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Guidelines for Developing and Documenting Alternative Conceptual Models, Model Abstractions, and Parameter Uncertainty in the Total System Performance Assessment for the License Application

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CHANGE HISTORY

Revision Number	Interim Change No.	Description of Change
00	00	Initial issue
00	01	ICN 01 addresses comments related to improving the discussion of the team approach and the role of the Subject Matter Expert (SME) in identifying and developing parameter distributions, alternative conceptual models and model abstractions. In addition, minor editing addressed errata identified in REV 00. Clarification of the relationship of these guidelines to AP-SIII.10Q, including applicability to process models and to various project departments. Clarification of the process for consideration of alternative conceptual models and the role of the Abstraction Team Lead.

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ACRONYMS

AMR	Analysis Model Report
AP	Administrative Procedure
ATL	Abstraction Team Lead
BDCF	Biosphere Dose Conversion Factor
BSC	Bechtel-SAIC Company, LLC
CDF	cumulative distribution function
CFR	Code of Federal Regulations
CRWMS	Civilian Radioactive Waste Management System
CSNF	commercial spent nuclear fuel
DIRS	Document Input Reference System
DOE	U.S. Department of Energy
DSNF	DOE owned spent nuclear fuel
EBS	Engineered Barrier System
EPA	U.S. Environmental Protection Agency
FEIS	Final Environmental Impact Statement
FEP(s)	feature(s), event(s), and process(es)
HLW	high level waste
HTOM	high thermal operating mode
KTI	key technical issue
LA	License Application
LTOM	low thermal operating mode
MGR	monitored geologic repository
MTS	Management and Technical Services
MVSR	Model Validation Status Report
NRC	U.S. Nuclear Regulatory Commission
PA	Performance Assessment
PASS	Performance Assessment Scope and Strategy
PDF	probability density function
PMR	process model report
PRA	probabilistic risk assessment
PSHA	probabilistic seismic hazard analysis
PTL	Parameter Team Lead
PVHA	probabilistic volcanic hazard analyses
QA	Quality Assurance

ACRONYMS (continued)

RG	Regulatory Guidance
RIB	Reference Information Base
RMEI	reasonably maximally exposed individual
SME	Subject Matter Expert
SSPA	Supplemental Science and Performance Analyses
SR	Site Recommendation
TDL	Technical Direction Letter
TDMS	Technical Data Management System
TH	Thermal Hydrology
TSPA	Total System Performance Assessment
VA	Viability Assessment
WIPP	Waste Isolation Pilot Plant
YMP	Yucca Mountain Project

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1. INTRODUCTION

The Total System Performance Assessment (TSPA) model for the Yucca Mountain Project (YMP) is based on a hierarchical system of model components, starting with conceptual models and moving through mathematical and representational models and resulting in applied or abstracted models. These model components are developed by the various subproject departments (e.g., Unsaturated Zone, Engineered Barrier System, Disruptive Events, Waste Form, etc.), and are then integrated into the TSPA. The following guidelines provide for a consistent treatment in developing, integrating, and documenting alternative conceptual models (Section 2), model abstractions (Section 3), and parameter uncertainties (Section 4) for use in the Total System Assessment–License Application (TSPA–LA).

These guidelines provide a supplemental level of detail that is useful for implementation of the existing administrative procedure (AP) AP-SIII.10Q, which governs the preparation of all model reports (including model abstractions) for the project. The treatment of uncertainty at the process model level will be addressed in the model reports, in the context of model validation, consistent with the requirements of Section 5.4.1 of AP-SIII.10Q. The scope of these guidelines is specifically limited to alternative conceptual models, model abstractions and uncertain parameters that are used in development of the TSPA model. The guidelines apply to all subprojects and departments preparing model reports or analyses that contribute alternative conceptual models, model abstractions and uncertain parameters that are to be used in development of the TSPA model.

These guidelines have been developed based on consideration of regulatory requirements (principally 10 CFR 63 and 40 CFR 197), which take precedence over other relevant documents. In addition to the regulations, pertinent NRC guidance documents (i.e., NUREG-1636 (Eisenberg et al., 1999 [DIRS 155354] hereafter in the text referred to as NUREG-1636), NUREG-1573, and RG 1.174), and existing administrative procedures for the Yucca Mountain Project (AP-SI.1Q, AP-SIII.3Q, AP-SIII.9Q, AP-SIII.10Q, and AP-AC.1Q) were considered during development of these guidelines. These guidelines also address issues and recommendations identified in *Uncertainty Analysis and Strategy* (Williams 2001 [DIRS 157389]) and *Evaluation of Uncertainty Treatment in the Technical Documents Supporting TSPA–SR.* (YMP 2001 [DIRS 155343]).

As required by AP-2.21Q, *Quality Determinations and Planning for Scientific, Engineering, and Regulatory Compliance Activities*, this work activity was evaluated for application to the Quality Assurance (QA) program, and the activity evaluation (BSC 2002a) determined that the development of this guidelines document is not subject to the QA program.

1.1 BACKGROUND

A TSPA is part of the information that will be provided to the Nuclear Regulatory Commission (NRC) to demonstrate that the repository post-closure performance will satisfy the regulatory requirements, as set forth in 10 CFR 63. The current standard for the demonstration is a *reasonable expectation*, rather than absolute proof, that the performance of the disposal system meets the regulatory requirements.

1.1.1 Regulatory Background

The NRC requirements for the performance assessment specifically discuss the treatment of uncertainty and the consideration of alternative conceptual models.

> 10 CFR 63.114 (b) Account for uncertainties and variabilities in parameter values and provide for the technical basis for parameter ranges, probability distributions, or bounding values used in the performance assessment
>
> 10 CFR 63.114(c) Consider alternative conceptual models of features and processes that are consistent with available data and current scientific understanding and evaluate the effects that alternative conceptual models have on the performance of the geologic repository.

In the preamble to 40 CFR 197, the Environmental Protection Agency (EPA) elaborates on the use of reasonable expectation and acknowledges that the primary means for demonstrating compliance with the standards is the use of computer modeling. The EPA then identifies an approach that quantifies uncertainties realistically, rather than one that involves conservative or bounding assessments.

> "Simplifications and assumptions are involved in these modeling efforts out of necessity because of the complexity and time frames involved, and the choices made will determine the extent to which the modeling simulations realistically simulate the disposal system's performance. If choices are made that make the simulations very unrealistic, the confidence that can be placed on modeling results is very limited. Inappropriate simplifications can mask the effects of processes that will in reality determine disposal system performance, if the uncertainties involved with these simplifications are not recognized. Overly conservative assumptions made in developing performance scenarios can bias the analyses in the direction of unrealistically extreme situations, which in reality may be highly improbable, and can deflect attention from questions critical to developing an adequate understanding of the expected features, events, and processes. For example, a typical approach to addressing areas of uncertainty is to perform "bounding analyses" of disposal system performance. If the uncertainties in site characterization information and the modeling of relevant features, events, and processes are not fully understood, results of bounding analyses may not be bounding at all. The reasonable expectation approach is aimed simply at focusing attention on understanding the uncertainties in projecting disposal system performance so that regulatory decision making will be done with a full understanding of the uncertainties involved." (66 FR 32102)

In addition to indicating EPA's preference for the use of reasonable expectation, the preamble links the understanding of uncertainty with the use of simplifications (i.e., abstractions) and the understanding of features, events, and processes (FEPs). FEPs are, in turn, directly related to the formulation of conceptual models. Consistent with the limitation of the scope of these guidelines to TSPA integration activities, issues related to FEPs will be addressed under provision of the Enhanced FEPs Plan (BSC 2002b).

As described above, the regulatory standard for TSPA–LA is one of reasonable expectation. In the preamble section of 10 CFR 63 (66 FR 55740), the NRC has decided to adopt EPA's preferred criterion of reasonable expectation for purposes of judging compliance with the postclosure performance objectives. This includes the considerations that alternative models are not be excluded simply because precise quantification is difficult. Within the context of reasonable expectation, these guidelines provide that not all work conducted by YMP for Total System Performance Assessment for Site Recommendation (TSPA–SR) will be revised for TSPA–LA. The previous work and its "Q" status was fully documented in *Total System Performance Assessment for Site Recommendation (TSPA–SR)* (CRWMS M&O 2000a [DIRS 153246]). Existing parameters or models from TSPA-SR will likely be used when the influence of the parameter or model on the dose at the accessible environment is minimal and the existing model is adequate for the purposes of the analysis, as required by AP-SIII.10Q. Consequently, conservative approaches may be used in the TSPA–LA for some model components and parameters. An additional body of work for the SR was documented in the *Supplemental Science Performance Assessment (SSPA)* (BSC 2001b, Volume 1 [DIRS155950] and BSC 2001c, Volume 2 [DIRS 154659]), and the *Total System Performance Assessment - Analyses for Disposal of Commercial and DOE Waste Inventories at Yucca Mountain – Input to Final Environmental Impact Statement and Site Suitability Evaluation (TSPA–FEIS)* (BSC 2001d [DIRS 156460]). Any parameters or models from this additional work that are used in the TSPA-LA will be revised as needed to achieve "Q" status for the TSPA–LA. This approach is consistent with the Bechtel-SAIC Company, LLC (BSC's) risk-informed prioritization efforts.

1.1.2 Project Treatment of Alternative Conceptual Models, Model Abstractions, and Parameter Uncertainty in TSPA–SR, SSPA, and TSPA–FEIS

Internal and external reviews of YMP documents developed for the Site Recommendation, including the TSPA–SR (CRWMS 2000a [DIRS 153246]), found inconsistencies in (a) the consideration of alternative conceptual models, (b) the development and documentation of model abstractions, and (c) the process and methods used to develop and document uncertainties. The treatment of alternative conceptual models, model abstractions, and parameter uncertainty in the TSPA–SR, SSPA, and TSPA–FEIS models and documents are summarized in Appendix A. These documents provide the basis for BSC's recent prioritization planning that has developed a risked-informed scope of work for the TSPA–LA.

The YMP has developed a strategy document that integrates recommendations from the internal and external review groups and panels concerning uncertainty. This document, *Uncertainty Analyses and Strategy* (Williams 2001 [DIRS 157389]), summarized the findings of these review groups and panels related to parameter uncertainty (Section 3.1, Williams 2001 [DIRS 157389]). In DOE's Technical Direction Letter (TDL) dated December 4, 2001 (DOE, 2002) this strategy document was identified as providing a good framework for accomplishing the goal of improving the treatment of uncertainty for TSPA–LA. However, DOE indicated in Item 4 of this TDL that more details were needed in order “to implement a consistent, comprehensive, and systematic strategy for the treatment of uncertainties.” In addition, Item 5 from this TDL provided for the development of a document that describes how the strategy would be implemented in TSPA–LA. This guidance document addresses both of these items. The following lists the eight-part strategy for improving the treatment of uncertainties in TSPA–LA (Section 3.2, Williams 2001 [DIRS 157389]), and the location in this document where the implementation of the strategy is discussed.

1. Developing a TSPA that meets the intent of "reasonable expectation" (see Section 4.1 of these guidelines)

2. Quantifying uncertainties in inputs to the performance assessment (see Section 4.2 of these guidelines)

3. Identifying a process that encourages the quantification of uncertainties and gains concurrence on approaches with the NRC (see Section 4.2 of these guidelines)

4. Providing the technical basis for all uncertainty assessment (see Section 2 and Section 4.2 of these guidelines)

5. Addressing conceptual model uncertainty (see Section 2 of these guidelines)

6. Developing a consistent set of definitions and methods for "bounds" and "conservative" estimates (see Sections 4.1 and 4.2 of these guidelines)

7. Developing and communicating uncertainty information that can be used by decisionmakers (see Sections 2.3, 3.3, and 4.3 of these guidelines)

8. Developing detailed guidance and providing for implementation (see Sections 2, 3, and 4 of these guidelines).

1.1.3 Key Technical Issue Agreements Addressing Program Improvements Related to Alternative Conceptual Models, Model Abstractions, and Parameter Uncertainty for TSPA–LA

The Department of Energy (DOE) and NRC have developed five Key Technical Issue (KTI) (3.38, 3.39, 3.40, 3.41, 4.01) agreements for program improvements related to alternative conceptual models, model abstractions, and parameter uncertainty for TSPA–LA. These KTI agreements call for:

- development of written guidance to provide for a systematic approach to developing and documenting alternative conceptual models, model abstractions, and parameter uncertainty in YMP documents being developed for TSPA–LA (KTIs TSPAI 3.38, TSPAI 3.40, and TSPAI 4.01);

- implementation of the guidance leading to an improved and consistent treatment of alternative conceptual models, model abstractions, and parameter uncertainty for TSPA–LA (KTIs TSPAI 3.40, TSPAI 3.41, and TSPAI 4.01); and
- TSPA–LA documentation of the treatment of alternative conceptual models, model abstractions and parameter uncertainty that reflects the written guidance (KTIs TSPAI 3.39, TSPAI 3.41, TSPAI 4.01).

This document provides the written guidance called for in these KTI agreements and the methodology for its implementation. Table 1-1 details these KTI agreements along with the section in this document where they are addressed. The documentation, justification, and comparisons called for in the KTI agreements will be provided in the respective model reports.

1.2 RELATIONSHIP OF GUIDELINES TO GOVERNING PROCEDURES

Since the issuance of the TSPA–SR and the KTI agreements, the governing quality procedure for analysis and model reports, Administrative Procedure (AP) AP-3.10Q *Analyses and Models*, has been superceded by procedures AP-SIII.9Q *Scientific Analysis* and AP-SIII.10Q *Models*. The governing procedures that address software control and development is AP-SI.1Q, *Software Management,* and the process for capturing data into the Technical Data Management System (TDMS) is AP-SIII.3Q, *Submittal and Incorporation of Data to the Technical Data Management System*. The *Scientific Process Guidelines Manual* (BSC 2001e [DIRS 157635]) has also been issued from the Chief Science Office and is pertinent to implementation of these guidelines. Investigators and modelers are required to attend updated training on these modeling-related procedures. Additionally, work is under way to address concerns with uncertainty propagation and model validation throughout the modeling process. These procedures, although applicable and governing the work stemming from these guidelines, do not specifically address all activities needed to satisfy the KTI agreements identified in Table 1-1.

The intent of these guidelines is to supplement the required training on the procedural requirements with subject-specific guidance. In case of conflicts between the governing procedures and these guidelines, the procedures will take precedence until the procedural conflict can be resolved either by revision of the procedure or these guidelines.

Definitions to address development, validations, documentation and traceability issues for models are provided in AP-SIII.10Q. For the purposes of these guidelines and the specific application to alternative conceptual models, model abstraction, and parameter uncertainty, the terms and definitions in NUREG-1636 *Regulatory Perspectives on Model Validation in High-Level Radioactive Waste Management Programs: A Joint NRC/SKI White Paper*, NUREG-1573 *Branch Technical Position On a Performance Assessment Methodology For Low-Level Radioactive Waste Disposal Facilities*, and Regulatory Guide (RG) 1.174 *An Approach for Using Probabilistic Risk Assessment in Risk-Informed Decisions On Plant-Specific Changes to the Licensing Basis,* are adopted to supplement the definitions provided in the APs.

1.3 GENERAL OVERVIEW OF GUIDELINES AND APPROACH

Sections 2, 3, and 4 provide specific guidance for the consistent treatment of alternative conceptual models, model abstractions, and parameter uncertainty in the TSPA–LA. The introductory material for each section briefly summarizes the scope of the guidelines for the particular topic. The first subsection addresses definitions and key concepts that are needed to implement the guidance. The second subsection addresses implementation process. The third subsection addresses communication of the results to external reviewers.

The TSPA Department will use these guidelines to supplement the governing APs on the documentation of alternative conceptual models, model abstractions, and parameter uncertainty that are directly used in the TSPA–LA Model. In addition, these guidelines document the process that the TSPA Department will use to integrate information from process models developed by other subproject departments into TSPA Model development.

1.3.1 Team Approach

A team approach will be used to provide for consistency in the implementation of these guidelines. Key team members will include the Parameter Team Lead (PTL), the Abstraction Team Lead (ATL), and Subject Matter Experts (SMEs). The PTL and ATL will manage the process of implementing these guidelines, and work closely with the SMEs to ensure a consistent understanding of how these guidelines will be implemented and documented. The SMEs are generally the principal investigators that are most knowledgeable about individual process models and their uncertain parameters. The SMEs will provide the technical expertise to identify, implement, and document the treatment of alternative conceptual models, model abstractions, and parameter uncertainty using the processes identified in these guidelines. The PTL, ATL and SMEs will be supported by Process Modeler(s) and TSPA Analyst(s). The Process Modeler will assist the SME in the development, documentation and validation of appropriate model abstractions. The TSPA Analyst will integrate the abstracted model(s) in the TSPA–LA. The functional roles for the different team members are as follows:

Parameter Team Lead (PTL) - Individual assigned responsibility to lead the process for ensuring the consistent treatment and documentation of parameter values, parameter distributions, and parameter uncertainty used in the TSPA–LA.

Abstraction Team Lead (ATL) - Individual assigned responsibility to lead the process for ensuring the consistent treatment and documentation of alternative conceptual models and model abstractions used in the TSPA–LA

Subject Matter Expert (SME) - Personnel that are most knowledgeable about individual process models and uncertain parameters associated with the process models. The SME is responsible for identifying and developing alternative conceptual models, model abstractions, and parameters (including values, distributions, and uncertainty) consistent with these guidelines for use in the TSPA–LA.

Process Modeler - Personnel assigned to assist the SME in developing and implementing process models and abstractions (where appropriate) for use in the TSPA–LA.

TSPA Analyst - Personnel assigned to integrate alternative conceptual models and model abstractions in the TSPA–LA model.

These functional roles may or may not correspond directly with the existing or future PA Project organizational structure. However, it is expected that individuals selected for the PTL and ATL roles will be designated by, and report to, the TSPA Department and PA Strategy and Scope subproject managers. The individual(s) selected will be authorized by the PA Project Manager. The SMEs will be designated by, and report to, the various departments and the respective subproject managers. This allows for the input and documentation to the TSPA–LA to be controlled within the PA Project.

1.3.2 Documentation Requirements

The technical basis for the treatment of model (conceptual and abstraction) and parameter uncertainties will be documented in the respective model reports. In order to enhance the transparency and traceability of the treatment of uncertainties, these guidelines require that the information describing the treatment of uncertainties be documented in an attachment to, or distinct section in, the individual model reports.

The use of the model abstractions and parameters in the TSPA–LA Model will be described and documented in the TSPA–LA model documentation per the governing procedure (APSIII.10Q). The documentation will include identification of the model abstractions and parameters, a listing describing the interfaces with the process models, and a description of any changes made by the TSPA Analyst to model abstractions provided by the SME. Any such changes by the TSPA Analyst must also be signed off by the appropriate SME and will occur within the context of the AP-S.14Q review process.

Table 1-1. KTI Agreements: Alternative Conceptual Models, Model Abstraction, and Parameter Uncertainty.

