conducted (Nuclear Regulatory Commission, 1999) that indicated the need for further refinement of the TPA code prior to its use to evaluate the DOE TSPA-VA. Refinements led to the current TPA Version 3.2 code (Mohanty and McCartin, 1998) and introduction of new sensitivity analysis techniques.[1] During development of the TPA Version 3.1 and 3.2 codes, increased attention was paid to making the TPA code more readily accessible to all staff members of the NRC and CNWRA. Improvements in the computational efficiency of the TPA code made it possible to port the code from the high-performance Unix workstations on which it had been developed, to the Windows-based personal computers used by most staff members. The effort toward making the code available to a broader user base led to the release of the code to DOE in support of NRC's openness policy of stakeholders access to NRC's models and support tools.

The three PAs conducted by the NRC and the publication of associated documents represent three confidence building cycles. A highly abstracted flow chart of the TPA confidence building process is shown in figure 2-1. The first two steps in the process involve updating PA tools based on design changes, new data, or new understanding of repository phenomonology. In the third step, the models and data are "frozen" while detailed studies are conducted with the TPA code, and the results and findings documented. Based on the results of sensitivity studies, evaluation of DOE TSPAs, and technical exchanges, NRC then assesses both its own confidence to review the LA as well as its confidence that the NRC TPA tools can withstand the scrutiny of a formal hearing process. NRC takes advantage of the DOE schedule to refine its PA tools using each cycle to identify shortcomings in the existing models and data, as well as topics that need further investigation and incremental understanding of processes, computational tools, and data. Aspects of the code such as the lack of reasonable conservativeness in models, lack of uniformity in the treatment of FEPs, or inadequate accounting of coupling among processes may require the confidence building cycle be repeated.

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[1] Mohanty, S., and T.J. McCartin, coordinators. *NRC Sensitivity and Uncertainty Analyses for a Proposed HLW Repository at Yucca Mountain, Nevada, Using TPA 3.1 Volume I. Conceptual Models and Data.* NUREG–1668. Volume 1. Washington, DC: Nuclear Regulatory Commission. To be published.

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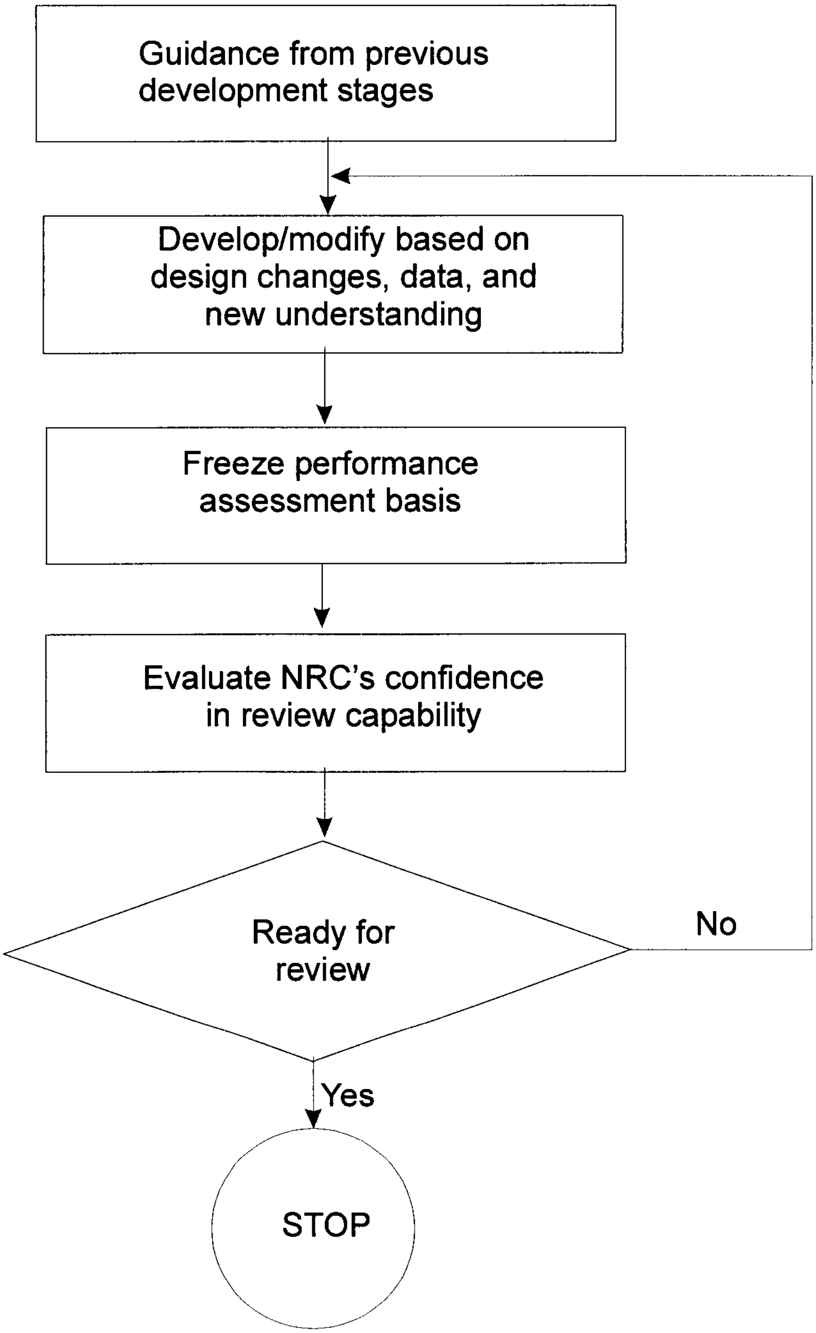

Figure 2-1. Confidence building cycle leading to license application review and evaluation of the performance confirmation program

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3 FUTURE PERFORMANCE ASSESSMENT CAPABILITY DEVELOPMENT AND CONFIDENCE BUILDING

Consistent with the confidence building cycle in figure 2-1, future iterations of PA tool development will be based on shortcomings identified in the last iteration of PA conducted by the NRC. To enhance confidence for the future iterations, it is necessary to (i) further develop and refine the PA tools, and (ii) document the entire process. The development of quantitative assessment tools will focus on DOE design changes, newly acquired site-specific data, and refinement of conceptual models. Complete scientific understanding of processes, fully validated computational tools, and complete and unambiguous site-specific data are not feasible. Hence, NRC will make licensing decisions under conditions of uncertainty. Therefore, the NRC basis for the decision must be well-documented. Documentation should emphasize completeness, transparency, and traceability of the results. When the development and documentation process have been subjected to stringent QA and review procedures and the results from calculations have been fully disclosed, confidence in the process will be demonstrated. This chapter identifies the documents needed to defend findings supported by the TPA code during the adjudicatory procedures attendant with licensing.

3.1 FURTHER DEVELOPMENT OF PERFORMANCE ASSESSMENT TOOLS

Future NRC efforts toward developing PA tools will be discussed in three sections that address (i) refining the TPA code, (ii) upgrading sensitivity analysis methodologies, and (iii) developing TPA pre- and post-processors. It is assumed that pre-LA consultation with DOE will continue and that the NRC will be informed of design changes well in advance of the release of the two TSPAs (TSPA-SR and TSPA-LA). Therefore, it is reasonable for the NRC to target its efforts on accommodating DOE design changes in the NRC PA tools. Modifications, however, can and should be less extensive than the first three TPA development phases because of the maturity[1] of the PA tools. Modifications should be conducted with care not to sacrifice the confidence gained through years of incremental refinement and testing. The ultimate goal is to show through evaluation and enhancement of assessment tools that there is sufficient confidence in PA to allow NRC to assess the DOE safety case. While modifications to the TPA code and other analysis tools continue, more attention should be given to quality management to assure a proper application of the methodology, models, database, and codes. The strategy for tool development is presented next.

3.1.1 Total-system Performance Assessment Code

The TPA code, which performs process-level calculations for the repository system, will be used as a major tool in reviewing the DOE TSPA. Based on several DOE/NRC technical exchanges and recent review of the TSPA-VA, it is believed that the TPA code is flexible enough to handle minor design changes in the engineered barrier system, new input data, and modest changes in the conceptual models. The code may not be capable, however, of readily incorporating and evaluating significant design changes without further modifications. A greater recognition should be made that the DOE dependence for safety may vary in time from one part of the disposal system to another as new knowledge is acquired. Therefore, the TPA code

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[1] As the code matures, the numbers of coding errors (bugs) found decreases exponentially as a function of time. Therefore, future changes to the code should be made with caution. A tracking mechanism to carefully document changes to the code should be implemented. Changes should be made in such a way that error will be localized. For example, if a better model is available to simulate flow and transport, the new transport code should be an option in the Total-system Performance Assessment code so the existing model can continue to be used if the user has a higher degree of confidence in it.