KTI #	NRC/DOE Agreement	Corresponding Section of This Document
TSPAI 3.38	DOE will develop written guidance in the model abstraction process for model developers so that (1) the abstraction process, (2) the selection of conservatism in components, and (3) representation of uncertainty, are systematic across the TSPA model. These guidelines will address: (1) evaluation of non-linear models when conservatism is being used to address uncertainty, and (2) use of decisions based on technical judgement in a complex system. These guidelines will be developed, implemented, and made available to the NRC in FY02.	Sections 2, 3 and 4 Abstraction Process (Section 3.2) Selection of conservatisms (Section 4.2) Representation of uncertainty (Section 4.2) Evaluation of non-linear models (Section 4.2) Use of decisions based on technical judgment (Section 4.2)
TSPAI 3.39	DOE will document the simplifications used for abstractions per TSPAI 3.38 activities for all future performance assessments. Justification will be provided to show that the simplifications appropriately represent the necessary processes and appropriately propagate process model uncertainties. Comparisons of output from process models to performance assessment abstractions will be provided, with the level of detail in the comparisons commensurate with any reduction in propagated uncertainty and the risk significance of the model. The documentation of the information will be provided in abstraction Analysis Model Reports (AMRs) in FY03.	Section 3 Represent necessary processes (Section 3.2) Propagation of uncertainties (Section 3.2) Comparison of output from process models (Section 3.2, AP-SIII.10Q) Documentation of information in model reports (Section 3.2) (Note: These guidelines provide the methodology for implementing this KTI agreement. Documentation, justification, and comparisons will be provided in the respective model reports)
TSPAI 3.40	DOE will implement program improvements to ensure that the abstractions defined in the AMRs are consistently propagated into the TSPA, or ensure that the TSPA documentation describes any differences. Program improvements may include, for example, upgrades to work plans, procedural upgrades, preparation of desktop guides, worker training, increased review and oversight. The program improvements will be implemented and made available to the NRC during FY02.	Section 3 Implement program improvements (Section 3.2) Ensure TSPA documentation documents differences (Section 3.2) Program improvements (Section 3.2)
TSPAI 3.41	DOE will provide the technical basis for the data distributions used in the TSPA to provide support for the mathematical representation of data uncertainty in the TSPA. The documentation of the technical basis will be incorporated in documentation associated with TSPA for any potential license application. The documentation is expected to be available to NRC in FY03.	Section 4 Provide technical basis (Section 4.2) Support mathematical representation of uncertainty (Section 4.2) (Note: These guidelines provide the methodology for implementing this KTI agreement. Documentation will be provided in the respective model reports)
TSPAI 4.01	DOE will document the methodology that will be used to incorporate alternative conceptual models into the performance assessment. The methodology will ensure that the representation of alternative conceptual models in the TSPA does not result in an underestimation of risk. DOE will document the guidance given to process-level experts for the treatment of alternative models. The implementation of the methodology will be sufficient to allow a clear understanding of the potential effect of alternative conceptual models and their associated uncertainties on the performance assessment. The methodology will be documented in the TSPA–LA methods and assumptions document in FY02. The results will be documented in the appropriate AMRs or the TSPA for any potential license application in FY03.	Section 2 Incorporate alternative conceptual models (Section 2.2) Does not result in an underestimation of risk (Section 2.2) Document guidance on treatment of alternative conceptual models(Section 2.2) Potential effects of alternative conceptual models and associated uncertainties (Section 2.2) Documentation in TSPA–LA (Section 2.2)

2. GUIDELINES FOR TREATMENT OF ALTERNATIVE CONCEPTUAL MODELS IN TSPA–LA

The requirements of 10 CFR 63 specifically address the use of alternative conceptual models.

> 10 CFR 63.114(c) "Consider alternative conceptual models of features and processes that are consistent with available data and current scientific understanding and evaluate the effects that alternative conceptual models have on the performance of the geologic repository."

The concept of alternative conceptual models is also addressed in NUREG-1636, Section A.3.

> "The conceptual model of the site, therefore, is often based on imperfect information resulting in considerable extrapolation of sparse quantitative data which, in turn, could possibly lead to large conceptual errors in the analysis. In view of this, it is especially important that alternate models be formulated and tested to account for possible biases in conceptual model formulation."

The discussions in NUREG-1573 regarding model uncertainty also address the issue of considering alternative conceptual models.

> "Treating model uncertainty requires making credible assumptions about likely processes and events, and expressing them through selection of appropriate conceptual models and input variables. Although system and subsystem models are designed to be "reasonably realistic," credible alternative models may be possible given: (a) limitations in available site data; (b) ambiguities in interpreting site features; and (c) inadequacies in understanding processes (e.g., physical, chemical, geologic, and meteorologic) relevant to long-term performance of engineered barriers and the site. In considering model uncertainty in demonstrating compliance, the LLW disposal facility developer should use the conceptual model that can be best defended based upon what is known about the site. Additional data may need to be collected to defend the selected model. Alternatively, it may be preferable to choose the most conservative conceptual model for demonstrating compliance. However, the evaluation should be performed in the context of providing a reasonable range of potential outcomes - incredible events, highly unlikely combinations of parameters, and unreasonable modeling assumptions should not be used. Additionally, it is important to recognize that the assumed future state of the system is not intended to correspond to all possible future site conditions, but is intended to test the robustness of the facility against a reasonable range of potential outcomes." (pp. 3-24, 3-25)

NUREG-1573, in discussing probabilistic assessments, further states:

> "When there are two or more equally reasonable and plausible conceptual models for the site, results of different conceptual models need to be compared and analyzed. Comparison of the results from different conceptual models provide a quantitative basis for evaluating the uncertainty and conservative nature of competing conceptual models." (p. 3-29)

Closely related is the following excerpt from RG 1.174, which both emphasizes the need to demonstrate that the choice for the initial conceptual model is adequate and that any alternative models considered are reasonable.

> "Whether the PRA is full scope or only partial scope, and whether it is only the change in metrics or both the change and baseline values that need to be estimated, it will be incumbent on the licensee to demonstrate that the choice of reasonable alternative hypotheses, adjustment factors, or modeling approximations or methods to those adopted in the PRA model would not significantly change the assessment. This demonstration can take the form of well formulated sensitivity studies or qualitative arguments. In this context, "reasonable" is interpreted as implying some precedent for the alternative, such as use by other analysts, and also that there is a physically reasonable basis for the alternative. It is not the intent that the search for alternatives should be exhaustive or arbitrary." (p. 1.174-14)

As indicated in the Introduction, the scope of these guidelines is specifically limited to conceptual models that are to be propagated for use or directly used in the TSPA model. The first activity in these guidelines is the identification of reasonable alternative conceptual models. These guidelines assume that alternative conceptual models either will have been addressed by the various subproject departments in the formulation of the process models, or will be presented as a separate model for consideration in the TSPA–LA. The second activity is the evaluation of the alternative conceptual models for implementation in the TSPA–LA. If implemented, the development, validation, and documentation of the alternative conceptual model will occur within the scope of the respective model reports and in accordance with the procedural requirements of AP-SIII.10Q. For those alternative conceptual models that are implemented, the third activity provides for evaluating the impact on system-level model results. The implementation of any alternative conceptual models will be presented in the TSPA–LA model documentation in accordance with AP-SIII.10Q. The third activity, evaluation of system-level impacts, does not involve model development and will be documented in the TSPA–LA technical report. The final activity, FEPs traceability, provides for the documentation and forward traceability of the handling of the FEPs included in the TSPA–LA.

A discussion of the treatment of alternative conceptual models in the TSPA–SR is provided in Appendix A (Section A.2).

2.1 DEFINITIONS AND CONCEPTS

These guidelines include use of a supplemental set of definitions consistent with AP-SIII.10Q. In many instances, the AP-SIII.10Q definitions are specific to their application for the project (e.g., the definition may be limited by such phrases as "for incorporation into an overall system model of the geologic repository;" or by the distinction between mathematical models and scientific analyses).

2.1.1 Definitions

The terminology provided in AP-SIII.10Q and the definitions listed below will be used in performing and documenting the alternative conceptual model process for the TSPA–LA. Terms designated as "(per AP-SIII.10Q)" are direct quotes from that procedure. The remainder of the definitions have been derived from other related sources (e.g., WIPP documentation, NUREGs) and are provided to clarify and supplement the existing proceduralized definitions.

Abstraction (per AP-SIII.10Q) - The process of purposely simplifying a mathematical model (component, barrier, or subsystem process model) for incorporation into an overall system model of the geologic repository. The products of model abstractions may represent reduction in dimensionality, elimination of time dependence, tables obtained from more complex models, response surfaces derived from the use of more complex models, representations of a continuous process or entity with a few discrete elements, etc.

Alternative Conceptual Models - Multiple working sets of hypotheses and assumptions of a system that are all acceptable (i.e., consistent with the purpose of the model, logically consistent with one another, in agreement with existing information, and able to be tested).

Applied Model - An analyst's application of the generic computational model to a particular system, using appropriate values for dimensions, parameters, and boundary and initial conditions. In waste management, the system is a waste disposal site, and so this model is also referred to as a site-specific model.

Computational Model - The solution and implementation of the mathematical model. The solution may be either analytical, numerical, or empirical. The computational model is generic until system-specific data are used to develop the applied model.

Conceptual Model - The set of hypotheses and assumptions that postulates the description and behavior of a system. These hypotheses and assumptions describe (a) the simplified physical arrangement of system components, (b) the initial and boundary conditions types, and (c) the nature of the relevant, chemical, physical, biological, and cultural phenomena.

Mathematical Model - The mathematical representation of a conceptual model. That is, the algebraic, differential, or integral equations that predict quantities of interest of a system and any constitutive equations of the physical material that appropriately approximate phenomena in a specified domain of the conceptual model.

Model, Abstraction (per AP-SIII.10Q) - A product of the abstraction process that meets the definition of a mathematical model.

Model-Form Uncertainty - Uncertainty in the most appropriate model form of a system. The uncertainty results from sparse observational data and lack of information available to corroborate or refute alternative models. Developing alternative models is one method to explicitly acknowledge model-form uncertainty.

Risk Dilution - A situation in which an increase in the uncertainty of the input parameters of a model may lead to a decrease in the mean of an output quantity.

2.1.2 Concepts

Model Hierarchy

The concept of model hierarchies is addressed in NUREG-1636 (Appendix A, Section A.3). In NUREG-1636, two steps in the model development process are recognized: formulation of the conceptual models and formulation of mathematical models that correspond to each of the conceptual models. To integrate the models into an overall system, a three level hierarchy is suggested. The first level consists of the very detailed models of the individual processes. At the second level, a subset of the detailed models with some simplifications (abstractions) is coupled to study and understand the interfaces between processes. In the third and final level, all component models are further simplified (abstracted) and coupled to formulate the total system performance model. In many cases, conceptual models may be expressed directly in their mathematical form. Regardless, without an expression in the mathematical form, there is not enough structure to quantitatively apply the conceptual model. This model hierarchy is consistent with PA pyramid utilized for YMP PA analyses (CRWMS M&O 2000a [DIRS 153246]).

Relationship of Definitions Provided in AP-SIII.10Q and NUREG-1636

Differences exist in the definitions provided in AP-SIII.10Q and those provided in NUREG-1636 and as presented above. The differences in AP-SIII.10Q largely reflect the project-specific application of the more generic NUREG definitions.

For instance, the definition of NUREG-1636 for *abstraction model* is " a conceptual model of a component, barrier, or subsystem that is purposely simplified to fit into a model of the overall geologic repository." By contrast, the definition in AP-SIII.10Q limits *abstraction* to "simplifying a mathematical model (component, barrier, or subsystem process model) for incorporation into an overall system model of the geologic repository", and defines *model, abstraction* as a product that "meets the definition of a mathematical model". The difference between NUREG-1636 and AP-SIII.10Q is the starting point of the abstraction, either the conceptual model or the mathematical model. However, the AP-SIII.10Q definition for *model, conceptual* allows for simplification (or abstraction) and idealizations, so the difference is largely semantic.

The distinctions in the AP-SIII.10Q definitions are necessary to distinguish between *model abstractions* and *scientific analysis*. From a strictly procedural standpoint, *model abstractions* result in mathematical models and are subject to the selection, development, validation, and documentation requirements listed in AP-SIII.10Q. Those that are in nature *scientific analysis* and apply more towards choices made within the context of formulating conceptual models fall under AP-SIII.9Q. This distinction is important for these guidelines because identification of an abstraction as a *model abstraction* also signifies that the associated uncertainty (both parameter and representational model uncertainties) be addressed and/or quantified, and as appropriate, be propagated into the TSPA–LA.

The definition for conceptual model in NUREG-1636 is somewhat more helpful in understanding these guidelines than the definition provided in AP-SIII.10Q. The NUREG-1636 definition is as follows:

> "A representation of the behavior of a real-world process, phenomenon, or object as an aggregation of scientific concepts, so as to enable predictions about its behavior." (Appendix C)

For alternative conceptual models to be implemented in the TSPA–LA, the usefulness of the NUREG-1636 definition lies in the concept of "a representation that enable predictions." By contrast, the AP-SIII.10Q definition suggests a somewhat less predictive quality:

> " A set of hypotheses consisting of assumptions, simplifications, and idealizations that describes the essential aspects of the system, process, or phenomenon."

For the purposes of these guidelines, the concepts expressed by the NUREG-1636 definition will be used as a supplemental definition to that provided in AP-SIII.10Q. In any case, to be of use to the TSPA–LA evaluations, the alternative conceptual model or its abstractions must be translated into a useable mathematical model.

Use of Alternative Conceptual Model

The consideration of alternative conceptual models is a regulatory requirement. The use of alternative conceptual models, as suggested by the statements in 10 CFR 63 and the regulatory guidance, the use of an alternative conceptual model is appropriate if

- It differs significantly from the initial conceptual model.
- It is consistent with available data and current scientific understanding.
- It is reasonable. As stated in RG-1.174, "In this context, reasonable is interpreted as implying some precedent for the alternative, such as use by other analysts, and also that there is a physically reasonable basis for the alternative. It is not the intent that the search for alternatives should be exhaustive or arbitrary." (p. 1.174-17)

2.2 PROCESS FOR TREATMENT OF ALTERNATIVE CONCEPTUAL MODELS IN TSPA–LA

The process will use a team approach (see example in Figure 2-1) for considering and implementing alternative conceptual models, as described below. This process closely parallels the approach for addressing model abstractions (Section 3) and for evaluating parameter uncertainty (Section 4).

To provide consistency in addressing alternative conceptual models, the implementation of these guidelines calls for the use of two essential participants: the Abstraction Team Lead (ATL) and the Subject Matter Expert (SME), (see Figure 2-1). The term, "Abstraction Team Lead," is intentional because the person directing the consideration of alternative conceptual models can be the same individual that is used to address model abstraction issues, as described in Section 3. If the ATL function is split between two or more persons, then close coordination of activities will be needed because of the interrelated nature of implementing the alternative conceptual models into the TSPA and model abstractions. The Parameter Team Lead (PTL), described in Section 4, will provide guidance on the incorporation of parameter uncertainty, as requested by the ATL and/or SME. A TSPA Analyst, and a Process Modeler, are also identified as participants and will provide technical support at the request of the ATL and SME.

The intent of these guidelines is that one ATL will be designated to address all alternative conceptual models from across the various subject areas. This will provide for consistency in the guidance given to the multiple SME's, the treatment of alternative conceptual models, and the implementation into the TSPA–LA. The ATL will direct the team in implementation of these guidelines, advise the SME on the appropriateness of proposed alternative conceptual models, and coordinate activities with multiple SMEs.

The process provides for review and concurrence by the ATL and the SME prior to implementation of the alternative conceptual models in the TSPA–LA. It also specifies that the implementation of the alternative conceptual model in the TSPA–LA be checked and reviewed by both the ATL and SME. This will allow for consistent guidance from and interface with the TSPA Department and the respective subproject departments. The cross-checking and review of the alternative conceptual model(s) will be performed as part of the technical checking under AP-SIII.10Q.

Requirements for development and documentation of alternative conceptual models to be propagated into the TSPA–LA are now addressed in AP-SIII.10Q. This procedure requires revision of the technical work plan and review of the work plan and model validation by the Chief Science Officer. For TSPA–SR, the description of the consideration and treatment of alternative conceptual models was placed in the AMRs. Effective with the implementation of these guidelines, the technical basis and the development and validation of the alternative conceptual model forwarded to the ATL for consideration and/or implementation in the TSPA–LA will be documented in the respective model reports. This documentation will be in the form of an attachment or distinct section to the model report, such that the updated documentation is more transparent than the existing documentation (see Section 1.3.2 regarding the use of attachments). The documentation for any alternative conceptual models implemented into the TSPA–LA will include a qualitative description and unambiguous mathematical description of the model. Alternative conceptual models that are forwarded to the ATL for consideration but not implemented and the basis for not implementing them will also be documented in the appropriate model report.

The TSPA–LA model report will document the basis for deciding that an alternative conceptual model brought forward by the SME was appropriate or inappropriate for implementation in the TSPA–LA. If implemented, the TSPA–LA model report will document how the alternative conceptual model was used in the TSPA–LA. The TSPA–LA model document will specifically denote any changes from the alternative conceptual model (as documented in the respective model reports) that were needed to integrate the model within the TSPA–LA framework. Additionally, an Appendix to the TSPA–LA documentation will list each of the alternative conceptual models used or implemented in the TSPA–LA and provide a brief description of the alternative conceptual models.

2.2.1 Process Implementation

The process for the treatment of alternative conceptual models consists of four basic activities: 1) identifying alternative conceptual models for consideration (if any), 2) evaluating any appropriate and reasonable alternative conceptual models, 3) evaluating system level impacts, and providing for FEPs traceability (see Figure 2-2).

Identify Alternative Conceptual Models

The first activity in the process is to determine whether any alternative conceptual models are consistent with available data and scientific understanding. The consistency with available data and scientific understanding, and the reasonableness of alternative conceptual models, was previously considered and documented by the SMEs as part of the TSPA-SR process, although in varying degrees of detail. In many cases the alternative conceptual models were either incorporated probabilistically, or the most conservative conceptual models were chosen. Repository design is an important area that may create alternative conceptual models for consideration in this process. Their evaluation will follow the same process detailed below.

Consequently, the identification of alternative conceptual models for TSPA-LA will involve the four steps identified below to determine the appropriateness of using any alternative conceptual models.

These steps will require the SMEs, in consultation with the ATL and TSPA Analysts in the TSPA Department, to carefully examine the existing models and supporting documentation used for the TSPA-SR, SSPA, and the TSPA-FEIS. The examination will then be fully documented in model reports. This documentation will at a minimum include a list of the alternative conceptual models reviewed by the SME, the decision made regarding consistency with available data and scientific understanding and reasonableness, and the basis for the decisions made. It will also document, if any, the sensitive or key parameters evaluated, the associated FEPS that were reviewed, the decision made regarding changes or development of alternative conceptual models, and the basis for the decision. The technical justification for determining that only one conceptual model is consistent or reasonable must also be documented. As the process evolves, the steps may be modified as appropriate.

<u>Step 1.</u> The ATL initiates a team meeting to discuss implementation and use of these guidelines. At this meeting, the ATL provides to the SME a list of key parameters, TSPA–SR and TSPA–FEIS key model components, and other project documents. The ATL will also review and discuss the application of the three criteria that determine whether an alternative conceptual model is appropriate. These criteria include: significant difference from the initial/existing conceptual model, consistency with existing data and current scientific understanding, and reasonableness (as defined by Regulatory Guide 1.174).

<u>Step 2</u>. A review by the SMEs of AMRs and PMRs to identify previously considered alternative conceptual models and to reevaluate their consistency with data in light of current project knowledge. For example, the various PMRs list several alternative conceptual models that were

not incorporated because (1) the models developed for TSPASR represented more realistic models than the alternative models; (2) they were not supported or were invalidated by existing observed data; or (3) sufficient data for developing and validating a representational model for the alternate conceptual model was not available or obtainable.

Step 3. A review by the SME of a list of model sensitivities/key parameters from the TSPA–SR, SSPA or other project documents (to be provided by the ATL) to identify where the use of alternative conceptual models would be most appropriate and suitable for implementation into TSPA–LA. Consistent with a risk-informed approach, alternative conceptual models will only be developed for areas with sensitive or key parameters. This would include a reexamination of FEPs that are related to key parameters to determine the appropriateness of modifying an existing screening decision (i.e., change from exclude to include) or identifying areas where an alternative treatment is appropriate. For example, the consideration of stress corrosion cracking may be represented by one or more alternative conceptual models that were not previously considered, since only the conservative model was chosen for use in TSPA–SR. The change from conservative or bounding estimates to realistic treatment (as described in Section 4 for addressing parameter uncertainty) may constitute an "alternative conceptual model" as defined above in that the hypothesis and assumptions used to construct the model form may have changed. Any changes to FEPs screening decisions or arguments will necessitate the FEPs team be notified in accordance with the Enhanced FEPs Plan (BSC 2002b). See also the following discussion on FEPs traceability.

Step 4. The SME will determine if one or more conceptual models differ significantly from the existing conceptual model, are consistent with available data and current scientific understanding, and are reasonable. This may be done either qualitatively, based on the SME's technical judgement, or quantitatively using existing or readily qualifiable software (i.e., consistent with the definition of a *scientific analysis* under AP-SIII.9Q). If the SME's judgement is that only one conceptual model is consistent with all information, then uncertainty from associated alternative conceptual models is also considered not significant, provided important parameter uncertainty is propagated in the model selected.