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should maintain flexibility in alternative design options, environmental conditions, and capability to perform calculations for spatially and temporally varying conditions.

The current NRC plan is to complete a major revision to the TPA code (Version 4.0) prior to release of the DOE TSPA-SR. Because the current Enhanced Design Alternative II (EDA II) (Howard, 1999) presented by the DOE is not anticipated to change in the near future, NRC can realistically modify the TPA code within the available time frame and prepare for reviewing the TSPA-SR. NRC may also improve the capability of the TPA code by adding new alternative conceptual models and expanding its flexibility in response to the comments made by the external reviewers of the TPA code.

The TPA code relies, in part, on information from several auxiliary codes,[2] either originally developed by the NRC and CNWRA or procured from outside sources, for the detailed analysis of repository components. Several of these supporting codes are integral to the TPA code and thus subjected to the same level of QA as the TPA code. However, there are several supporting codes (e.g., MULTIFLO and UDEC) providing input used in the PA calculations, that are continuously upgraded. Developing and testing such codes should be synchronized with the TPA code development, and these codes should undergo equivalent quality and reliability checks. Overall, for all supporting codes providing input to the TPA code, a uniform application of the QA procedure should be a priority.

As in previous versions of the TPA code, development of future versions of the TPA code will closely follow TOP-018, which adopts the software guidelines described in NUREG/BR–0167, "Software Quality Assurance Program and Guidelines" (Nuclear Regulatory Commission, 1993). In addition to fulfilling TOP-018 requirements for software QA, good engineering practices and software industry standards for the development of commercial software should be followed.

According to the current schedule, less than one year (figure 1-1) is available to plan, develop, test, and prepare supporting documents for the TPA Version 4.0 code, which will be used to review the DOE TSPA-SR. As mentioned earlier, the code development effort will include refinements to NRC models and code modifications to ensure that the DOE new design and site data can be evaluated using the TPA code. The supporting documents are discussed in later sections. One year and two months (figure 1-1) is available between the submission of the TSPA-SR and TSPA-LA documents. During this period, the NRC primary focus should shift to code testing, code verification, software validation, and preparation of supporting documents. It is assumed that DOE will not make major repository design changes during this time. NRC will develop the TPA Version 5.0 code only if the TPA Version 4.0 code is incapable of accommodating design changes and new data obtained during the post-TSPA-SR period.

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[2] The supporting codes currently used directly in the Total-system Performance Assessment code or that provide inputs are (i) MULTIFLO (Lichtner and Seth, 1996) for near-field chemistry calculations, (ii) GENII (Napier et al., 1988) for pathway dose calculation, (iii) SNLLHS (Iman et al., 1980) for Latin Hypercube Sampling, (iv) NEFTRAN (Olague et al., 1991) for radionuclide transport calculation, (v) UDEC (Itasca Consulting, Inc., 1996) for computing volume of damaged rock in the drift, (vi) ORIGENII (Ludwig and Renier, 1989) for radionuclide inventory calculations, and (vii) EQ3/6 (Wolery, 1992) for geochemical modeling of aqueous system. GENII, SNLLHS, and NEFTRAN codes are directly used as a part of the TPA code.

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3.1.2 Sensitivity Analysis Tools

Sensitivity and uncertainty analyses have been conducted by the NRC to show which parameters have the greatest effect on the behavior of the TPA code and which specific parameter uncertainties contribute most to uncertainties in estimated performance and, therefore, might pose a threat of noncompliance with the performance objectives. Under the present TPA code architecture, sensitivity analyses are conducted outside the TPA code. NRC employs several methods, some using commercially developed software or software developed in-house.[3] Because of limitations of each sensitivity approach, NRC evaluated various standard methods and investigated new techniques as a part of the process of selecting suitable methods. Limitations exist with all methods such as inaccuracy in identifying and ranking influential parameters, inability to incorporate correlated input parameters, and inability to deal with a large set of input parameters. A wider range of techniques should be evaluated and new ways to address current limitations should be explored.