Evaluate Alternative Conceptual Models

Following the initial activity of identifying possible alternative conceptual models, SME and process modeler will develop appropriate mathematical models and model abstractions, based on the alternative conceptual models, to evaluate the behavior of the repository system. The responsible SME, in consultation with the ATL, will evaluate whether any identified alternative conceptual models for the subsystem process model should be developed for further implementation in the TSPA–LA. If not, the considerations and the basis for the decision to not implement the alternative conceptual model in the TSPA–LA will be documented by the SME in the model report. If the decision is to recommend implementing the alternative conceptual models in the TSPA–LA, then the following steps may apply. As the process evolves, the steps may be modified as appropriate.

Step 1. The ATL and PTL (or designees) provide assistance in determining and recommending appropriate methods for propagating necessary uncertainty and variability in the alternative conceptual model(s) (see Section 4 on parameter uncertainty).

Step 2. The SME provides results from process models to be used as a basis for demonstrating whether the alternative conceptual model(s) produces significantly different results for the subsystem component model. Alternative conceptual models will be implemented in TSPA–LA only for subject areas with sensitive or key parameters. The SME also provides a method and/or data to be used to validate the alternative conceptual model(s).

Step 3. The SME and Process Modeler develop the mathematical expression and/or model abstraction of the alternative conceptual model(s), validate, and document the results, all in accordance with the requirements of AP-SIII.10Q. If the mathematical expression or model abstractions of the alternative conceptual models are not straight forward, then the use of conservatism (consistent with the guidelines provided in Section 4 of this document on the use of conservatism) is an acceptable option and will be documented accordingly. If an alternative conceptual model can be formulated to produce results that are commensurate with existing subsystem components and site data, the differences in performance between the alternative conceptual models will be described and quantified where practicable (e.g. using standard statistical measures such as "goodness of fit" (Chi-square test, Kolmogorov-Smirnov test, etc.)).

Step 4. This work is submitted to the ATL for technical review and comments regarding the potential suitability for implementation in the TSPA–LA. If all alternative conceptual model(s) result in performance similar to the current subsystem component used in the TSPA–LA, as determined by the SME in consultation with the ATL, then the alternative conceptual model uncertainty is insignificant and no further evaluation of the alternative conceptual model(s) for system level impacts is needed. The SME and Process Modeler then address the ATLs comments and document the basis for the decision regarding the disposition of the ACML, as described in Step 5. If the performance of the alternative conceptual model(s) is different from the initial conceptual model, and the alternative conceptual model(s) will be recommended to the ATL for evaluation of system level impacts and implementation into the TSPA–LA, then the SME and Process Modeler further develop abstractions as appropriate to address the ATL's concerns. The SME also develops and provides a confidence distribution to the ATL for potential use in weighting of the alternatives, using the approach in NUREG-1563 as appropriate, and describes any controversy regarding the acceptability of the alternative conceptual models.

Step 5. The SME then documents the alternative conceptual model(s) considered in the model report in accordance with AP-SIII.10Q. To validate the alternative conceptual model(s), the comparison of the results will be to data or by some other appropriate method as described in AP- SIII.10Q, rather than to the results of the existing process model. This is because differences from the nominal case process model results would be expected i.e., the alternative conceptual model(s) should be "significantly different" from the initial model. The SME then dispositions the information and resulting data in accordance with AP-SIII.3Q. The SME then transfers control of the alternative conceptual model(s) to the ATL for evaluation of system level impacts and possible implementation into the TSPA–LA.

Evaluate System Level Impact and Implement in the TSPA–LA

The ATL will be responsible for determining which, if any, alternative conceptual models to implement in the TSPA–LA and for recommending the approach for implementation. This activity includes evaluating whether the results of the TSPA–LA are sensitive to the alternative conceptual model(s), choosing which alternative models to implement and/or to further quantify model uncertainty, and for determining the approach for implementation. Criteria of significance will need to be developed for systematic inclusion/exclusion of alternative conceptual models, much like the work done for FEPs, because of the potentially onerous number of combinations of alternative conceptual models in the TSPA. Clearly, not all combinations will provide useful information. The linkage of effects of multiple alternative conceptual models will also be considered in defining the analyses to be run with alternative conceptual models. In support of the ATL's decision, the TSPA Department, through the TSPA analyst, will determine and document the system level impact of any alternative conceptual models implemented in the TSPA–LA, as requested by the ATL. The steps for the evaluation and implementation follow.

Step 1. The ATL reviews the alternative conceptual model recommendations from the SME. If no alternative conceptual models are recommended by the SME, or if all alternative conceptual model(s) predict behavior similar to the existing subsystem component used in the TSPA–LA, or if the TSPA is not sensitive to which alternative conceptual model is used, then the ATL may determine that alternative conceptual model uncertainty is insignificant and no further evaluation of the alternative conceptual model(s) for system level impacts is needed. (See Step 4 under Evaluate Alternative Conceptual Models above). In this case, the ATL will determine which of existing conceptual models (existing or alternative) to carry forward to the TSPA–LA. The ATL will advise the SME of the determination, the determination will be documented in the model report by the SME, and a brief summary of this determination will be included in the TSPA–LA documentation by the ATL. If the SME disagrees with the ATL's determination, the SME may elevate the determination to the PA Manager for resolution.

Step 2. If one or more alternative conceptual models are to be further evaluated for system level impacts, the ATL will advise the TSPA Analyst to either further quantify or not quantify alternative conceptual model uncertainty and provide only a qualitative discussion of the uncertainty. The ATL will also provide and document any recommendations for implementation. The basis for these recommendations will be documented in the TSPA–LA report. The decisions of the ATL should be based on the sensitivity of the TSPA–LA model results to changes in the subsystem model component being evaluated.

Step 3. Should the system level impact of any alternatives appear important enough to quantify for the TSPA–LA, one of two approaches will be used. For those alternative conceptual models for which little controversy exists (i.e., it is the SME's judgement that either representation would be generally considered reasonable or acceptable to the scientific community at large) and have significant system-level impact, the TSPA Department will incorporate the conceptual models into the TSPA–LA model. A parameter will be used to select between the two or more alternatives. This selection parameter will have a distribution assigned based on confidence in the applicability of the various alternative conceptual models. The distribution will be provided based on the SME's judgement and/or any available expert elicitation information. The potential risk dilution from implementing multiple alternative conceptual models will be evaluated in this step.

For controversial alternatives and/or for those with significant system-level impact, the TSPA Analyst may choose to run the full TSPA simulation for each alternative and report the results.

Alternatively, the ATL may choose to implement only the most conservative of the alternative conceptual models along with the existing conceptual model, and provide a basis for the decision which verifies that the selected conceptual model is truly conservative when incorporated in the TSPA–LA.

Step 4. The TSPA Analyst obtains the controlled information necessary to implement the alternative conceptual model(s) and documents the integration and the results generated within TSPA–LA, and returns the documentation to the ATL. The work is reviewed by the ATL and the SME.

Step 5. The ATL ensures that the implementation, development and validation of the alternative conceptual model (along with the decision to use the alternative conceptual model and the basis for that decision) is documented in the TSPA–LA model report, with appropriate referencing to the documentation provided in the supporting model report.

FEPs Traceability

Because of the use of the FEPs process for TSPA–SR, relevant FEPs have been included in conceptual models used as the basis for TSPA–SR and/or SSPA. The basis for excluding certain FEPs from further consideration has been previously documented in the FEPs-related AMRs.

Because of the interrelationship of the FEPs process and the formation of conceptual and alternative conceptual models, these guidelines will also implement the review of AMRs that directly support the TSPA–SR and the subsequent documentation to provide forward traceability for included FEPs. This activity will necessitate that all abstraction model reports (or equivalent AMRs that feed TSPA, in those cases where the abstraction AMR may be being merged into the process AMR) be updated. This FEPs traceability activity involves three steps. As the process evolves, the steps may be modified as appropriate.

Step 1. The SME(s) (or designees) responsible for model reports that directly feed the TSPA will identify those FEPs that are screened in through the work included in the respective AMR. This identification will be done in consultation with the relevant FEP AMR leads and in conjunction with implementation of the Enhanced FEPs Plan (BSC 2002b).

Step 2. The SME(s) (or designees will provide a summary for each included FEP of how it has been included (e.g., explicit modeling, incorporation in parameter range, etc.) for the TSPA–LA. This summary can be in an attachment or distinct section to the AMR. This summary will be consistent with the guidance provided in the Enhanced FEP Plan (BSC 2002b). The Enhanced FEPs Plan (BSC 2002b) details the FEPs screening process. The FEPs developed in conjunction with alternative conceptual models, will be screened in the same manner.

Step 3. Provide the same summary information to the relevant FEP AMR lead so that it can be included in the FEP AMR or other appropriate document.

2.2.2 Roles and Responsibilities

The alternative conceptual model team will include the ATL and a TSPA Analyst(s), and the SME and process modeler. It is intended that a single ATL will be used to lead the entire alternative conceptual model process. The team will also include an SME selected by the appropriate Department Manager, and an appropriate Process Modeler. In many instances, it will be desirable for the alternative conceptual model team members to be identical to and/or to interface regularly with the team addressing model abstraction issues and/or parameter uncertainty. The PA Project Manager or designee will assign these roles.

<u>Department Manager(s) Tasks</u>:

1. The PA Project Manager (or designee) will select the ATL and the TSPA Analyst from within the TSPA Department

2. The respective subproject Department Managers(s) will select the SME(s) and the Process Modeler(s)

<u>ATL (or designee) Tasks</u>:

1. Initiate a team meeting to discuss implementation of these guidelines.

2. Provide the SME with a list of key models and key parameter uncertainties.

3. Coordinate the alternative conceptual process and interface with personnel performing any related model abstraction and parameter uncertainty activities.

4. Advise the SMEs and Process Modeler on the alternative conceptual models to be used in TSPA to determine the viability of implementing them into TSPA–LA., based on significant difference, consistency with data, and reasonableness.

5. Determine whether alternative conceptual models result in significantly different behavior and whether to include them in the TSPA–LA. Determine the method for implementing them, based on consultation with the SME. In the event that the SME disagrees with the ATL's decisions, the matter may be elevated by the SME to the PA Manager for resolution.

6. Advise the Process Modeler during development, validation, and documentation of the alternative conceptual model. Advise and assist the TSPA Analyst during implementation of the alternative conceptual model into the TSPA.

7. Advise the TSPA Department regarding the need to further quantify alternative conceptual model uncertainty.

8. Review and check the alternative conceptual model and results before and after integration into the TSPA–LA.

9. Ensure documentation of the integration and use of the alternative conceptual models in the TSPA–LA model report, with text annotation of any changes in the model abstraction needed to facilitate integration into the TSPA–LA.

10. Ensure that the alternative conceptual models have been developed and documented in the model report and TSPA–LA document according to applicable modeling and software control procedures.

PTL (or designee) (see Section 4.2) Tasks:

1. Provide insight to the ATL, TSPA Analyst(s), SME, and Process Modeler with regard to key parameters identified from the process described in Section 4 and provide guidance on the propagation of uncertainty and variability through the alternative conceptual model process.

TSPA Analyst(s) Tasks:

1. Attend team meeting which addresses implementation of these guidelines.

2. Assist the Process Modeler in developing the alternative conceptual model, particularly with regard to interfacing with other TSPA models and components.

3. Integrate versions of the alternative conceptual model(s) in the TSPA–LA model.

4. Document the modeling decisions, basis for the decisions, and use in the TSPA–LA, along with any changes required to integrate the alternative conceptual model, in accordance with project procedures governing models and the use of software.

SME Tasks:

1. Attend team meeting which addresses implementation of these guidelines.

2. Identify alternative conceptual models that will be recommended to the ATL for consideration in the TSPA–based on the criteria of significant differences, consistency with data, and reasonableness. In the event that the SME disagrees with the ATL's decisions, the matter may be elevated by the SME to the PA Manager for resolution.

3. Assist the Process Modeler in implementing appropriate methods for propagating necessary uncertainty and variability (see Section 3 on model abstractions and Section 4 regarding parameter uncertainty). Provide results from process models to be used as a basis for comparison. Provide any site data or standard data sets or other methods, to be used for validation of the alternative conceptual model.

4. Confer with and assist the Process Modeler during development, validation, and documentation of the alternative conceptual model. Confer with the TSPA Analyst, as needed, during integration of the alternative conceptual model into the TSPA.

5. Perform review of the alternative conceptual model before and after integration into the TSPA–LA.

6. Transmit to the ATL final copies of the developed and documented alternative conceptual models for integration into the TSPA. Provide a distribution that describes an estimate of the confidence in each of the alternative conceptual models.

7. Document the development and validation of the alternative conceptual model in the AMR in an attachment or distinct section format to allow for extended documentation as needed.

8. Interface with personnel performing any related model abstraction and parameter uncertainty activities.

9. Ensure that the alternative conceptual model is developed and documented in accordance with applicable project procedures governing models and use of software.

10 Implement and document the FEPs traceability activity as described above.

Process Modeler Tasks:

1. Attend team meeting which addresses implementation of these guidelines.

2. Assist the SME in reviewing process models and determining the viability of any alternative conceptual models to be forwarded to the ATL.

3. Modify the Technical Work Plan as necessary to include development, validation, and documentation of the alternative conceptual model(s) as required per AP-SIII.10Q.

4. Determine the relevant observations or literature to justify or support the alternative conceptual model (e.g., justification for a set of appropriate values to use in the model, sensitivity study, or previous use of the alternative conceptual model) and document the supporting information. Assist SME in determining significant difference, consistency with data, and reasonableness.

5. Request that the SME assist in determining appropriate methods for propagating necessary uncertainty and variability (see Section 4 on parameter uncertainty) and provide results from process models, site data, or standard data sets to be used as a basis for comparison and/or validation of the alternative conceptual model.

6. Develop and validate the model or model abstraction by comparing results to the site data and/or a standard data set, and document the results in accordance with applicable project procedures governing models and use of software.

7. Document the development and validation of the alternative conceptual model in the AMR.

8. Assist the TSPA Analyst with integration and documentation of integration of the alternative conceptual model into the TSPA–LA.

2.3 COMMUNICATION TO DECISION MAKERS

How to communicate structural (i.e., model) uncertainty along with parametric uncertainty in probabilistic analyses is still an open issue in the risk analysis literature. Given the choices that must be made regarding which models to include in the TSPA and the method of model integration, the Project is left with the task of communicating the level of uncertainty that these choices impart on the final results.

Without an explicit or clearly acceptable means of quantifying those uncertainties, it is critical that any communication of results includes a discussion of the consideration of alternative conceptual models, for both technical and policymaker audiences. The approach discussed in this document is to provide a separate attachment or distinct section in the model report for discussion of key components of the model.

In addition to the description and documentation of the decision process used to determine the "consistency" of the alternative conceptual model as described above in the implementation process, for each alternative conceptual model judged to be "consistent" and "reasonable", the attachment or distinct section to the model report will include a discussion of:

Uncertainty: Provide a brief discussion of uncertainties in results derived from the alternative conceptual models in comparison to the current TSPA model component, referring to the appropriate reports and graphs where the detailed results can be found.

Confidence: Provide a discussion of the level of confidence the Project has that the calculated uncertainties appropriately reflect the real world conditions. This would include discussion of the state of understanding of physical processes, amount and quality of data available, and accuracy of models used to represent the physical system.

Impact of Uncertainty: Provide a discussion of how uncertainty impacts the overall estimates of system and subsystem performance. This would include discussions, as appropriate, of how performance might change if future information supports specific alternative conceptual models or modifications to parameter distributions.

The discussion in the model report attachment or distinct section will include the rationale for the models chosen and a description of those unmodeled conditions that the assessment does not consider. This would also include items excluded for various reasons or events deemed to be implausible. The qualitative description of what is not explicitly modeled provides a higher level of confidence to what is being modeled. Furthermore, the implications on results of what is excluded will also be identified and documented. Much of this communication has already been created and documented by the Project, however the information is currently dispersed among a variety of different Project documents. Consequently, the discussion could be a summary of the past work with clear reference to the original source documentation.

In addition to the detailed discussions, a method for communicating a summary of the current understanding of model uncertainty to decision-makers is discussed in Section 4.3.3 of *Uncertainty Analyses and Strategy* (Williams 2001 [DIRS 157389]). At the decision-maker level, it will be important to develop means of expressing results and their uncertainties in a concise, summary manner.

The choice and/or method of integration of the alternative conceptual model or model abstractions in the TSPA–LA will be documented in the TSPA–LA model report. The information will include identification of the model abstraction, listing of interfaces with other system model components, and documentation of any changes made by the TSPA Analyst from the alternative conceptual model abstraction provided by the SME that were needed to implement the alternative conceptual model abstraction. The basis for determining the use and type (i.e., conservatism or weighting) of the model abstraction will also be included in the documentation. Specific reference to the supporting model report prepared by the SME and/or Process Modeler will be provided.

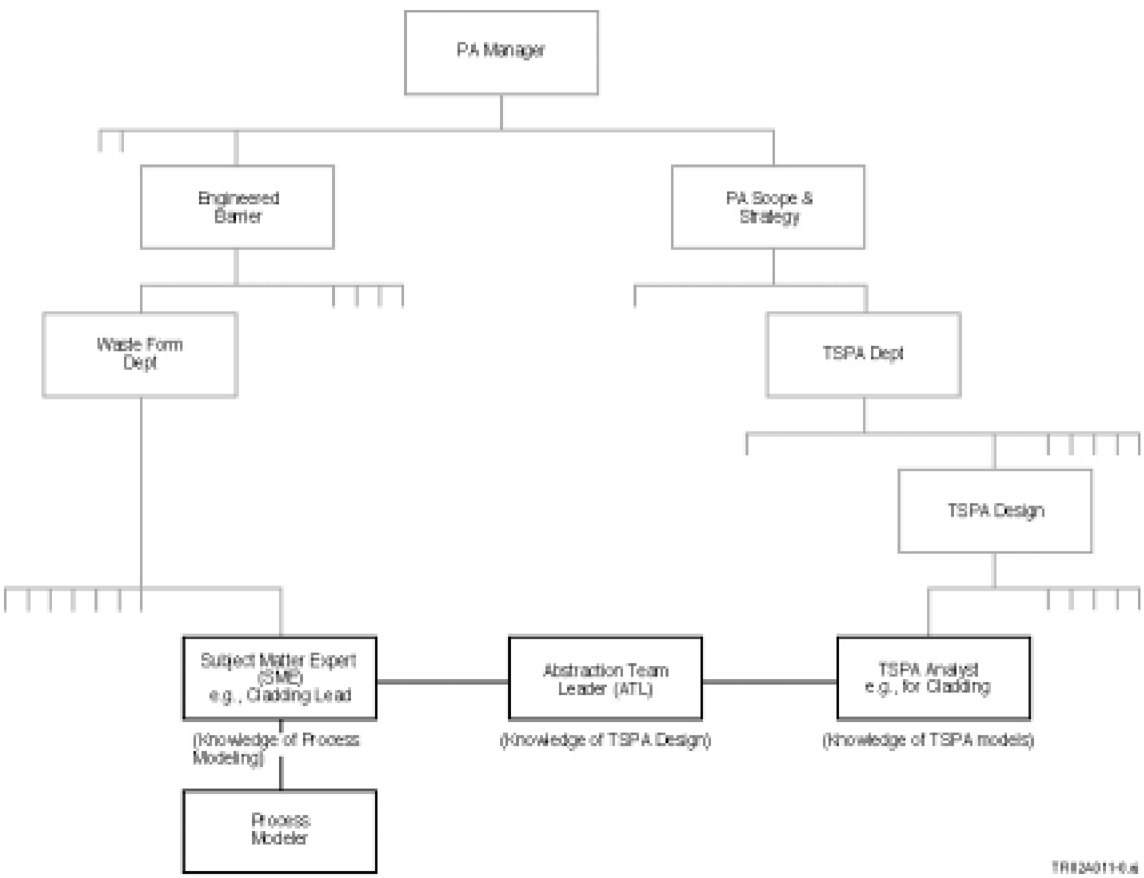

Figure 2-1. Alternative Conceptual Model Development Team (Example).