Because of the significance of sensitivity analyses in PA, it is important that TOP-018 requirements for sensitivity analysis codes be implemented and documented with the same rigor as for the TPA code. For the verification of industry-accepted software packages (e.g., S-plus), well-chosen examples and underlying assumptions and limitations may be summarized in the documents reporting the sensitivity analyses methods. For these industry-accepted software, it may be possible to rely on the examples in the manuals, though these examples should be verified and documented to ensure relevance (assumptions and limits) and applicability to the analysis of TPA outputs.

It is anticipated that with the approach of the LA, the PA focus will gradually change toward sensitivity analyses and modifications to the TPA code will slow.

3.1.3 Pre- and Post-Processors

Pre- and post-processors facilitate interaction with complex codes such as the TPA and the sensitivity analyses by facilitating the manipulation of input data and the display of results without having to execute operating system commands or use an ASCII text editor. Efforts are currently underway to develop two post-processors for systematic presentation of results from PA calculations. The first post-processor implements the parameter tree and intermediate output tree approaches for identifying combinations of parameters and intermediate outputs that have the most influence on the performance measure. The second post-processor implements a simplified input-output diagram method that will permit the staff to study the effects of a variety of design alternatives on repository performance. Additionally, as part of stakeholder confidence building, an interactive visualization tool should be made available through the Internet to provide the staff and the stakeholders access to sample results from a range of realistic TPA analyses. Remote access of information from a centrally located database via the Internet has been made possible by very recent developments.

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[3] The sensitivity analysis methods currently used by the Nuclear Regulatory Commission (NRC) and Center for Nuclear Waste Regulatory Analyses staffs are regression-based, parameter tree, factorial design-based, Fourier Amplitude Sensitivity Test and differential analysis. NRC has relied on commercially developed software packages such as S-Plus (StatSci, 1993) for the regression-based methods used as the primary sensitivity analysis methods in IPA Phase 2 (Wescott et al., 1995).

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3.2 DOCUMENTATION

The NRC independent quantitative PA analyses should be able to be scrutinized by the stakeholders. Documentation should facilitate evaluation of the PA approach and promote acceptance by the scientific community. PA results may be presented in a wider context and expressed in a form tailored to the intended audience, including the lay public. NRC interaction with the scientific community and the public can be assisted by adopting a system of documentation that remains stable with time so the reviewer will have a "historical perspective." Documentation of results should be complete and transparent. Results, decisions, and calculations should be traceable to their sources. Several documents are proposed to address completeness, transparency, and traceability. The structure of documentation is shown in figure 1-2. As indicated in table 1-2, document development should begin during preparation for the TSPA-SR review and be finalized during preparation for the TSPA-LA review.

3.2.1 Features, Events, and Processes Screening Document

As part of the NRC PA program, greater effort should be devoted to developing a formal approach to FEPs screening both to provide guidance to the DOE and to record the process by which FEPs were included or excluded from the TPA code. NRC may provide guidance to DOE prior to the receipt of the TSPA-LA if the NRC selection of FEPs is significantly different from the DOE. NRC conducted a review of scenario selection approaches (Bonano and Baca, 1994). Additional work should be performed to reflect the NRC's current TSPA approach and identify new FEPs. Conducting a systematic scenario development and FEPs screening will also give NRC staff the necessary experience to review DOE scenarios. NRC may also use its own selection of FEPs in future development of the TPA code.

Documentation of all steps in a FEPs screening methodology is necessary to ensure that relevant, possible, future evolutions of the repository are properly considered by DOE and NRC and to provide the traceability needed to facilitate future revisions. The FEPs document should reflect that (i) sufficient background material is available when selecting FEPs in the PA and (ii) all steps in the FEPs screening methodology are correctly and consistently executed. A visual representation of linkage between the FEPs in the repository system will facilitate communication with the stakeholders. Methods commonly used to illustrate the interaction of FEPs are fault and event trees, influence diagrams, and the rock engineering system (Eng et al., 1994; Stenhouse et al., 1993). These methods will help document the reasoning for decisions to include or exclude processes. This document should also include the chain of decisions that led to the final selection of FEPs.

3.2.2 System-Level Documentation

System-level documentation for the PAs should support all aspects of assessments such as the underlying models and data and should be developed following software engineering life cycle practices. Although NRC recently attempted to comprehensively document its PA capability [TPA Version 3.2 User's Guide (Mohanty and McCartin, 1998) and the sensitivity analysis reports (Nuclear Regulatory Commission, 1999; Mohanty et al.,1999)], these documents represent only a portion of the documentation recommended by Thompson (1999)[4] at the external review of the TPA code. Documentation should include an overview

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[4] Thompson, B.G.J. 1999. External Review of Total-system Performance Assessment (TPA) Version 3.2 Code: Module Description and User's Guide and Related Sensitivity Analyses Applications.

(figure 1-2), written for technically literate persons who may be unfamiliar with PA, of interactions between DOE and NRC on the repository program and a guide through the documents that support the NRC PA methodology. The overview document also should describe, at a fundamental level, the interactions between subsystems and explain the procedures to include or exclude a process, or the decision to treat a highly coupled process as several independent processes. Other proposed documents include a theory manual, user manual, programmer manual, and several QA documents. The theory manual would describe the theoretical basis for the models and modeling methods, and include a detailed description of each model along with references to the scientific studies that support the model. The manual should clearly describe the methods implemented to bound and characterize uncertainties and identify assumptions and uncertainties. Additionally, the theory manual should document the NRC thinking on the likelihood that model and parameter uncertainties can be reduced further to achieve an additional safety margin. The programmer manual will describe the development and maintenance of the computer codes to be used in the project. The programmer manual will include information on software design specifications, code structure, file descriptions, data requirements, acceptance tests, and maintenance procedures and will be a valuable document for future code developers. The user manual will describe the code and provide the necessary information for successful installation and operation of the computer program.

3.2.3 Process-Level Documentation

Documentation at the process level should discuss the detailed analyses conducted to develop abstracted models and to select associated parameter values. A series of documents prepared by the subject-matter experts should provide bases for all abstracted models used in the TPA code. An effective system of long-term record keeping is important to ensure that the decisions on issues, such as how conservative the models should be or how much accuracy can be sacrificed in breaking a complex coupled process into a combination of simpler process, can be placed in a broad, historical context. Currently, no such document is maintained by the NRC or CNWRA. Staff should recognize that the DOE has kept options open, so that emphasis on safety may shift in time from one part of the disposal system to another. Therefore, flexibility in the model should be maintained until the LA. For example, the selection of Alloy C-22 as the corrosion-resistant material substantially extended the estimated waste package life and has shifted the focus of the TSPA toward emphasizing natural barriers (e.g., saturated zone chemistry and hydrology). The DOE focus could revert to emphasizing the engineered barrier system if new failure modes are found to substantially decrease WP life. Therefore, flexibility in the models should be maintained so that, when warranted, the WP life can be studied with appropriate consideration of dominant processes affecting radionuclide releases at early times.

3.2.4 Documentation of Supporting Data

It is essential that the data used in the TPA code are recorded and transmitted in a form suitable for creating computer input data files, interpreting results, and archiving. Figure 3-1 shows an example of a data transmittal form, which would be required for each parameter. A standard form would contain the description of the probability distribution function type and attributes, a justification for its selection, and approvals by the data contributor, modelers, and the manager of the database. A computerized data handling system would greatly reduce the chance of errors in creating and maintaining the database.

TPA Parameter Characteristics for Yucca Mountain Postclosure Assessment

1. Submitted
By: ______________________ Date: ____________

2. Parameter Full Name, Complete Definition, and Mathematical Symbol

Full Name: FMULT factor to account for an in-drift flow diversion

Complete Definition: The fraction of water infiltrating to the repository from the unsaturated zone above the repository that will enter the waste package (WP) and contribute to the release of radionuclides. Water dripping toward the drift may be diverted around the drift due to capillary action and down the side of the drift, or may not enter the WP for other reasons.

Mathematical Symbol (if any): Fmult

3. SI Units: [unitless]

4. Probability Density function (PDF) for the Parameter

PDF Type: Lognormal

Bounds:
None [ ], or
Value bounds [X], or
Quantile bounds [ ]

Upper bound: 0.2
Lower bound: 0.01

Attributes [examples: a, b, c, μ, σ)] as appropriate for type:
(List on back of page or on separate page if need more space.)