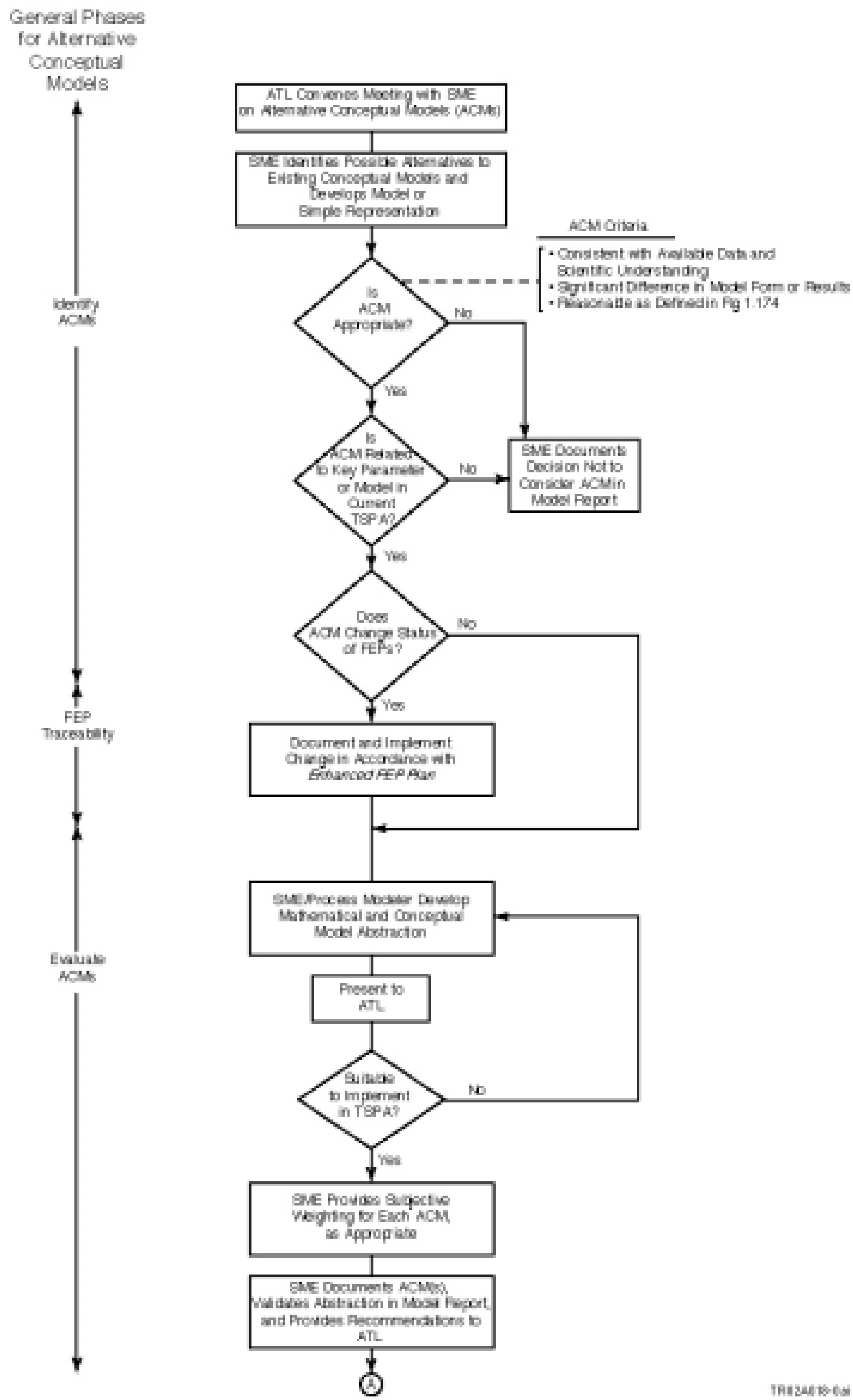

Figure 2-2. Process for Treatment of Alternative Conceptual Models in TSPA–LA.

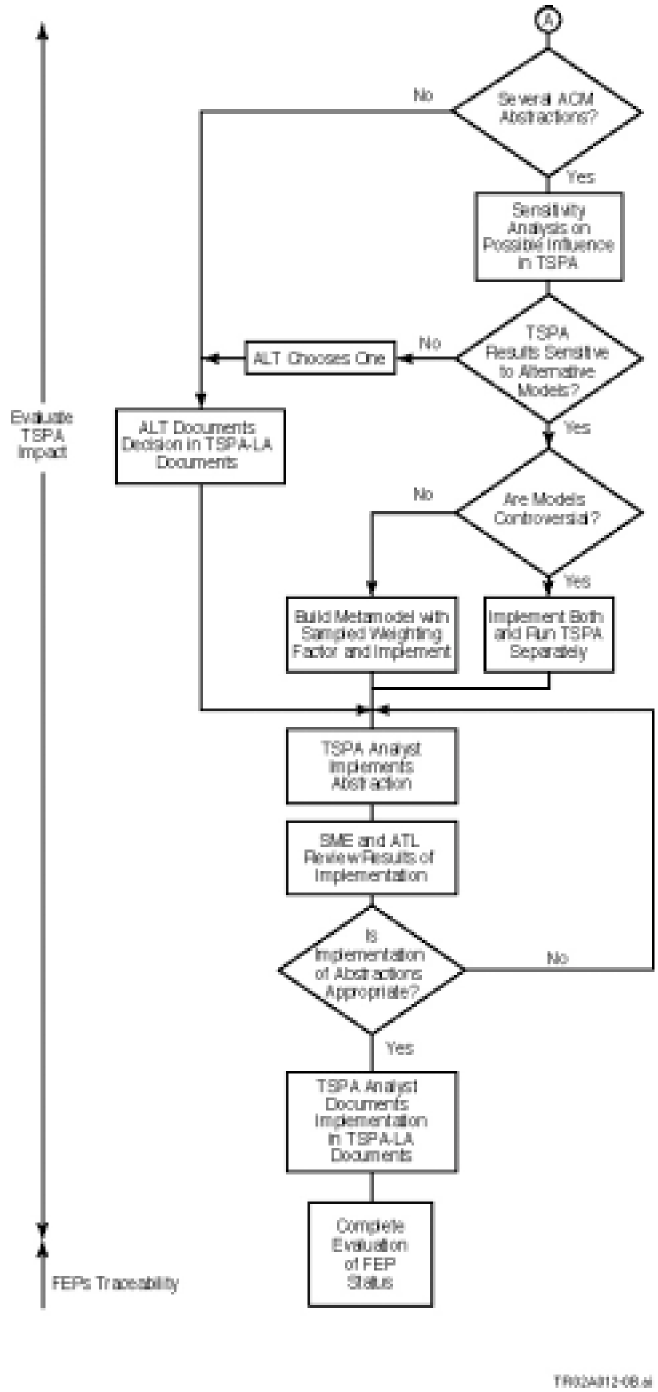

Figure 2-2 (continued). Process for Treatment of Alternative Conceptual Models in TSPA–LA.

3. GUIDELINES FOR TREATMENT OF MODEL ABSTRACTIONS IN TSPA–LA

The requirements of 10 CFR 63 specifically address the issues of uncertainty and variability in parameter values and the use of alternative conceptual models (10 CFR 63.114(b) and (c)). However, the use of abstractions or simplification of models is not directly addressed by the NRC. The regulatory recognition of abstractions (or simplifications) as part of the concept of "reasonable expectation" lies in the preamble to 40 CFR 197, which is more fully cited in Section 1 of this document. The NRC has decided to adopt EPA's preferred criterion of reasonable expectation for purposes of judging compliance with the postclosure performance objectives (66FR55740), and by inference, EPA's perspective on the use of model abstractions. The pertinent excerpt from the preamble to 40 CFR 197 is as follows:

> “Simplifications and assumptions are involved in these modeling efforts out of necessity because of the complexity and time frames involved, and the choices made will determine the extent to which the modeling simulations realistically simulate the disposal system's performance. If choices are made that make the simulations very unrealistic, the confidence that can be placed on modeling results is very limited. Inappropriate simplifications can mask the effects of processes that will in reality determine disposal system performance, if the uncertainties involved with these simplifications are not recognized.” (66 FR32102)

The concept of abstraction (or simplification) is also addressed in NUREG-1636, Section A.3. In the description of model hierarchies in NUREG-1636, simplification occurs at each step of the modeling process. As stated in the Introduction of this document, the scope of these guidelines are limited to model abstractions that are directly used in the TSPA model. This corresponds with the third and final level of model development identified in NUREG-1636,

> "In the third and final level, all component models are further simplified and coupled to formulate a total-system performance assessment (TSPA) model."

NUREG-1636 also emphasizes that not all processes need to be reduced to their third level of simplicity for inclusion in the system model because some of the processes may be so central to the final result that they have to be included in full detail. This suggests that NUREG-1636 recognizes that the issue of model abstractions and model integration represents a continuum of activity, rather than discrete, readily identifiable steps.

The first activity in these guidelines is the identification of those model components that are suitable for model abstraction. The second activity is to involve the SME in the selection of the model abstractions. The third activity involves developing, validating, and documenting the model abstractions in accordance with the procedural requirements of AP-SIII.10Q. The fourth, and final activity, is the integration of the model abstraction into the TSPA–LA and documentation in the appropriate TSPA–LA related reports.

A summary of the use of abstractions in the TSPA–SR is provided in Appendix A (Section A.3). The summary tables in Appendix A (Tables A-2, and A-3) can be used for identifying which model components were considered suitable for model abstraction in TSPA–SR, and could be similarly represented.

3.1 DEFINITIONS AND CONCEPTS

These guidelines include use of a supplemental set of definitions consistent with AP-SIII.10Q and a new taxonomy for identifying abstraction methods and techniques. In many instances, the AP-SIII.10Q definitions are specific to their application for the project (e.g., the definitions may be limited by such phrases as "for incorporation into an overall system model of the geologic repository"; or by the distinction between mathematical models and scientific analyses).

3.1.1 Definitions

The revised terminology provided in AP-SIII.10Q and listed below will be used in performing and documenting the model abstraction process for the TSPA–LA. Definitions quoted from the procedures are noted as "(per AP-SIII.10Q)". The remainder of the definitions have been derived from other related sources (e.g., WIPP documentation, NUREGs, and RG1.174) and are provided to clarify and supplement the existing proceduralized definitions

Abstraction (per AP-SIII.10Q) - The process of purposely simplifying a mathematical model (component, barrier, or subsystem process model) for incorporation into an overall system model of the geologic repository. The products of model abstractions may represent reduction in dimensionality, elimination of time dependence, tables obtained from more complex models, response surfaces derived from the use of more complex models, representations of a continuous process or entity with a few discrete elements, etc.

Alternative Conceptual Models - Multiple working sets of hypotheses and assumptions of a system that are all acceptable (i.e., consistent with the purpose of the model, logically consistent with one another, in agreement with existing information, and able to be tested).

Applied Model - An analyst's application of the generic computational model to a particular system, using appropriate values for dimensions, parameters, and boundary and initial conditions. In waste management, the system is a waste disposal site, and so this model is also referred to as a site-specific model.

Conceptual Model - The set of hypotheses and assumptions that postulates the description and behavior of a system. These hypotheses and assumptions describe (a) the simplified physical arrangement of system components, (b) the initial and boundary conditions types, and (c) the nature of the relevant, chemical, physical, biological, and cultural phenomena.

Computational Model - The solution and implementation of the mathematical model. The solution may be either analytical, numerical, or empirical. The computational model is generic until system-specific data are used to develop the applied model.

Mathematical Model - The mathematical representation of a conceptual model. That is, the algebraic, differential, or integral equations that predict quantities of interest of a system and any constitutive equations of the physical material that appropriately approximate phenomena in a specified domain of the conceptual model.

Model, Abstraction (per AP-SIII.10Q) - A product of the abstraction process that meets the definition of a mathematical model.

Model-Form Uncertainty - Uncertainty in the most appropriate model form for a system. The uncertainty results from sparse observational data and lack of information available to corroborate or refute alternative models. Developing alternative models is one method to explicitly acknowledge model-form uncertainty.

Model, Process (per AP-SIII.10Q) - A mathematical model that represents an event, phenomenon, process, component, etc., or series of events, phenomena, processes or components. A process model may undergo an abstraction into a system model.

Model, System (per AP-SIII.10Q) - A collection of interrelated models that represents the overall geologic repository or overall component subsystem of the geologic repository.

Scientific Analysis (per AP-SIII.10Q) - A documented study that 1) defines, calculates, or investigates scientific phenomena or parameters; 2) evaluates performance of components or aspects of the overall geologic repository; or 3) solves a mathematical problem by formula, algorithm, or other numerical method. A scientific analysis may use a previously developed and validated mathematical model, within the mathematical model's intended use and stated limitations, but may not revise the mathematical model in order to complete the scientific analysis. A scientific analysis may involve numerical manipulations that are not part of a validated mathematical model, but only if: 1) the choice of method for such manipulation is evident from standard practice and does not require justification and 2) the analysis results are not to be used to support licensing compliance arguments that require the additional confidence that would be attained by documenting the work as a model.

Scientific Analysis, Abstraction (per AP-SIII.9Q) - A product of the abstraction process that meets the definition of a scientific analysis and does not meet the definition of a mathematical model.

3.1.2 Concepts

Relationship of Definitions Provided in AP-SIII.10Q and NUREG-1636

Differences exist in the definition of abstraction provided in AP-SIII.10Q and those provided in NUREG-1636. These differences largely reflect the specific-project application in AP-SIII.10Q of more generic definitions provided in NUREG-1636. These were previously described in Section 2.1.2.1 of this document.

Propagation of Variability and Uncertainty

In the preamble to 40 CFR 197, the use of model abstractions and concerns regarding propagation of uncertainty are linked.

> "Inappropriate simplifications can mask the effects of processes that will in reality determine disposal system performance, if the uncertainties involved with these simplifications are not recognized." (p. 32102)

Consequently, the model abstractions used in the TSPA–LA must capture the important uncertainty or variability of the initial model, and the abstraction must be validated in a manner appropriate for its intended use. Model abstractions will be validated by comparing the results of the model abstraction against the results of the original model to demonstrate incorporation of important uncertainty and variability. The comparison of the propagated uncertainty and variability between the initial model and the model abstraction will be documented to ensure transparency and traceability.

Model Hierarchy and Use of Abstractions in TSPA–LA

The concept of model hierarchies and abstraction is addressed in NUREG-1636 (Section A.3). Two steps in the model development process are recognized: formulation of the conceptual models, followed by formulation of mathematical models that correspond to each of the conceptual models. To integrate the models into an overall system, a three level hierarchy is suggested, though the models may not be explicitly discretized in this manner. The first level consists of the very detailed models of the individual processes. This is, in some sense, an abstraction of the actual physical system. At the second level, a subset of the detailed models with some simplifications (abstractions) is coupled to study and understand the interfaces between processes. In the third and final level, component models are further simplified (abstracted) and coupled to formulate the total system performance model. In this approach, abstraction occurs at each step of the modeling process. This is consistent with the approaches and taxonomies used by other total system modeling efforts (Sisti and Farr, 1998; Frantz, 1998).

Model abstractions are based on individual techniques or a combination of multiple techniques, depending on the initial complexity of the process model and the level of detail desired in the abstraction. Sisti and Farr (1998) and Frantz (1998) propose a taxonomy of abstraction methods that addresses anything done to move from the real world, to a conceptual model, then to a mathematical model and/or computational model, and then to the applied or abstracted model. This is consistent with the model hierarchy and approach presented in NUREG-1636.

Frantz (1998) suggests that model abstraction techniques can be categorized into three broad classes - Model Boundary Modification, Model Behavior Modification, and Model Form Modification. Of these three categories, Model Boundary Modification is most closely aligned with the formation of conceptual models, and Model Behavior Modification is more commonly associated with the formation of the detailed mathematical or representational models. The primary area of focus for these guidelines, however, is in the area of Model Form Modification.

The first class of model abstraction techniques is termed Model Boundary Modification, which primarily focuses on changing the variables or boundaries that are external to the model itself. It is primarily based on modification of the input variable space. Of the techniques used in the process models for the TSPA–SR, parameter reduction based on FEP screening would be categorized as a Model Boundary Modification. In general, the techniques identified as Model

Boundary Modifications do not directly result in formulation of a mathematical model and are, therefore, likely to be considered scientific analysis abstractions as defined by AP-SIII.9Q.

The second class of model abstraction techniques is termed Model Behavior Modification. This type of model abstraction involves aggregating some aspect of the model such as states of the system, temporal elements, entities, or functions of the entities. An example of the regulatory use of model behavior modification is the mandated use of the Reasonably Maximally Exposed Individual (RMEI) (aggregation of the characteristics of the various individuals residing near Lathrop Wells), as described in 10 CFR 63. Because of this regulatory requirement, the RMEI concept is used in the Biosphere model in the determination of biosphere dose conversion factors. Other examples of Model Behavior Modification abstraction techniques used in the process models include temporal aggregation (e.g. time steps used to evaluate the impact of igneous eruptions through time). The development of the thermal response abstraction involves aggregation of results; thus, it also is a type of Model Behavior Modification. A more extensive discussion of these first two classes of abstractions can be found in Frantz (1998).

The focus of these guidelines is on the third level of abstraction, as described in NUREG-1636. Generally, these abstractions are in the category of Model Form Modification. This is by far the most common category of model abstractions used directly for the TSPA–SR. It is characterized by a simplification of the input-output transformations within a model or model component. The same set of inputs may be used to support both the initial and abstracted models, with the primary difference in the abstraction being the manner in which the parameter values are determined. In some cases, the results from the process model (as opposed to the original inputs) may be used as the basis of the abstraction. Typically, Model Form Modifications result directly in a mathematical model and will therefore need to address uncertainty propagation under AP-SIII.10Q, which includes the need for model validation consistent with the intended use of the model abstraction.

Several possible techniques or combination of techniques can be used as demonstrated by their use in TSPA–SR (Appendix A, Section A.2), these include:

Look-up Tables in which a transformation function is represented by a set of values. The input value to the table is used as an index value for a table of values, and the generated output value is determined by retrieving the indexed value(s). Multidimensional tables are referred to as response surfaces.

Probability Distributions in which the computation of a parameter value is replaced with a generated number, with the use of various probability distributions. The distributions may take several different forms. Multiple examples of the use of this technique are listed in Appendix A. Probability distributions can be used to replace more complex model components (in which case they are being used as an abstraction technique) or they can also be used for a more realistic representation of uncertainty (e.g., replacing conservatism with a probabilistic approach).

Linear Function Interpolation represents a step between simple look-up tables and full polynomial representations. A typical technique is to use a look-up table whose entries are points, or breakpoints, on the polynomial curve. This reduces the polynomial function to a series of straight-line curves or other more-readily interpolated mathematical functions.

Metamodeling involves the use of several techniques such as parametric polynomial response surface approximations, splines, radial basis functions, kernel smoothing, spatial correlation models, and frequency-domain approximations.

The use of model abstractions is part of the TSPA modeling process. The use of model abstractions can be an appropriate method to gain computational efficiency at the system level. The use of model abstractions is particularly appropriate when the abstraction does not pertain to a key or sensitive parameter or sensitive model component in a performance assessment. Model abstractions for key or sensitive parameters or model components may also be appropriate within certain constraints. These constraints include: 1) that the model abstraction must provide for propagating the uncertainties inherent in the underlying process model, and 2) that the model abstractions should also yield results that are consistent with level of resolution of the other TSPA model components that the model abstraction feeds. Model abstractions that address key model components and/or key parameters will likely need a greater degree of resolution than those that do not. The development and documentation of model abstractions is governed by the requirements of AP-SIII.10Q.

3.2 PROCESS FOR MODEL ABSTRACTION IN TSPA–LA

The model abstraction process will use a team approach (Figure 3-1) for performing model abstractions that closely parallels the approach described for both addressing alternative conceptual models (Section 2) and considering parameter uncertainty (Section 4). To provide consistency in determining which model components can be abstracted and the method(s) used to address them, the implementation of these guidelines calls for the use of two essential participants. These essential participants are the ATL and the SME (see Figure 3-1). The intent of these guidelines is that one ATL will be designated to address all model abstraction issues across the various subject areas. This will provide consistency in the guidance given to the multiple SME's, treatment of model abstractions, and the propagation of uncertainties and variability into the TSPA–LA.

The intent of these guidelines is that the ATL will also serve as the team lead for addressing alternative conceptual models, due to the interrelationship of these two subject areas. The process provides for review and concurrence by the ATL and the SME prior to use of the model abstraction in the TSPA–LA. It also specifies the review by the ATL and SME of the integration of the model abstraction into the TSPA–LA. This will allow for consistent guidance from and interface with the TSPA Department to the respective subproject departments. The cross-checking and review of the model abstractions will be performed as part of the technical review under AP-SIII.10Q.

The changes specified below for controlling the integration of model abstractions within the TSPA–LA simulations will not necessarily enforce the consistent use of parameters in developing each of the model abstractions for TSPA–LA by the various process model departments. Without the oversight of the ATL, the various model abstractions may be produced in parallel with others and differences may occur prior to the TSPA–LA integration step.

However, the use of the ATL as a central point of contact in the checking process will allow these differences to be identified and assist in minimizing differences to the extent practicable. This will also allow for documentation of any such differences in the individual supporting model reports and in the TSPA–LA.

Requirements for model abstraction documentation are now addressed in AP-SIII.10Q, including revision of the technical work plan as needed, and review of the work plan and model validation by the Chief Science Officer. For TSPA–SR, the description of the technical basis for the abstractions was placed in the AMRs. Effective with the implementation of these guidelines, the underlying technical basis for the model abstraction and the development and validation of the model abstraction will be documented in the respective model reports. This documentation will be provided as an attachment or distinct section to the model report such that the documentation is more transparent (see Section 1.3.2 regarding the use of attachments). The documentation will include both a qualitative description and an unambiguous mathematical description of the model abstraction. The TSPA–LA model report will document precisely how the model abstraction was used in the TSPA–LA. The TSPA–LA model report will specifically denote any changes from the model abstraction as documented in the respective model report that were needed to integrate the model abstractions within the TSPA–LA. Furthermore, the TSPA–LA model report will demonstrate that the model abstraction as incorporated into the TSPA–LA has adequately propagated the important uncertainties and variabilities.

3.2.1 Process Implementation

The model abstraction process for TSPA–LA is summarized in Figure 3-2. The following process will be used to identify, develop, propagate, and document the use of model abstractions in TSPA–LA.

Identify Possible Model Abstractions

The designated ATL and TSPA Analyst(s) will meet to review the conceptual models, process models, and model abstractions used in the TSPA–SR and TSPA–FEIS. In addition, the ATL and TSPA Analyst(s) will meet with the PTL (see Section 4.2) to review parameter uncertainty in the existing models. The ATL and TSPA Analyst will review the process models and model components to:

- Identify any process models or model components that may appropriately be addressed using abstractions in TSPA–LA.
- Identify any new or additional model components needed for the TSPA–LA.
- Consider the findings of the TSPA–SR, SSPA, previous sensitivity studies, or other project documentation to identify the importance of the model component and the specific parameters to the estimated mean dose, mean groundwater concentrations, and descriptions of barrier capabilities.
- Consider the results of work being performed for parameter uncertainty and the need to propagate uncertainty and variability.

- Consider the level of resolution needed from the model abstraction by considering the level of resolution of the other TSPA model components that the model abstraction feeds. Model abstractions that address key model components and/or key parameters will likely need a greater degree of resolution than those that do not.

The ATL will then initiate a team meeting to discuss the implementation and use of these guidelines. At this meeting, the ATL provides to the SME a list of key parameters, TSPA–SR and TSPA–FEIS key model components and other applicable project documents. The ATL will also provide a list of model components where additional model abstraction may be warranted. Note this basis for importance may change as the TSPA–LA model is developed, and will need to be reevaluated during the TSPA–LA analysis period.

The SME may identify technical issues in proceeding with a recommended model abstraction or may propose alternatives that would be more suitable for model abstraction. The SME will provide such information to the ATL for further consideration. It is important to note that the TSPA–LA is intended to be an iteration of the SR model suite, and new abstractions will not be incorporated without a thorough consideration of their overall significance.

In some cases, it may be determined that addressing parameter uncertainty and variability may be difficult if an abstraction is used, or that other sensitivities prevent the use of a model abstraction. In that case, a more detailed representational model (such as the initial model considered) will be recommended for use and the decision will be documented in the model report.

Develop Model Abstractions

In constructing the model abstraction, the SME and Process Modeler will consider the level of resolution of the process model, which is the basis and/or provides input to the model abstraction. They will also consider the level of resolution in the TSPA–LA model components that the model abstraction will address (as identified by the ATL and PTL. Consequently, the SME and Process Modeler will work in consultation with the ATL and TSPA Analyst during the model abstraction development. This includes soliciting and receiving written recommendations from the ATL and PTL regarding selection of any conservative components, parameter uncertainties, evaluation of linear and non-linear models when conservatism is used, and handling of any important parameter uncertainties and variabilities. The SME and Process Modeler are responsible for developing, validating, and documenting the model abstraction in the respective model report per the requirements of AP-SIII.10Q. The basis of the abstraction and the techniques used will be documented in such a way that they are clearly identifiable and readily explained to an external reviewer.

The steps below describe the process developed by the TSPA Department to construct the model abstraction. As the process evolves, the steps may be modified as appropriate.

Step 1. The SME (or designee) considers the ATL requests and recommendations regarding the model abstraction. The SME also determines the basis to justify or support the model abstraction (e.g., justification for a set of appropriate values to use in the model abstraction, sensitivity study, or previous use of the model abstraction) and documents the supporting information. The SME then determines the methods and techniques to be used for the model abstraction. The methods selected should be consistent with recommendations from the PTL for propagating uncertainty and variability.

Step 2. The SME provides results from process models to be used as a basis for demonstrating that the model abstraction results are appropriately representative, including the propagation of important variabilities and uncertainties. The SME will be responsible for demonstrating that the effects of the input included in the model abstraction capture the important effects of the input as identified in the process models.

Step 3. The SME and Process Modeler develop and validate the model abstraction by comparison to the results of the process model, and document the results, all in accordance with the requirements of AP-SIII.10Q.

Step 4. The SME then provides the ATL with sufficient documentation to review the work. In the event that the SME disagrees with the ATL's comments or recommendations and the issue cannot be resolved with the ATL, the matter may be elevated by the SME to the PA Manager for resolution. After the ATL's review is complete, the SME documents the model abstraction in the model report in accordance with AP-SIII.10Q and dispositions any resulting data in accordance with AP-SIII.3Q. The SME is responsible for ensuring that the model abstraction complies with the project procedural requirements for software control and electronic control of data. The SME then transfers control of the model abstraction process to the ATL.

Integrate the Model Abstraction into TSPA–LA and Document

As the process evolves, the steps may be modified as appropriate.

Step 1. The TSPA Analyst obtains a controlled copy of any software and data needed to implement the model abstraction per AP-SI.1Q and AP-SIII.3Q. In consultation with the ATL, the TSPA Analyst integrates the model abstraction into the TSPA–LA. The TSPA Analyst documents the integration activities and the results stemming from the integration of the abstraction within TSPA–LA.

Step 2. The ATL and the SME perform a joint review of the integration activities and the model abstraction results. In the event that the SME disagrees with the ATL's response to comments or recommendations and the issue cannot be resolved with the ATL, the matter may be elevated by the SME to the PA Manager for resolution. The ATL iterates with the TSPA Analyst until the model abstraction is properly implemented and documented. If any changes were made for the purpose of integration, the TSPA Analyst will ensure compliance with any applicable software control procedures per AP-SI.1Q and information and data storage procedures per AP-SIII.3Q. The ATL documents the ATL's and SME's joint concurrence on the appropriateness of the final model abstraction.

Step 3. The ATL ensures that the initial development and validation of the model abstraction (along with the decision to use the abstraction and the basis for that decision), is documented in the supporting model report. The ATL also ensures that the integration of the model abstraction into TSPA–LA is appropriately documented in the TSPA–LA model report.

3.2.2 Roles and Responsibilities

The model abstraction team will include the ATL and a TSPA Analyst(s). It is intended that a single ATL will be used to oversee the entirety of the model abstraction process. The PTL (see Section 4) will also be a part of the model abstraction team. The team will also include a SME(s) determined by the respective Department Manager(s), and a designated Process Modeler(s), neither of which will report directly to the TSPA Department. In many instances, it will be desirable for the model abstraction team members to be identical and/or to interface regularly with the team addressing alternative conceptual model issues and/or parameter uncertainty. The PA Project Manager will assign these roles.

ATL (or designee) Tasks:

1. Identify conceptual models, process models, and model components that may be suitable for abstraction. This may be done by reviewing the process models and classifying the component and elements of the process model with regard to the taxonomy described above. Previous reports and work that have identified key parameters, sensitivity analysis, and the list of abstractions provided in Appendix A may be used to identify possible model abstractions.

2. Initiate team meeting to discuss implementation of these guidelines.

3. Advise the SMEs and Process Modeler on the model abstractions to be used in TSPA–LA to determine the viability of performing the abstraction.

4. Advise the Process Modeler during development, validation, and documentation of the model abstraction. Advise and assist the TSPA Analyst during integration of the model abstraction into the TSPA–LA.

5. Review the model abstraction before and after integration into the TSPA–LA. In the event that the SME disagrees with the ATL's comments or recommendations and the issue cannot be resolved with the ATL, the matter may be elevated by the SME to the PA Manager for resolution.

6. Ensure documentation of the integration and use of the model abstraction in the TSPA–LA model report, with complete documentation of any changes in the model abstraction needed to facilitate integration into the TSPA–LA.

7. Coordinate model abstraction process and interface with personnel performing any related alternative conceptual model and parameter uncertainty activities.

8. Ensure that model abstractions have been developed and documented according to applicable modeling and software control procedures.

PTL (or designee) Tasks:

1. Provide insight and recommendations to the ATL, TSPA Analyst(s), SME, and Process Modeler with regard to parameter uncertainty (see Section 4) and provide guidance on the propagation of uncertainty and variability through the model abstraction process.

TSPA Analyst(s) Tasks:

1. Attend team meeting to discuss implementation of these guidelines.

2. Assist the ATL in reviewing process models, identifying, and categorizing any feasible model abstractions or techniques.

3. Assist the Process Modeler in developing the model abstraction, particularly with regard to interfacing with other TSPA models and components.

4. Integrate model abstractions in the TSPA model.

5. Document modeling decisions, the basis for the decision, and the use in the TSPA and any changes required to integrate the model abstraction in accordance with existing project procedures governing models and the use of software.

SME Tasks:

1. Attend team meeting which addresses implementation of these guidelines.

2. Identify technical issues related to performing the abstraction in light of the recommendations from the ATL and propose alternate recommendations as appropriate.

3. Assist the Process Modeler in implementing appropriate methods for propagating necessary uncertainty and variability (see Section 4 on parameter uncertainty and Section 2 on alternative conceptual models). Provide results from process models to be used as a basis for demonstrating that the model abstraction results are appropriately representative including the propagation of uncertainty and variability.

4. Confer with and assist the Process Modeler during development, validation, and documentation of the model abstraction in TSPA–LA. Confer with the TSPA Analyst, as needed, during integration of the model abstraction into TSPA–LA.

5. Review the model abstraction before and after integration into the TSPA–LA. In the event that the SME disagrees with the ATL's comments or recommendations and the issue cannot be resolved with the ATL, the matter may be elevated by the SME to the PA Manager for resolution.

6. Transmit to the ATL final copies of the developed model abstractions for integration into the TSPA after concurrence with the ATL has been documented.

7. Document the development and validation of model abstraction in the AMR in an attachment or distinct section.

8. Interface with personnel performing any related parameter uncertainty activities.

9. Ensure that the model abstraction is developed and documented in accordance with applicable project procedures governing models and use of software.

Process Modeler Tasks:

1. Attend team meeting to discuss implementation of these guidelines.

2. Assist the SME in reviewing process models and determining the viability of performing the abstraction in conjunction with recommendations from the ATL and TSPA Analyst.

3. Modify the Technical Work Plan as necessary to include development, validation, and documentation of the model abstraction as required per AP-SIII.10Q.

4. Determine whether site-specific observations or relevant literature exists to justify or support the model abstraction (e.g., justification for a set of appropriate values to use in the model abstraction, sensitivity study, or previous use of the model abstraction). Document the supporting information.

5. Request that the SME assist in determining appropriate methods for propagating necessary uncertainty and variability (see Section 4 on parameter uncertainty), and that the SME provide results from process models to be used as a basis for demonstrating that the model abstraction results are appropriately representative.

6. Develop and validate the model abstraction by comparing results of the model abstraction to the results of the process model, and document the results in accordance with applicable project procedures governing models and use of software.

7. Document the development and validation of the model abstraction in the model report.

8. Assist the TSPA Analyst with integration and documentation of integration of the model abstraction into TSPA.

3.3 COMMUNICATION TO DECISION MAKERS

The development of a model abstraction and technical basis for performing the abstraction will be documented in an appropriate model report. The documentation will include text appropriate for describing the modeling process, the understanding of any important uncertainties and variability derived from the process model, and the technical justification or basis for performing the model abstraction. The documentation will then provide a comparison between the results of the process model and the model abstraction and demonstrate that important parameters and related uncertainties and variabilities are appropriately represented in the results of the model abstraction.

The integration of the model abstraction in the TSPA–LA will be documented in the TSPA model report. The information will include identification of the model abstraction, a listing of interfaces with other system model components, and documentation of any changes made by the

TSPA Analyst to the model abstraction. The basis for determining that use of the model abstraction was appropriate will also be included in the documentation. Specific reference to the supporting AMR prepared by the SME and/or process modeler will be provided.

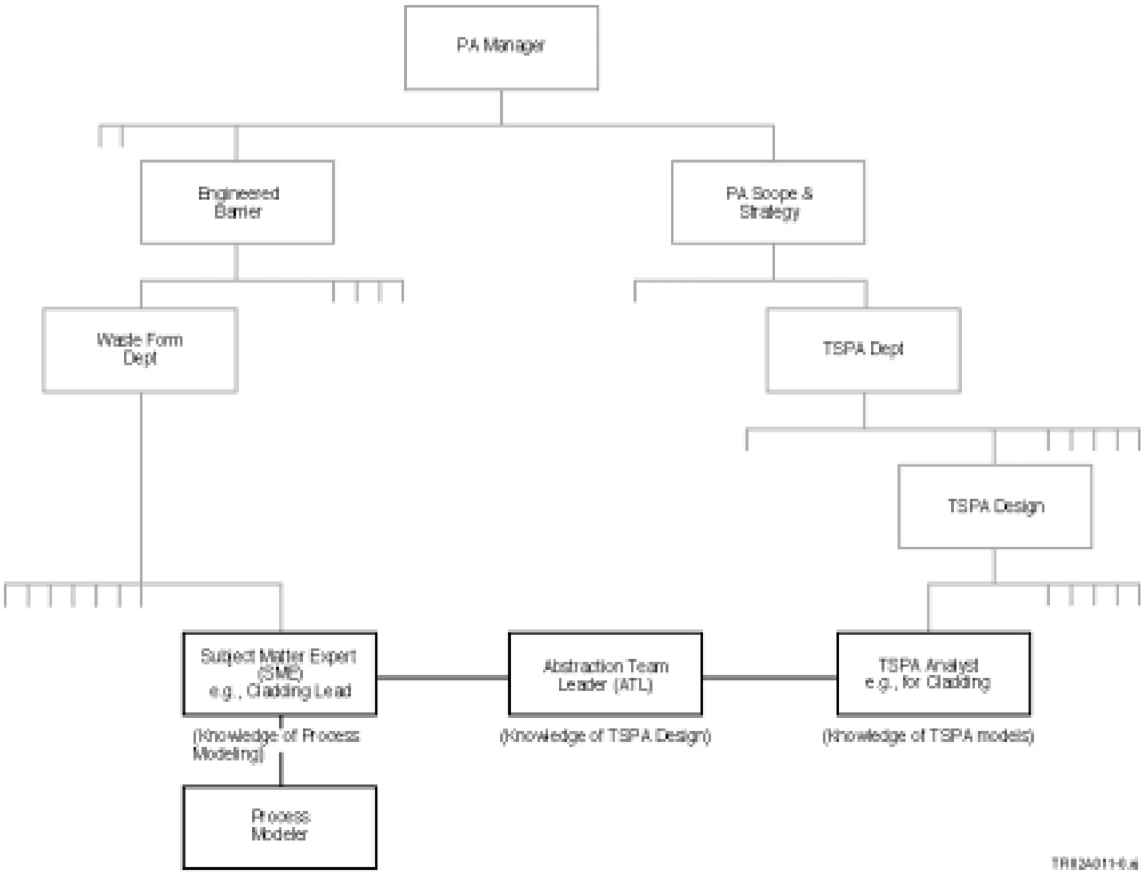

Figure 3-1. Model Abstraction Development Team (Example).

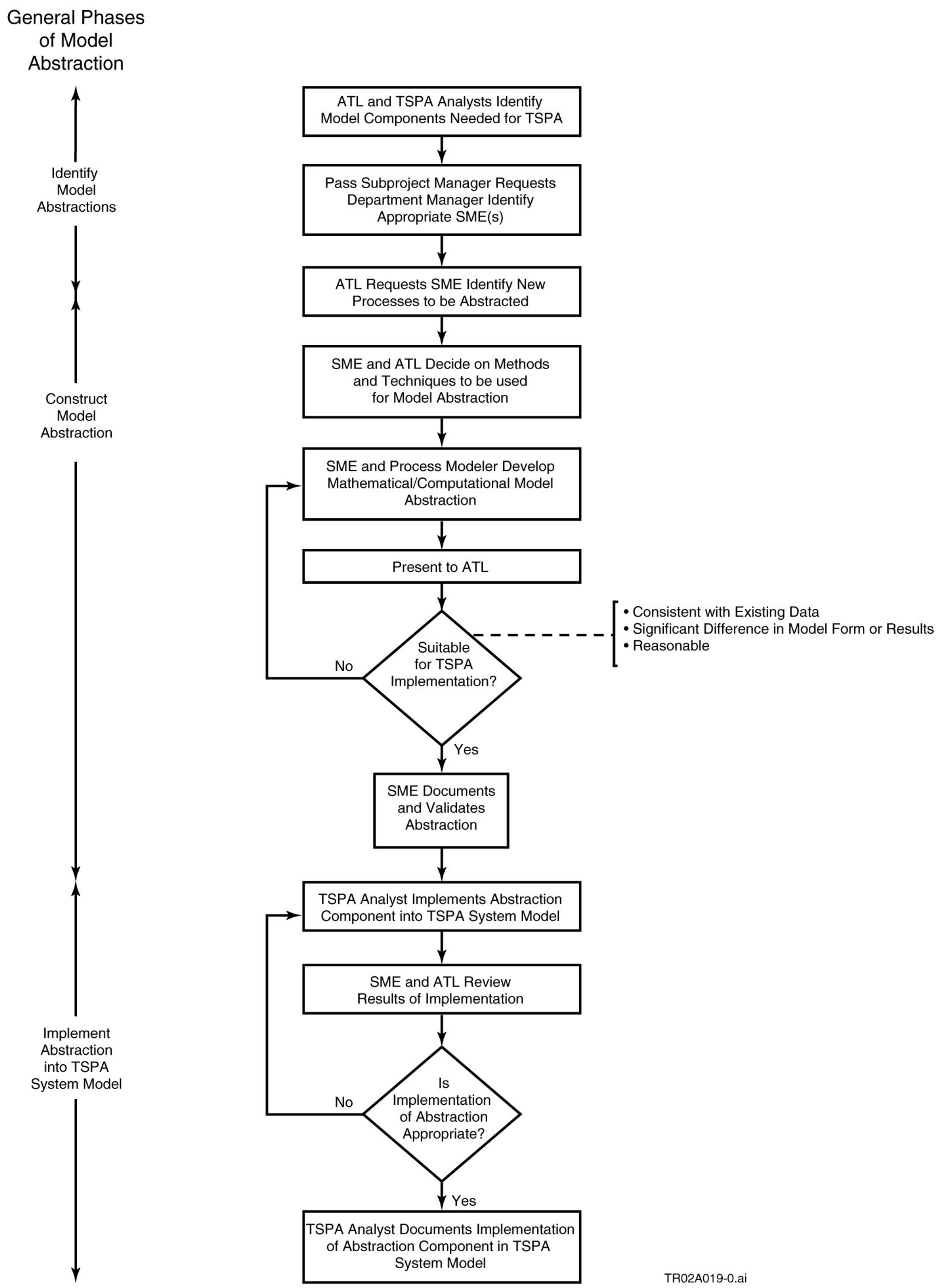

Figure 3-2. Process for Treatment of Model Abstractions in TSPA–LA.