5. Dependence (if any) on Another Parameter Via a Correlation Coefficient

Independent [X], or
Dependent on parameter: ______________________
(Full Name)
with Correlation Coefficient (between - 1 and +1): ____________

6. Reasons for this choice of PDF (Please provide justification for the given information, including PDF type, attributes, bounds, the principal sources of uncertainty, underlying assumption, simplification and qualifying conditions, and attach a plot of the PDF and data points used. Alternatively, please provide a reference where this information may be found).

7. TPA Information: (TO BE COMPLETED BY TPA DEVELOPER)

Short name of the parameter in TPA: FmultFactor
Long name (up to 32 characters): Flow Multiplication Factor
Data are compatible with TPA model constraints.

Checked by: ______________________ Date: ____________

Data have been correctly entered into the TPA code database.

Checked by: ______________________ Date: ____________

Figure 3-1. Example of a data submission form

3.2.5 Documentation of Model/Code Verification

Model or code verification is concerned with the completeness and correctness with which the system model is translated from descriptive or mathematical representations into the computer program.[5] Strictly speaking, program verification means to demonstrate, via a mathematical proof, that the program is consistent with its specifications (Ralston et al., 1983). Verification is of particular importance for computer codes for the PA of radioactive waste disposal because conventional methods of model validation are not easily implemented for these codes. Verification requirements and selection of appropriate verification techniques are typically established at the onset of the project to facilitate these activities throughout the software development life cycle, which includes software requirements, design, development use, and maintenance (American Nuclear Society, 1987). NUREG/CR–3378 (Duda, 1984) is an example of model/code verification documentation. Because neither the verification requirements nor appropriate techniques have been identified to date, effort should be made to conduct model/code verification as a part of software validation.

Code inter-comparisons can gradually enhance code reliability by providing evidence that different codes developed and used by different groups produce consistent results when applied to the same problem (Eisenberg et al., 1999). While intercomparison exercises do not address all aspects of software development, they do provide specific hints where detailed verification of a participating code might be particularly useful. Results of code comparisons are often published at the end of the project, which would provide visibility; however, there is no international or other PA code comparison program scheduled at this time.

3.2.6 Documentation of Software Validation

Software validation ensures that software performs properly prior to its use in regulatory reviews. The software validation process is clearly defined in Technical Operating Procedure (TOP)-018. According to TOP-018, the software validation process begins when the software is mature. The test procedure should demonstrate that (i) all relevant data and information have been given due consideration, together with associated uncertainties; (ii) the models used have been adequately tested; (iii) a well-defined and rational assessment procedure has been followed; and (iv) results have been fully disclosed and subjected to QA and review procedures. The software validation process will consist of tests that provide evidence of correct and successful implementation of algorithms, as appropriate. Software validation also includes benchmarking or comparative testing against results from other software. TOP-018 requires that a software validation test plan (SVTP) be developed that includes computational demonstrations (e.g., through test cases) of proper and correct implementation of mathematical formulas and algorithms in the PA tools. The SVTP also requires that a software validation test report (SVTR) be prepared to document the results of software validation. The report is intended to include test cases for all modules, the overall code, and interpretation of the results. NRC will ultimately determine if the software has been adequately validated for use in licensing.

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[5] Verification must be clearly distinguished from validation. Model validation is demonstration of suitability of a model to accurately represent a stipulated component (e.g., waste package) or aspect (e.g., heat flow) of a real system. Eisenberg et al. (1999) provide a detailed description of model validation. Validation deals with building the right model whereas verification deals with building the model right (Whitner and Balci, 1989).