4. GUIDELINES FOR CONSISTENT TREATMENT OF PARAMETER UNCERTAINTY

The NRC requirements for the performance assessment are stated in 10 CFR 63.114 and specifically require the treatment of uncertainty and variability:

> 10 CFR 63.114 (b) Account for uncertainties and variabilities in parameter values and provide for the technical basis for parameter ranges, probability distributions, or bounding values used in the performance assessment.

The following section provides guidelines for consistent treatment of parameter uncertainty for TSPA–LA. The following sub-sections (1) provide a consistent set of applicable definitions for terms used when describing the process for consistent treatment of uncertainty, (2) review a few concepts and assumptions related to parameter uncertainty, (3) describe a process that will provide consistent treatment of parameter uncertainty (called epistemic uncertainty herein) and variability (called aleatory uncertainty) for TSPA–LA, and (4) assign specific tasks to a parameter development team.

A summary of the past use of uncertainty parameters in the TSPA–FEIS is provided in Appendix A (Section A.4).

4.1 DEFINITIONS AND CONCEPTS

4.1.1 Definitions

These guidelines include use of a supplemental set of definitions consistent with AP-SIII.10Q. In many instances, the AP-SIII.10Q definitions are specific to their application for the project (e.g., the definition may be limited by such phrases as "for incorporation into an overall system model of the geologic repository;" or by the distinction between mathematical models and scientific analyses). The remainder of the definitions have been derived from other related sources (e.g., WIPP documentation, NUREGs) and are provided to clarify and supplement the existing proceduralized definitions. These supplemental definitions have been modified based on the need to address parameter uncertainty and on the definitions provided in other regulatory guidance

> **Aleatory Uncertainty** - Uncertainty in the parameter space of the conceptual model for which sufficient knowledge is unobtainable such that the corresponding parameters are treated as chance occurrences of features, events, and processes. These parameters may be conveniently used to form scenarios related to chance either in designing the TSPA simulation or within a component of the TSPA model. For example, this inexactness can arise because both volcanic disruption and no volcanic disruption are possible states of the disposal system that need to be considered, because the micro-structure of the material and the micro-environment vary across a waste package surface, or because different individuals vary in their tolerance to contaminants. This type of parameter inexactness is also called Type A, stochastic, irreducible, or variable uncertainty. Both aleatory and stochastic formally refer to randomness in processes (e.g., radioisotope decay), but the general lack of knowledge about the state of the system (e.g., volcanic disruption or no volcanic disruption) is now also associated with these words. The term

"variable uncertainty" emphasizes the variability among individual characteristics of a population. This type of inexactness cannot be reduced through further testing and data collection (e.g., variability of a population to the tolerance of contaminants cannot be reduced through further testing); it can only be better characterized, and, thus, this first type of parameter uncertainty is also referred to as irreducible uncertainty.

Alternative Conceptual Models - Multiple working sets of hypotheses and assumptions of a system that are all acceptable (i.e., consistent with the purpose of the model, logically consistent with one another, in agreement with existing information, and able to be tested).

Applied Model - An analyst's application of the generic computational model to a particular system, using appropriate values for dimensions, parameters, and boundary and initial conditions. In waste management, the system is a waste disposal site, and so this model is also referred to as a site-specific model.

Computational Model - The solution and implementation of the mathematical model. The solution may be analytical, numerical, or empirical. The computational model is generic until system-specific data are used to develop the applied model.

Conceptual Model - The set of hypotheses and assumptions that postulates the description and behavior of a system. These hypotheses and assumptions describe (a) the simplified physical arrangement of system components, (b) the initial and boundary condition types, and (c) the nature of the relevant, chemical, physical, biological, and cultural phenomena.

Data - Subset of information that is collected, organized, and used to prepare values for parameters.

Epistemic Uncertainty - Uncertainty in the parameter space of the conceptual model for which some knowledge is obtainable. For the corresponding imprecisely known parameters, the imprecision can be expressed as a degree of belief of what the true value should be as related to the conceptual model. The second type of inexactness arises from a lack of knowledge about a parameter because the data are limited or there are alternative interpretations of the available data. The parameter is not variable because of an intrinsic characteristic of the entity but because an analyst does not know what the precise value of the parameter should be. This type of inexactness is also called Type B, state of knowledge, or reducible uncertainty. Epistemic refers to the "state of knowledge" about a parameter. The state of knowledge about the exact value of the parameter can increase through testing and data collection such that the uncertainty is "reducible." Developing a probabilistic distribution for a parameter is the usual way to explicitly describe epistemic uncertainty.

Information - A collection of cognitive and intellective material. Information includes both observational data and communicated knowledge derived by inference and interpretation.

Fixed Parameter - Parameter that is considered precisely known (i.e., constant) for the intended purposes of TSPA analysis.

Informational Entropy - A "measure of information" that is proportional to the sum (or integral) of the product of the probability of a data point (or continuous function) and the log of the probability (i.e., $U \propto -\sum p_i \log p_i$ where U is informational entropy and p_i is the probabilistic representation of the uncertainty in a quantity). This measure of information quantifies the connection between probability and uncertainty. Of all the distributions that can be chosen based on the information at hand, the one distribution that maximizes U is the only selection that does not unwittingly add more information.

Mathematical Model - The mathematical representation of a conceptual model. That is, the algebraic, differential, or integral equations that predict quantities of interest of a system and any constitutive equations of the physical material that appropriately approximate phenomena in a specified domain of the conceptual model.

Model-Control Parameter - Parameter used to control the numerical solution of the mathematical model (e.g., convergence control or time-step control).

Model-Form Uncertainty - Uncertainty in the most appropriate model form for a system. The uncertainty results from sparse observed data and lack of information available to corroborate or refute alternative models. Developing alternative models is a method to explicitly acknowledge model form uncertainty.

Parameter - Parameters are the underlying elements ($\mathbf{x} = x_1, x_2, \ldots x_n$) of a parameter space D(**x**). The individual parameters x_n may be vectors or tensors, but are usually scalar quantities. As a parameter varies so does the result. Parameters that reflect epistemic uncertainty are coefficients of a mathematical model. Parameters that reflect aleatory uncertainty define choices in the selection of scenarios in a TSPA analysis or selection of various models within components of the TSPA model.

Parameter Database - Database of parameters that are used in the TSPA simulation. The parameters have been developed by interpreting data stored in the primary databases of the Yucca Mountain Project and/or general scientific knowledge.

Parameter Uncertainty - Uncertainty in the most appropriate value for a parameter expressing epistemic uncertainty. The uncertainty results from sparse observed data and lack of information able to corroborate or refute alternative parameter values.

Scenario - A subset of the set of all features, events, and processes considered in a model. Specifically, for a mathematical model it is a subset of the parameter space.

Scenario Uncertainty - Uncertainty in the most appropriate scenarios for a system. The uncertainty results from the omission of features, events, or processes (FEPs) of a system (i.e., completeness errors) and imperfect aggregation of FEPs (aggregation errors).

Uncertainty - As relates to performance assessment, uncertainty is the inexactness in the most appropriate (a) set of features, events, and processes (FEPs) or scenarios formed from these FEPs to include in further analyses, (b) conceptual, mathematical, computational or applied model form used to represent the FEPs, or (c) parameter value to use for a mathematical, computational, or applied model.

Uncertain Parameter - An imprecisely known parameter; one that cannot be assigned a single, universally accepted scalar, vector, or tensor value.

Uncertainty Analysis - The description of the model form and parameter uncertainty (i.e., uncertainty assessment), the propagation of this uncertainty through a model or model system (i.e., uncertainty propagation) and the subsequent use of analytical or numerical techniques to determine the impact of the uncertainty on model results.

4.1.2 Concepts Associated with Parameter Uncertainty

Characterizing Parameter Uncertainty

Characterizing the uncertainty in parameter **x** requires developing a joint probability density function, $F(\mathbf{x})$. In TSPAs for Yucca Mountain, the joint distribution is approximated by the product of distributions of the individual parameter $F_1(x_1) \bullet F_2(x_2) \bullet \ldots F_n(x_n)$ (i.e., the parameters are assumed to be independent parameters). The distribution (either cumulative distribution function [CDF] or probability density function [PDF]) of a parameter, x_n, represents both what we know and what we do not know about that parameter and should reflect the best, current knowledge of the range and likelihood of the appropriate parameter value when used in the particular context in a TSPA.

Aleatory and Epistemic Parameters

Conceptually, the parameter space can be divided into aleatory and epistemic parameters. Distinguishing between these two types of uncertainty is not important to estimates of *mean* risk (Pate-Cornell, 1996), but can be important to understanding the results and how the uncertainties might be better characterized (and possibly reduced) by the collection of more data. The desire to maintain a separation between aleatory and epistemic uncertainty affects the design of the analysis (e.g., separate analysis of volcanic disruption and no volcanic disruption). It may also affect the design of individual components (e.g., the component modeling corrosion of the waste package). If the TSPA does not maintain a separation between aleatory and epistemic uncertainty for a specific parameter, then the total uncertainty is expressed as a combined distribution. The usefulness of making this distinction and the choice for which parameters will be treated as aleatory will be made and documented when developing submodels or components of the TSPA and designing the TSPA analysis (e.g., selecting scenarios to propagate through the TSPA system model). The description of parameter uncertainty of all the remaining parameters (designated as either epistemic parameters or combined epistemic/aleatory parameters) is discussed in the remainder of Section 4.

General Process of Defining Distributions

The goal of the uncertainty analysis is to obtain the best characterization of uncertainty possible with the information and resources that are available, while avoiding unnecessary risk dilution in the system performance. There are three important aspects to developing a distribution from available data and information in order to reach this goal. First, use objective techniques that are easily understood by others. Second, use techniques that do not imply more information is available (and, thus, certainty) about a parameter than is actually the case. Both aspects can be obtained by using the theory of informational entropy (Tierney, 1990; [DIRS 125989]; Jumarie, 1990 [DIRS 157701]) and will be used to the extent practicable. Third, evaluate the overall effect of the uncertainty distributions in an attempt to minimize unnecessary risk dilution of system performance.

In general, the process for using the data and information to characterize the parameter uncertainty must be tailored to the type of data available and the parameter's use in TSPA computational models. Hence, to appropriately characterize uncertainty (i.e., assign a distribution, $F(x_n)$) within the context of the assumptions and requirements of the TSPA analysis, a TSPA Analyst familiar with the TSPA Model and a SME, familiar with data and information available, must jointly define a distribution. The guidelines below ensure this interaction is coordinated by the PTL. Only one PTL would be selected to coordinate the assignment of all parameter values. A database administrator assists the PTL in carrying out his/her duties (Figure 4-1).

Documentation of Parameter Values

For TSPA–SR, the description of the underlying reasoning for a parameter value was placed in the appropriate/relevant AMR. For SSPA, a brief description was included in Volume 1 of the SSPA report (BSC 2001b, Volume 1 [DIRS 155950]). Effective with the implementation of these guidelines, the underlying reasoning for the parameter selection will remain in the respective model report but as an attachment or distinct section such that the documentation can be more transparent. Additionally, the TSPA–LA documentation will summarize all the parameter values and distributions in an Appendix, and the particular use of the parameter in TSPA–LA models will be described in the TSPA–LA model documentation.

For TSPA–SR and SSPA, parameters were manually placed in the input files or directly into coded equations. Effective with the implementation of these guidelines, the parameter uncertainty process will include development of a TSPA parameter database, or modification of existing databases (such as RIB or TDMS), consistent with existing QA procedures regarding input data, for controlling the entry of parameters. A TSPA parameter database facilitates retrievability by (a) providing consistent distributions among the computational models; (b) placing responsibility for maintaining correct parameter entries with a limited number of personnel; (c) providing a uniform interface for software used by TSPA Analysts; and (d) providing a uniform interface for SMEs communicating with the TSPA Department. The parameter database is expected to contain the following information on parameters, as applicable: (a) ID of entry; (b) qualitative description of parameter, (c) quantitative description of distribution, (d) units (preferably SI system); (e) sources of underlying data; (f) flag denoting whether or not parameter is active, (g) date of most recent change; and (h) name of person making the entry or update.

The TSPA, as currently configured, relies heavily upon extensive abstractions of process models of various phenomena (Section 3). The TSPA Parameter Database will be developed for linkage with GoldSim during TSPA analyses. The database will not track the parameters in the process models nor have the objective of ensuring that the values used in the TSPA models are necessarily consistent with parameters of the process models. However, the consistency of parameter from process model through abstraction to TSPA issues will be addressed in the model reports defining parameter values and developing the abstractions as described in Section 3, which will be provided by the respective departments responsible for developing process models and abstractions.

Conditions Where Bounds and Conservative Estimates are Appropriate

As described in Section 3.1.4 of *Uncertainty Analyses and Strategy* (BSC, 2001a), the treatment of uncertainty in the TSPA–SR was in accord with the recommendations made by the TSPA Peer Review Panel (Budnitz et al 1999 [DIRS 102726]), who provided their perspectives after review of the TSPA-VA (CRWMS M&O 1998 [DIRS 108000]; CRWMS M&O 1997 [DIRS 100842]). The general guidance can be summarized as the following: Provide a defensible selection from among alternative conceptual models and explain the technical basis for the selection in the AMR; when there are sufficient data to do so defensibly, quantify uncertainties in parameters (e.g., with probability distributions); otherwise, in the absence of sufficient data, develop conservative or bounding estimates that can be defended technically.

In 10 CFR 63, the NRC requires the analysis for TSPA–LA to be based on *reasonable expectation* Additionally, within the context of reasonable expectation and per 10 CFR 63.304, it is not defensible to "exclude important parameters from assessments and analyses simply because they are difficult to precisely quantify to a high degree of confidence". Consequently, the DOE intends to make use of work that was conducted for TSPA–SR, if appropriate in relation to a risk informed decision process. This means that not all work conducted by YMP for TSPA–SR will necessarily be revised for the license application. More specifically, existing models or parameters from the TSPA–SR may be used when the influence of the model or parameter on the mean dose, and mean groundwater concentrations at the accessible environment are minimal, there is adequate barrier capability description, and the existing model is adequate for the purposes of the analysis, as required by AP-SIII.10Q. Consequently, conservative estimates may be used in the TSPA–LA for some model parameters. Other parameter values will be further developed making realistic estimates of the distribution as described below.

In addition, sensitivity analysis where one (or a group of) parameter(s) is varied one at a time (e.g., evaluation of enhanced or degraded barriers), may involve the use of conservative or bounding estimates to discern their importance. The parameter values for this type of sensitivity analysis will be dependent on the analysis purpose. Normally, conservative values will be selected at either the minimum or maximum of the distribution developed below, as appropriate; however, other values may be selected if clearly documented.

Relationship between Uncertainty Analysis and Statistical Analysis

As practiced, both statistical analysis and uncertainty analysis are applications of probability theory. However, statistical analysis uses probability theory to analyze sampled data. Uncertainty analysis uses probability theory to quantify our current knowledge and understanding of the most appropriate parameter value to use in a particular analysis as developed from the data. For example, an investigator first develops a distribution for the parameter, using data that has been statistically analyzed. The investigator then must provide further interpretation to develop the parameter and describe the uncertainty. Once the parameter uncertainty has been described, the uncertainty is propagated through the TSPA model, and the significance of the uncertainty analyzed to complete the uncertainty analysis.

4.2 PROCESS FOR TREATMENT OF PARAMETER UNCERTAINTY IN TSPA–LA

The following generalized process developed from past work (DOE 1996 [DIRS 100975]; Howarth et al., 1998 [DIRS 157700]) is intended to promote (a) traceability (ensuring that the parameters used in the TSPA model have a referenced source to provide a traceable link to underlying data); (b) retrievability (ensuring that parameters can be retrieved, preferably in computer form); (c) verification and parameter review (ensuring that the parameters used are complete and consistent with PA model assumptions); and (d) documentation of parameters (ensuring that the parameters are defined and parameter distributions are documented).

4.2.1 Process Implementation

The following activities will be used to identify, develop, and document the use of parameters and associated uncertainties in TSPA (Figure 4-2).

Identify and Categorize Computational Model Parameters

To initially start this process and for any newly developed component models for TSPA–LA, the PTL and TSPA Analysts of the Performance Assessment Scope and Strategy (PASS) Subproject will describe the computational model (implemented mathematical model) in the TSPA and identify parameters that are necessary to perform the calculations for the TSPA. The PTL will categorize the parameters as either model-control parameters or model configuration parameters. Model-control parameters will be officially tracked when a simulation is warehoused in YMP's Technical Data Management System (TDMS) and will not be further tracked by the PTL. Model configuration parameters will be further categorized by the PTL as fixed or uncertain parameters. Uncertain parameters for which there are few data and are important to the TSPA may be evaluated through formal elicitation per the project's administrative procedures. The PASS Subproject Manager, in consultation with PTL and other Department Managers, will select those parameters requiring assignment through formal expert elicitation (see AP-AC.1Q). The parameters will be categorized as uncertain but specified through expert elicitation.

Identify Subject Matter Experts (SMEs)

At the request of the PASS Subproject Manager, Department, Managers will identify the appropriate SME to provide all pertinent data and information for evaluating uncertain parameters of the TSPA models.

Describe TSPA Model Component and Pertinent Data

The TSPA Analyst will describe the pertinent TSPA model component and pertinent parameters to the SME and PTL (Figure 4-2). In turn, the SME describes the pertinent data for developing model parameters to the TSPA Analyst and PTL. An SME may supplement the site-specific data with (a) other qualified data approved for use according to appropriate QA procedures, and (b) other information necessary to fully characterize the uncertainty. The use of other information will be used when reviewing the Model Report, as described when documenting the parameters (Figure 4-3). The source of underlying information will be documented on a Parameter Entry Form (Figure 4-4) or equivalent memorandum. The forms will be assembled in an electronic database. The initial categorization of the parameter as either model control, fixed, or uncertain, will be presented by the PTL.

Construct Distributions for Uncertain Parameters

In consultation with the TSPA Analyst and SME, the PTL develops a parameter distribution for uncertain parameters as follows. As the process evolves, the steps may be modified as appropriate.

<u>Step 1</u>. Determine whether relevant site-specific observational data exists for the parameter in question. If observational data exist, go to Step 2; if no or limited observational data are found, go to Step 3.

<u>Step 2</u>. Determine the size of the combined observational data. If the number of values in the data set is sufficient, as defined by the PTL, use the data directly to evaluate the parameter range and distribution (e.g., construct a truncated Student-t distribution, construct a piecewise-linear cumulative distribution function (CDF), or construct a discrete CDF). Otherwise, go to Step 3.

<u>Step 3</u>. Request that the SME provide subjective estimates of:

(a) The range of the parameter (i.e., the minimum and maximum values taken by the parameter) and

(b) One of the following (in decreasing order of preference):

  (1) Percentile points for the distribution of the parameter (e.g., the 25th, 50th [median], and 75th percentiles),

  (2) Mean value and standard deviation of the distribution, or

  (3) Mean value.

The range and distribution for the parameter must take into account the model form and the treatment of aleatory and epistemic uncertainty in the TSPA analysis. For example, if the TSPA model does not discretize spatially and temporally, then the parameter distribution will account for this temporal and spatial variability (aleatory uncertainty) in a suitably averaged manner.

<u>Step 4</u>. The PTL, in consultation with the SME and TSPA Analyst, will construct a distribution depending upon the kind of subjective estimate, along with any technical or scientific basis for that estimate, that has been provided. The construction will be in accordance with informational entropy theory to the extent practicable. These may include the following distributions, or other distributions as justified by the available data:

(a) Uniform PDF over the range of the parameter,

(b) Piecewise-linear CDF based on the subjective percentiles,

(c) Beta PDF based on the subjective range, mean value, and standard deviation,

(d) Normal PDF (truncated) based on the subjective mean value and standard deviation,

(e) Exponential PDF (truncated) based on the subjective range and mean value.

Step 5. The three members of the parameter development team review the distribution created. The process of producing a distribution is repeated, possibly after supplying more information and data, and further explanation of the TSPA model and parameter until a meaningful distribution is produced. Concurrence by all three members of the team is signified by signatures on the Parameter Entry Form or equivalent memorandum (Figure 4-4). Normally, the PTL facilitates disputes in assigning a distribution unless he/she is part of the dispute. The TSPA Department Manager may then either resolve the dispute informally by appointing an outside facilitator or formally as specified in the QA procedures.

Document Parameters

The PTL submits the signed form to the Database Administrator, who updates the TSPA parameter database with the endorsed values and distribution for the parameter. After the database is updated, the Database Administrator creates appropriate output files for use in TSPA simulations.

The SME will include a plot of the distribution and document reasoning for the selected shape and range of the parameter distribution in the appropriate model report, including a discussion of how aleatory uncertainty was included, if necessary. The use of unqualified data as corroborative information in the development of the distribution will be reviewed along with the model report.

In addition, the PTL, with assistance from the Database Administrator, will prepare a parameter report, to be published as an appendix to the TSPA report, that describes the general process for selecting parameter values and distributions, defines plots and parameter values, and lists the parameters used in the TSPA report.

4.2.2 Roles and Responsibilities

The functional roles and responsibilities for the five participants needed to implement the parameter uncertainty process are described below. The team members include three parameter team members (PTL, SME, and TSPA Analyst), a Database Administrator to support the PTL, and a support role for the PASS Subproject Manager. The PA Project Manager or his designee will assign these roles.

PTL Tasks:

1. Confer with TSPA Analysts on the parameters required for computational model components used in TSPA.

2. Identify means to categorize parameters (e.g., fixed, model-control, expert elicitation, uncertain) and appropriate manner of defining and controlling values for each category.

3. Request data from SMEs to develop parameters.

4. Coordinate discussion of parameter in TSPA by TSPA Analyst and discussion of available information by SME to develop parameter value.

5. Based on informational entropy theory, develop parameter distribution in consultation with TSPA Analysts and SME.

6. Submit parameters and their uncertainty as described by distributions, including source to Database Administrator, in memorandum of transfer or approved Parameter Entry Form.

7. Produce periodic parameter report or appendix documenting parameters for periodic PA simulations in conjunction with Database Administrator.

8. Provide assistance to ATL regarding the propagation of uncertainty and variability as part of the alternative conceptual model and model abstraction process.

<u>TSPA Analyst(s) Tasks</u>:

1. Present an unambiguous description of the TSPA model and pertinent parameters to SME and PTL.

2. Perform modeling and statistical analysis as requested by the PTL to support the development of the parameter distribution.

<u>SME(s) Tasks</u>:

1. Gather project-specific data and all other qualified data to describe a specific parameter of the TSPA model of the Yucca Mountain disposal system.

2. Gather any other corroborative information, including non-qualified data that helps develop the distribution for a specific parameter.

3. Confer and assist the PTL as needed to determine and verify the appropriateness of the selected distribution

4. Describe the use of the parameter in a component of the TSPA model and the basis for the distribution in the appropriate AMR. Display at least the CDF for the parameter.

<u>Parameter Database Administrator (or designees) Tasks</u>:

1. Set up and administer the parameter database.

2. Operate software used to maintain the parameter database.

3. Enter data and verify data entry, approved by the PTL, into the parameter database.

4. Maintain the history of modifications to the database files, and a dictionary defining items in the database.

5. Produce output appropriate for use by TSPA software.

6. Assist in preparing a periodic parameter report with the PTL.

PASS Subproject Manager Tasks:

1. Ensure department managers select appropriate SMEs to confer with the PTL in developing distributions.

2. In consultation with PTL, determine when formal expert elicitation (AP-AC.1Q)will be used to define parameter distributions.

4.3 COMMUNICATION OF UNCERTAINTIES

For purposes of communicating with and within the TSPA Department, the SME and TSPA Analysts will display at least the cumulative distribution function (CDF) of parameters in the model report. When others are preparing documents for a wider audience, the PTL will help the author(s) in selecting the most appropriate graphical display and textual information for the parameter distributions and provide citations to the source information. Examples for developing and using text descriptions and graphics for a wide audience are provided in Section 4.3 of *Uncertainty Analyses and Strategy* (Williams 2001 [DIRS 157389]), and can be used for guidance in determining appropriate presentation methods.

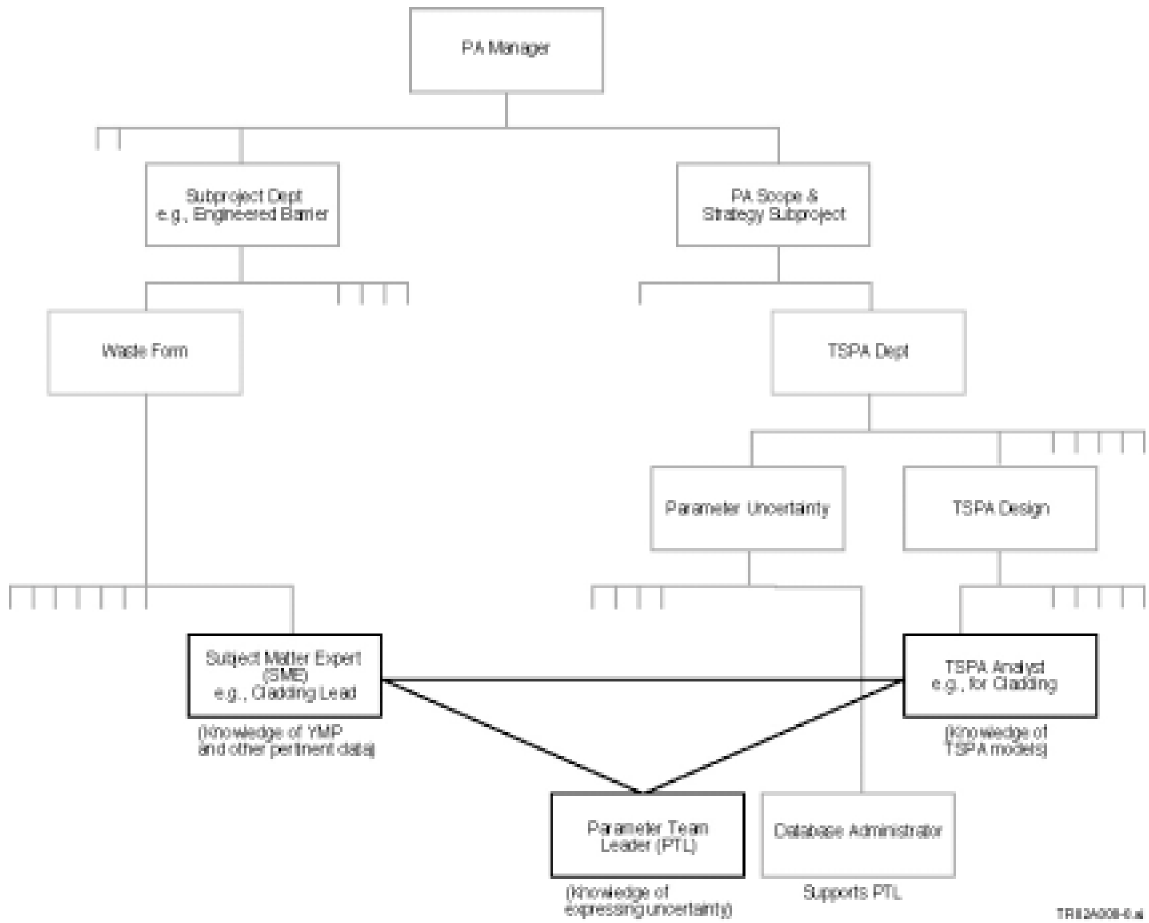

Figure 4-1. Parameter Development Team (Example).

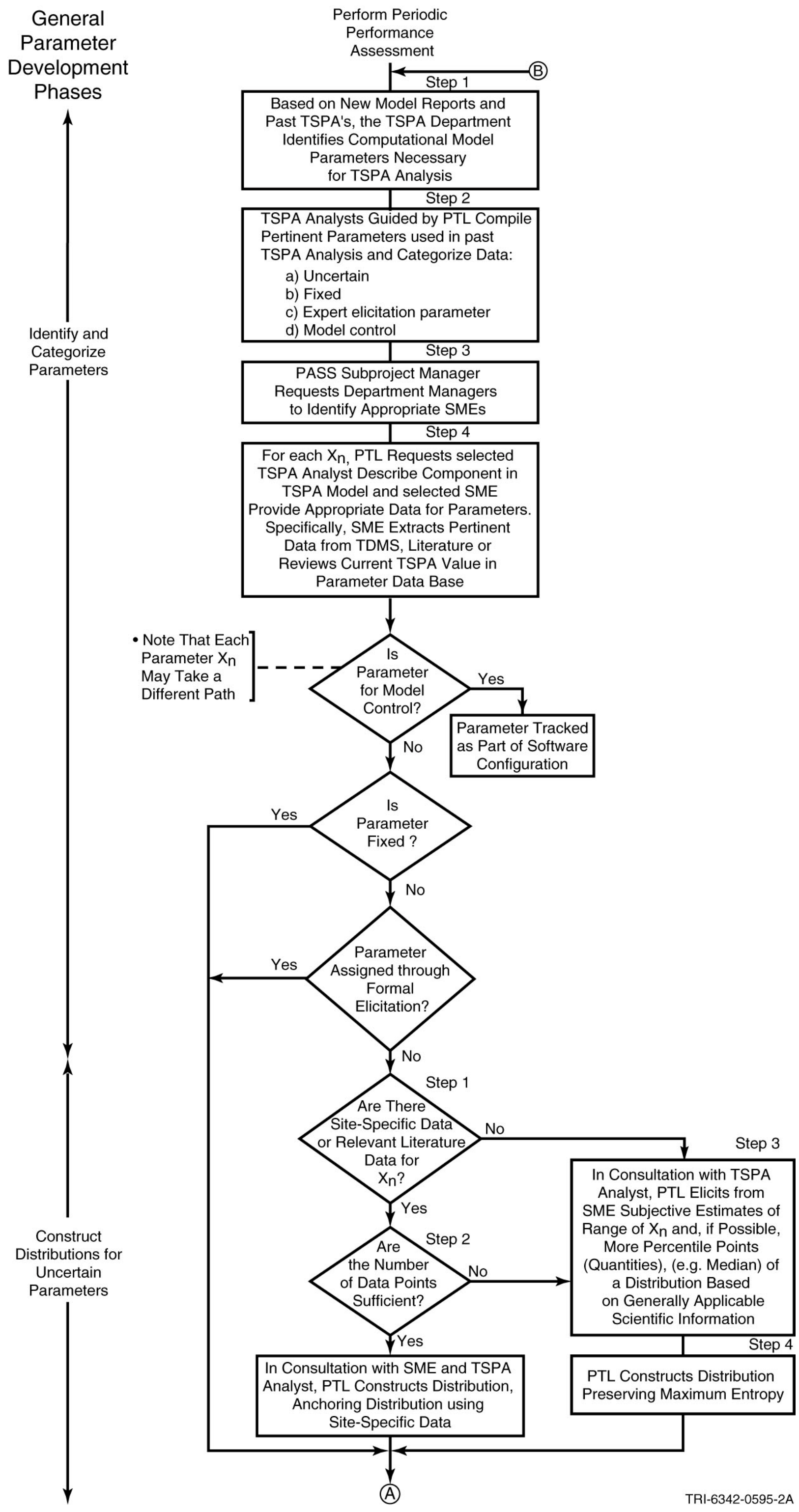

Figure 4-2. Steps in the Description of Parameter Uncertainty.

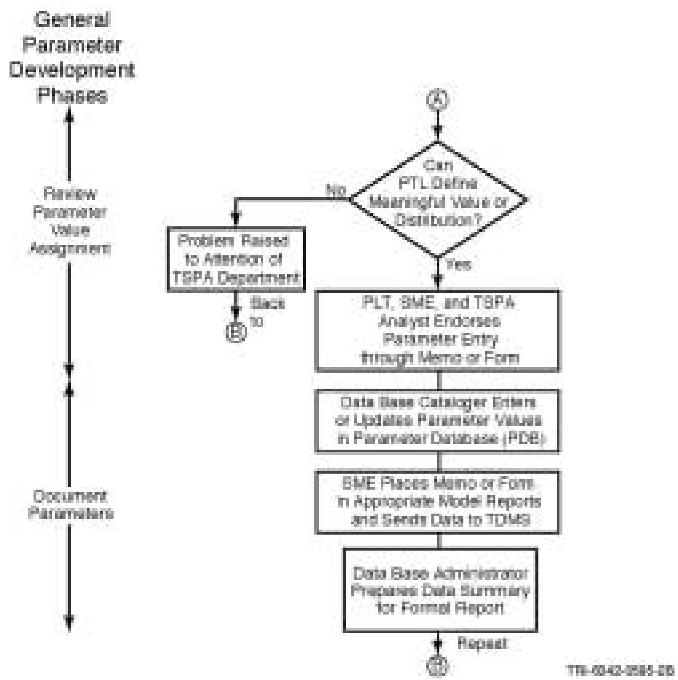

Figure 4-2 (continued). Steps in the Description of Parameter Uncertainty.

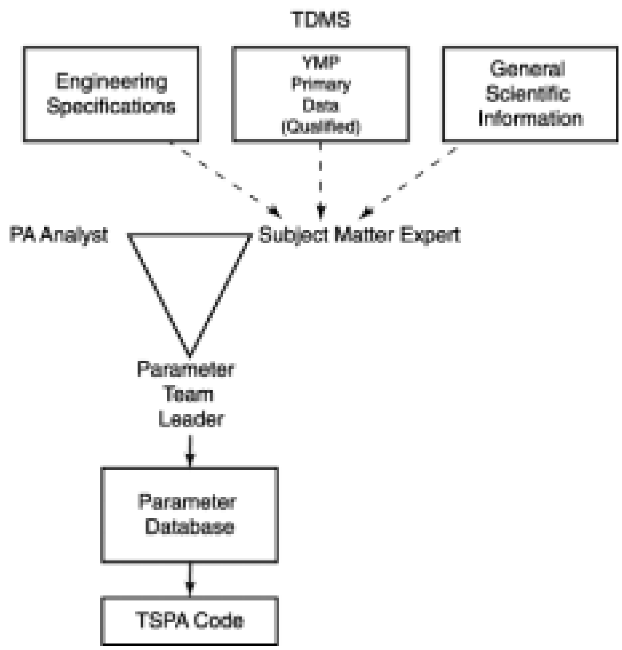

Figure 4-3. Flow of Information to Parameter Database and TSPA Model.

YMP	**Parameter Entry Form**
	Form Number: TBD **Effective: TBD**
	Procedure: N/A Revision: ________ Page 1 of ___

☐ Modification ☐ Error Correction ☐ New ☐ Deactivation

Parameter:	________________	Id:	________________
Material:	________________	Idmtrl:	________________
Model:	________________	Idpram:	________________
Category:	________________	Units:	________________

Distribution:

Type: Mean: ________________

Median: ________________

Std Dev: ________________

Values: Attachment: Y N

Source:
Interpretation:
Qualified Data?: Y N Attachment: Y N

Parameter Entry Approved By:

________________________ ________________________
Parameters Team Lead (Print) Parameters Team Lead Signature/Date

Concurrence:

________________________ ________________________
Subject Matter Expert (Print) Subject Matter Expert Signature/Date

________________________ ________________________
TSPA Analyst (Print) TSPA Analyst Signature/Date

Entered By: ________________ ________________ ________
(Print) *Signature* Date

Entry Checked by: ________________ ________________ ________
(Print) *Signature* Date

Data Control PA Database ☐ Other ________________ TDMS File Code: ________
(i.e., input file)

Figure 4-4. Parameter Entry Form.

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APPENDIX A

ALTERNATIVE CONCEPTUAL MODELS, MODEL ABSTRACTIONS, AND PARAMETER UNCERTAINTIES IN PREVIOUS TSPA ANALYSES

This appendix provides a brief summary of two predecessor documents that address the treatment of uncertainty in a TSPA. The first of these documents, *Evaluation of Uncertainty Treatment in the Technical Documents Supporting TSPA–SR* (YMP 2001 [DIRS 155343]) prepared by the Management and Technical Services (MTS) contractor to DOE, evaluated the treatment of uncertainty in the TSPA–SR (and supporting analysis/model reports (AMRs) and process model reports (PMRs)), and provided recommendations related to improving the identification, categorization, evaluation, and quantification of uncertainties. The second document, *Uncertainty Analyses and Strategy* (Williams 2001 [DIRS 157389]), provides the strategy that is intended to be used to improve the treatment of uncertainty in the development of the TSPA–LA.

In addition, this appendix summarizes an internal evaluation of the use of model abstractions in the TSPA–SR and identifies the YMP review of AMRs for model validation compliance with AP-3.10Q, *Analyses and Models* as documented in *Model Validation Status Report* (BSC 2001g [DIRS 156257]) (MVSR).

A.1 BACKGROUND AND APPENDIX ORGANIZATION

Uncertainty in TSPA arises from three sources: (1) uncertainty in what can happen as expressed by consideration of relevant features, events, and processes (FEPs) (conceptual model uncertainty), (2) uncertainty in the model form for the probability and consequence models used in TSPA (representational or abstraction model uncertainty), and (3) uncertainty in the parameters of these probability and consequence models (parameter uncertainty). Section A.2 provides a brief summary of how alternative conceptual models were addressed in the TSPA–SR. Section A.3 summarizes the use of model abstractions in the TSPA–SR. Section A.4 discusses the treatment of parameter uncertainty in the TSPA–SR, and the Supplemental Science and Performance Analyses (SSPA) documentation.

A.2 ALTERNATIVE CONCEPTUAL MODELS IN TSPA–SR

Conceptual model uncertainties arise from incomplete understanding of the processes being modeled. The principal way of addressing this type of uncertainty is to develop and evaluate alternative conceptual models that include a spectrum of viable conceptualizations. Valid alternative conceptual models must be capable of explaining the available data.

The review conducted by the MTS and documented in *Evaluation of Uncertainty Treatment in the Technical Documents Supporting TSPA–SR* (YMP 2001 [DIRS 155343] indicated that discussions of the consideration of alternative conceptual models were sometimes documented in the AMRs and PMRs that support the TSPA models and calculations. In many cases alternative conceptual models were considered, but not utilized because: (1) they were not supported or were invalidated by existing observed data; (2) there was insufficient data for developing and validating a representational model for the alternate conceptual model; (3) the models developed for TSPA represented more realistic models than the alternative models; or (4) only the more conservative model was forwarded for use in the TSPA.

One example where an alternative conceptual model was developed and then used in the TSPA–SR was the saturated zone flow model. In developing the saturated zone flow model, two conceptual models were used to develop two representational models. One model assumed isotropic permeability fields. The second model included large-scale horizontal anisotropy of permeability in the volcanic units of the saturated zone to the southeast of the potential repository. These conceptual models were considered to be equally likely. Therefore, both representational models were used in the TSPA–SR calculations for saturated zone flow.

In the TSPA–SR, there are examples of alternative conceptual models being incorporated directly into a probabilistic analysis. In the probabilistic seismic hazard analyses (PSHA), alternative tectonic models were developed and incorporated directly into the hazard analysis. In the probabilistic volcanic hazard analysis (PVHA), alternative conceptual models related to the igneous event probability were evaluated, weighted, and incorporated into a composite probability distribution for an igneous event occurrence.