3.2.7 Time Frame for Development of Documents

Ten supporting documents have been proposed, not counting the reports on process-level analyses and data produced by the subject-matter experts. The hierarchy of these documents is shown in figure 1-2 but does not indicate the order in which these documents need to be developed. The proposed documents (figure 1-1 and table 1-2) are prioritized to support timely development of the TPA code and its dependent codes. Recognizing the limited time available to complete these tasks, primary focus should be on the high-priority documents (table 1-3). Four documents should be produced, at least in draft, during calendar year 2000 and finalized for the TSPA-LA in the following years. Resources committed to these documents will be based on budgetary and time constraints. The FEPs screening document preparation can begin promptly because it does not depend on the other documents. NRC can start to prepare the overview document based on its past PAs and current knowledge of the DOE design and site data for the proposed repository. The development of the theory, user, and programmer manuals should follow completion of the TPA Version 4.0 code. However, work can begin prior to the completion of this code because no changes to the basic framework of the TPA code are anticipated that could alter user and system requirements. Additionally, these documents can be built on information presented in the TPA Version 3.2 Code User's Guide[6]. The theory manual is expected to include both system-level and process-level (abstracted models) documentation following the style used in the TPA Version 3.2 Code User's Guide. Code verification can start after completion of the TPA Versions 4.0 and 5.0 code development. However, prior to completion of the code development, identification should begin of appropriate analytical or numerical solutions, against which the code should be compared. Preparation of the SVTP should also start early for a carefully composed plan to be presented for review. If formal documentation of all tests conducted to date at the CNWRA and NRC is begun early in the process, then preparation of the SVTP and SVTR can be expedited. The documentation has been maintained either in the form of scientific notebooks or software change report entries beginning with development of the TPA Version 3.1 code. The actual software validation should start after the completion of the TPA Version 4.0 code and its associated documents. The sensitivity analysis reports will be prepared only after completion of each TPA code development and test effort. The draft documents should be modified in FY 2001, concurrent with the TPA Version 5.0 code development. During the post-TSPA-SR review period, the staff effort is expected to primarily focus on the SVTR and finalization of the other documents.

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[6] Mohanty, S., and T.J. McCartin, coordinators. *Total-system Performance Assessment (TPA) Version 3.2 Code: Module Description and User's Guide*. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses. 1998.

4 CONCLUSIONS

NRC has been developing an independent PA capability to fulfill the obligations of providing guidance to DOE during site characterization, construction, operation and closure; select critical portions of the DOE LA and pre-licensing documents for intensive review; and support development of a technical framework for its regulations. NRC's independent PA capability includes development of PA tools that involve complex mathematical models and computer codes. This report identifies where the NRC quantitative PA efforts should be focused to assure its readiness for reviewing the DOE TSPAs to support the SR, the LA, and for the performance confirmation program.

This report proposes that continued development of several PA tools and preparation of supporting documents are necessary to fully support these tools. Recognizing the limited time available to complete these tasks before the scheduled submittal of the DOE-LA, the following observations and recommendations are made.

- NRC already has significant computational capability through development of several versions of the TPA code and sensitivity analysis tools. Further improvements to the TPA code prior to the SR and LA reviews should be limited to making necessary process-level refinements and accommodating the DOE design changes to the proposed repository and newly acquired site data.

- The documents needed to support the PA tools should be prepared during the 2 ½ yr period prior to the scheduled LA submittal. Preparation of several of the proposed documents will require substantial participation from various KTIs.

- The software validation process for the PA tools required by TOP-018 should begin promptly. This process, which involves preparation of a plan, software comparison, and preparation of a report, is anticipated to be time-consuming and somewhat resource-intensive. Hence, work in this area should start promptly so the TPA code will be ready for the LA review in the year 2002. To implement the software validation process effectively, modifications to the codes will be frozen.

NRC is currently consulting with OGC to determine the documentation needed to support its independent quantitative PA for reviewing the DOE LA. If the OGC determines that complete documentation of NRC's PA tools is necessary, it may not be feasible for NRC to prepare all of the proposed documents on time. However, those documents designated as high priority (table 1-3) should be completed as a minimum.

Finally, it is emphasized that demonstrating compliance with regulatory criteria is solely DOE's responsibility. The NRC effort to develop an independent PA capability is focused on evaluating DOE submittals and site characterization activities. Thus, PA is not conducted to remedy perceived deficiencies in the DOE program. The NRC task, however, will remain difficult because as DOE strives to reduce unnecessary conservatism, NRC will need a higher level of confidence in its own models and data that are used to make regulatory judgements regarding the DOE demonstration of compliance. The NRC confidence in its PA tools will play a key role in achieving the required level of confidence in the DOE models and data (i.e., reasonable assurance that radiological health and safety and the environment will be adequately protected). Therefore, NRC should continue to build confidence in its PA tools.

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