While alternative conceptual models were used in some cases, as the above examples illustrate, YMP (2001 [DIRS 155343]) concluded that for most key models a clear description of the conceptual model(s), the bases of the models, and the related uncertainties, are lacking or difficult to find. The documentation hierarchy utilized for the SR contributed to this lack of transparency.

A.3 MODEL ABSTRACTIONS IN TSPA–SR

As part of the response to KTI agreements dealing with the consistent treatment of model abstractions (see Table 1.1 – TSPAI 3.38, TSPAI 3.39, and TSPAI 3.40) an internal review of model abstractions used in the TSPA–SR was conducted. This review focused on the AMRs supporting the TSPA–SR as indicated in Table 3.1-1 of the TSPA–SR model document (*Total Systems Performance Assessment (TSPA) Model for the Site Recommendation,* CRWMS M&O 2000b [DIRS 148384]), and the hierarchy of analyses and models used to support the TSPA–SR as shown in Figure 6-1 for the *Total System Performance Assessment (TSPA) Model for the Site Recommendation* (CRWMS M&O 2000b [DIRS 148384]). These AMRs were reviewed to develop a list of model abstractions. The resulting list was forwarded to Process Model Report (PMR) Leads and Performance Assessment Representatives for their review and comment. During this review, guidance provided resulted in the identification of several additional abstractions. The identified model abstractions were then grouped into five abstraction categories. These abstraction categories included:

> **Probability Distributions** - Probability distributions refer to the replacement of the results of more complicated numerical models with a distribution. Specification of parameters by a single representative value or range of values represents a subset of the probability distribution approach to abstraction.
>
> **Simplified Numerical Models** - Simplified numerical models are more efficient codes that are used in the TSPA model to replace more complex process (numerical) models.

Functions - The use of functions to replace more complicated numerical models is a frequently used method to develop abstractions. The typical method is to determine how a new parameter varies with respect to a known parameter and then create a function that closely matches this variation.

Response Surfaces - Response surfaces are multivariate functions that return values for unknown parameters based on any number of input values. Since there is no limit to the number of mutually orthogonal dimensions in imaginary space, response surfaces in n-dimensions may be used to predict multivariate relationships.

Parameter Reduction - Justification is given in the form of conceptual models and/or FEPs arguments that limit or reduce the number of parameters/events considered in the TSPA. The abstractions identified using this method fall within the subset of "scientific analysis abstraction" as defined in AP-SIII.10Q because they do not result in a mathematical model (see Section 3.1.1 for definitions).

The review of project documents indicated that the nominal case for the TSPA–SR used 26 model abstractions. In addition, three AMRs not meeting the narrower definition of "model abstraction" (i.e., defined as a mathematical model in AP-SIII.10Q) were identified bringing the total number to 29. It should be noted that additional model abstractions were used to address the igneous disruption case, and numerous abstractions were used to develop individual process models. These additional model abstractions were outside the scope of the abstraction review, which was focused on the abstractions used directly in the nominal case for the TSPA–SR.

A summary of the types of abstractions used for the nominal case is presented in Table A-1, based on the primary abstraction technique used. Table A-2 lists the AMRs that were classified as model abstractions. Table A-3 lists those AMRs classified as abstractions but not meeting the narrower definition of "model abstraction." A basic description of each abstraction as well as outputs to the TSPA are given in the column labeled "Description of Model Abstraction." In addition, the abstraction type and the dependent process are shown. In actuality, the TSPA model abstractions may have used combinations of abstraction techniques; for simplicity, Table A-1 categorizes each AMR as only one of the types used.

In addition to the internal review to identify model abstractions used in the nominal case of the TSPA–SR, the YMP conducted a formal review of all AMRs to determine the extent to which model validation was achieved in compliance with Administrative Procedure AP-3.10Q, *Analyses and Models*. This review was accomplished as part of the response to Corrective Action Request BSC-01-D-001 (Clark 2001; Krisha 2001) and is documented in *Model Validation Status Report* (BSC 2001g [DIRS 156257]) (MVSR). In the MVSR, 128 models were identified and their validation status was determined. The 128 models identified included models that did not support the TSPA–SR (i.e. the output from these models was not used as input to the TSPA–SR model), and multiple models that were combined into a single abstraction (e.g., three identified models were embedded in the GENII-S dose assessment code). While there is not a one-to-one correlation between the results of the internal review to identify model abstractions used in the TSPA–SR, and the results documenting models/model validation status in the MVSR, both of these sources provide information on model abstractions used in the TSPA–SR.

A.4 PARAMETER UNCERTAINTY IN TSPA–SR, SSPA, AND TSPA–FEIS

As indicated in the introduction to this appendix the treatment of uncertainty in the TSPA–SR was examined in two reports. The first report, *Evaluation of Uncertainty Treatment in the Technical Documents Supporting TSPA–SR* (YMP 2001 [DIRS 155343]) prepared by the Management and Technical Services (MTS) contractor to DOE, evaluated the treatment of uncertainty in the TSPA–SR (and supporting analysis/model reports (AMRs) and process model reports (PMRs)), and provided recommendations related to improving the identification, categorization, evaluation, and quantification of uncertainties. The second report, *Uncertainty Analyses and Strategy* (Williams 2001 [DIRS 157389]), provides the strategy that is intended to be used to improve the treatment of uncertainty in the development of the TSPA–LA.

The MTS study (YMP 2001 [DIRS 155343]) concludes that the Yucca Mountain Project (YMP) has numerous good examples of parameters that are based on data that were measured directly, and has good examples of uncertainty treatment of these data that include discussions of measurement errors, representativeness, and related issues. The MTS study also indicates that there are a number of cases in the AMRs where parameter uncertainty is not characterized and a bounding parameter value is chosen. In other cases, parameter values are chosen that are indicated to be representative, or parameter ranges were addressed using probability distributions. The MTS study concludes that the basis for the selection of the specific values or distributions is unevenly presented.

For TSPA–SR, over 300 parameters were considered uncertain and described by probability distributions. When there was significant uncertainty in parameters (or the particular model or representation), the analyst/modeler was directed to use the “conservative” estimates in order to not bias the results to be potentially optimistic projections of total system performance. As described in Section 3.1.4 of *Uncertainty Analyses and Strategy* (Williams 2001 [DIRS 157389]), the project guidance for treatment of uncertainty in the TSPA–SR was in agreement with the recommendations made by the TSPA Peer Review Panel (Budnitz et al 1999 [DIRS 102726]), after review of the TSPA-VA (CRWMS M&O 1998 [DIRS 108000]; CRWMS M&O 1997 [DIRS 100842]). The general guidance can be summarized as the following: Provide a *defensible* selection from among alternative conceptual models and explain the technical basis for the selection in the AMR; when there are sufficient data to do so defensibly, quantify uncertainties in parameters (e.g., with probability distributions); otherwise, in the absence of sufficient data, develop conservative or bounding estimates that can be defended technically. The consequence of this approach was a mix of conservative and realistic inputs. In some cases, the TSPA Analysts provided informal guidance to the project investigators on how to develop an uncertainty description; in other cases, they did not. Thus, consistency in the uncertainty description is lacking, as noted by the MTS study.

A specific goal for the SSPA (BSC 2001b, Volume 1 [DIRS 155950]; BSC 2001c, Volume 2 [DIRS 154659]), which followed the TSPA–SR, was to evaluate the impact of uncertainty in the parameters. Therefore, for many parameters, the uncertainty distribution was redefined. As discussed in detail in Section 2.2 of *Uncertainty Analyses and Strategy* (Williams 2001 [DIRS 157389]), the SSPA work developed a full range of uncertainty and , if available, used “non-QA” data (e.g., information from outside the YMP) in developing these distributions. For the SSPA, the DOE identified, considered, and evaluated the most recent and relevant information about Yucca Mountain and the potential repository system that was available from all sources, inside and outside the YMP, regardless of the "Q" status of the data. This information was used to quantify uncertainties, provide insights for updating conceptual and numerical models, and provide additional lines of evidence about the possible future behavior of a repository. To the extent possible, the information was incorporated in an updated supplemental TSPA model and evaluated for two thermal operating modes.

The process for evaluating unquantified uncertainties involved: (1) identifying unquantified uncertainties to be evaluated; (2) developing more representative, quantified descriptions of those uncertainties; and (3) evaluating the implications of those newly quantified uncertainties for repository performance. The impacts of the new representations for previously unquantified uncertainties were then evaluated through updated process models, and supplemental TSPA analyses using the updated uncertainty treatment. The representations were implemented and the form and rationale for them documented. The implications of these new representations for process-level model results are discussed in Sections 3 through 14 of Volume 1 of the SSPA (BSC 2001b, Volume 1 [DIRS 155950]). For many of these quantified uncertainties, supplemental TSPA sensitivity analyses were also conducted, as described in Volume 2 of the SSPA (BSC 2001c [DIRS 154659]). These included subsystem performance analyses, TSPAs, and analyses similar to those documented and discussed in the TSPA–SR (CRWMS M&O 2000 [DIRS 153246]). The significance of these analyses is described in Section 2.2 and 2.3 of *Uncertainty Analyses and Strategy* (Williams 2001 [DIRS 157389]). Section 2.2 addresses the significance of the newly quantified uncertainties and Section 2.3 discusses the key remaining uncertainties that have not yet been quantified.

Table A-4 lists the approximately 340 uncertain parameters used in the *Total System Performance Assessment - Analyses for Disposal of Commercial and DOE Waste Inventories at Yucca Mountain – Input to Final Environmental Impact Statement and Site Suitability Evaluation* (TSPA–FEIS), which is the most recently available TSPA model document (BSC 2001d [DIRS 156460]). The number of parameters listed for TSPA–FEIS includes changes made from TSPA–SR for the SSPA analyses (see Section 2.1 of *Uncertainty Analyses and Strategies* (Williams 2001 [DIRS 157389]). It also addresses several additional issues related to promulgation of 40 CFR 197 (i.e., calculation of dose at 18 km boundary, consideration of biosphere dose conversion factors (BCDFs) for reasonably maximally exposed individuals (RMEI), the specified representative volume of groundwater, use of commercial spent nuclear fuel to represent naval fuel in the inventory), inclusion of a new version of WAPDEG (that includes microbial-induced corrosion and aging multipliers for inside-out corrosion and temperature-dependent general corrosion), and corrections to the thermo-hydrologic process models for the low temperature operating mode of the repository.

To some extent for probability models, and especially for consequence models, the inexactness in parameters can be divided further into uncertainty from limited knowledge on the various states of a system and uncertainty from the precise value for a model parameter. These two types of uncertainty are referred to as aleatory and epistemic uncertainty.

Aleatory uncertainty, sometimes called aleatory variability, relates to features, events, and processes that are random in character and cannot be known in detail. As a result, aleatory uncertainties are not reducible with additional data or knowledge. Examples are the location, timing, and magnitude of the *next* earthquake to occur in a region; the fracture-scale permeability structure and its lateral variability over dimensions of the repository; identifying which waste packages will have manufacturing defects that lead to early failures; the molecular-level variation in crystalline structure of Alloy-22 across a waste package surface or among multiple waste packages. All of these processes are captured to some extent in the risk analysis, but they are represented by random processes that are described by "effective" parameters (e.g., bulk permeability) or average rates (e.g., earthquake probabilities, rates of manufacturing defects) that include an aleatory component of uncertainty that will never be resolved. Aleatory variability can occur over both spatial and temporal scales.

Epistemic uncertainties are lack-of-knowledge uncertainties arising because our scientific understanding is imperfect. They are therefore reducible with the gathering and interpretation of additional data and other pertinent information. Examples are average earthquake recurrence rates on a particular fault; rates of general corrosion (passive dissolution) of Alloy-22 as a function of pH and temperature; and changes in bulk rock strength as a function of thermal stresses.

Distinguishing between these two types of uncertainty is not important to estimates of *mean* risk (Pate-Cornell, 1996), but they can be important in the application of the performance assessment model and in assessing the degree to which residual uncertainties might be reduced with the collection of additional data. For example, laboratory testing of multiple metal coupons in a long-term corrosion test may result in a distribution of corrosion rates for a given chemical and temperature environment. The manner in which that observed distribution can be used as a probability distribution on corrosion rate in the performance assessment model varies between two extremes. One extreme is assuming that observed distribution is due entirely to random variability (aleatory variability) and can be applied to all patches on a waste package and to all waste packages (i.e., the spread in rates is due entirely to random variability in patches in waste packages due to true, but unknowable, differences in the metal at different locations). The second extreme is to assume that the observed distribution is due entirely to epistemic uncertainty (i.e., the true corrosion rate on each patch and each waste package is actually the same, but our lack of knowledge keeps us from knowing exactly what that rate is). In the former case (100% aleatory variability), the gathering of additional data will not lead to a reduction in uncertainty, while in the latter case (100% epistemic uncertainty), the gathering of additional data will lead to a large reduction of uncertainty. Because of the importance of corrosion rate to performance assessment results, making a distinction between these two uncertainties can in this case be important.

The second type of inexactness arises from a lack of knowledge about a parameter (either scalar, vector, or tensor quantity of a model) because the data are limited or there are alternative interpretations of the available data. The parameter is not variable because of an intrinsic characteristic of the entity but because an analyst does not know what the precise value of the parameter should be. This type of inexactness is termed Type B, epistemic, state of knowledge, or reducible uncertainty. "Epistemic" refers to the "state of knowledge" about a parameter. The state of knowledge about the exact value of the parameter can increase through testing and data collection such that the uncertainty is “reducible.”

The MTS study (YMP 2001 [DIRS 155343], Section 3.4) provides a summary discussion of the treatment of aleatory and epistemic uncertainty in the probabilistic seismic hazard analysis (PSHA), which is one of the clear treatments of these two types of parameter uncertainty in YMP. As described in Section 6.5.2 of the AMR *Characterize Framework for Seismicity and Structural Deformation at Yucca Mountain, Nevada,* the PSHA methodology is formulated to represent the randomness inherent in the natural phenomena of earthquake generation and seismic wave propagation. Integration is carried out over these aleatory uncertainties to get a single hazard curve. The size, location, and time of the next earthquake on a fault and the details of the resultant ground motion at a site of interest are examples of quantities considered aleatory. Epistemic uncertainties, on the other hand, are expressed in the PSHA by incorporating multiple assumptions, hypotheses, models, or parameter values. These multiple interpretations are propagated through the analysis, resulting in a suite of hazard curves. Results are presented as curves showing statistical summaries (e.g., mean, median, fractiles) of the exceedance probability for each ground motion amplitude. A second example of clear treatment of epistemic and aleatory uncertainty can be found in Section 6.1 of *Incorporation of Uncertainty and Variability of Drip Shield and Waste Package Degradation in WAPDEG Analysis* (CRWMS M&O 2000c [DIRS 146546]).

The general consensus is that maintaining a separation between aleatory and epistemic uncertainty is valuable (Paté-Cornell, 1996 [DIRS 107499]; Apostolakis, 1989 [DIRS 107710]; Helton, 1994 [DIRS 107739]). This desire to maintain a separation between aleatory and epistemic uncertainty strongly affects the design of the analysis (e.g., separate analysis of volcanic disruption and no volcanic disruption). It may also strongly affect the design of individual submodels (e.g., the component modeling of corrosion of the waste package). However, it is not always useful or enlightening to maintain this separation for all parameters. If the analysis design of the TSPA model does not maintain a separation between aleatory and epistemic uncertainty for a certain parameter, then the uncertainties are not separated and the total uncertainty is expressed as a combined distribution. For example, in the TSPA, the disposal system is not discretized such that variability in the adsorption coefficient (Kd) can be modeled under various chemical conditions. Rather, the probability distribution used for Kd includes both aleatory and epistemic uncertainty. The separation of parameter uncertainty into aleatory or epistemic uncertainty may or may not occur for any one particular variable for the license application, but the process described here will help ensure that appropriate AMRs and the TSPA–LA report document how the two forms of parameter uncertainty are handled and ensure that the parameter distribution reflects how the underlying model is used in the TSPA analysis.

Table A-1. Abstraction Types and their Frequency in TSPA–SR.

Abstraction or Model Abstraction	Type of Abstraction	Frequency
Model Abstractions {26}	Probability Distributions (including those specified only as representative values or ranges)	10
	Simplified Numerical Models	4
	Functions	9
	Response Surfaces	3
Scientific Analysis Abstractions {3} (see Table A.3)	Parameter Reduction	3
Total Number of Abstractions in TSPA–SR		**29**

Table A-2. Model Abstractions Used by the TSPA–SR for the Nominal Scenario.

PA Dept	Document Number, Short ID, DIRS Number	Document Title	Model Abstraction Type	Description of Model Abstraction	Inputs to Model	Dependent Processes
BIO	ANL-MGR-MD-000003 B0055 [DIRS: 152536]	Disruptive Event Biosphere Dose Conversion Factor Analysis Rev 01	Probability Distributions	Development of biosphere dose conversion factors.	Transport parameters, transfer coefficients, exposure times, ingestion/inhalation exposure parameters, erosion and leaching data	Biosphere model
BIO	ANL-NBS-MD-000007 B0075 [DIRS: 153206]	Abstraction of BDCF Distributions for Irrigation Periods, Rev 0/ICN 1	Probability Distributions	Fourteen radionuclides were identified in a predecessor AMR to have significant Biosphere Dose Conversion Factors (BDCFs) build-up factors from prior irrigation. The purpose of this AMR was twofold. First, to develop and fit, for each radionuclide, an analytical approximation for the abstracted BDCF distributions over the period of time considered for irrigation. Second, to incorporate into this approx. the soil loss data. The result is to provide PA with an abstraction for soil build up effects on BDCFs to be used to calculate dose.	Irrigation times, scale factors, statistical mean & standard deviation, and in some cases the shift for various radionuclides	Biosphere model
BIO	ANL-NBS-MD-000008 B0080 [DIRS: 153207]	Distribution Fitting to the Stochastic BDCF Data, Rev 00 ICN 01	Probability Distributions	The BDCF data are provided as data sets. Each data set is comprised of 150 stochastic realizations of BDCFs evaluated for a given radionuclide after a predefined period of previous irrigation. Each data set was analyzed to derive statistically justifiable distribution (abstractions) to the individual data sets of the BDCFs. These abstractions that define the BDCF distributions by a limited number of parameters (two or three) will be used in the TSPA numerical predictive capability for assessing performance of the proposed Yucca Mountain repository. In particular, they will be used in the TSPA numerical predictive capability to calculate dose with its uncertainty from radionuclide concentrations in groundwater.	Predictions of future climate, irrigation, radionuclide physical parameters	Biosphere model

Table A-2. Model Abstractions Used by the TSPA–SR for the Nominal Scenario. (Continued)

PA Dept	Document Number, Short ID, DIRS Number	Document Title	Model Abstraction Type	Description of Model Abstraction	Inputs to Model	Dependent Processes
EBS	ANL-EBS-HS-000003 E0130 [DIRS: 154594]	Abstraction of NFE Drift Thermodynamic Environment and Percolation Flux, Rev 00, ICN 02	Simplified Numerical Model	Abstraction of the thermal hydrology (TH) model that characterizes the in-drift thermodynamic environment. Creates time-history data as output. Outputs to the TSPA model include infiltration rates averaged for TSPA bins and for specific locations.	Inputs include averaged temperature, liquid saturation, relative humidity, evaporation rate, and percolation flux.	WAPDEG, waste form model
EBS	ANL-EBS-MD-000031 E0000 [DIRS: 150418]	Invert Diffusion Properties Model, Rev 01	Function	A model to show how resistivity and diffusivity can be estimated as a function of water content and temperature.	Resistivity, porosity, saturation, cementation factor	EBS Transport model and EBS Radionuclide Transport Abstraction
EBS	ANL-EBS-MD-000042 E0045 [DIRS: 129280]	In-Drift Colloids and Concentration, Rev 00	Function	A model for GoldSim to calculate colloid concentration as a function of ionic strength, as well as for determining the stability of smectite and iron-(hydr)oxide colloids as a function of both ionic strength and pH. It employs bounding relationships that are closely tied to the colloid generation and characterization experimental programs conducted at ANL and LANL and to documented colloid characteristics of a variety of groundwaters. The abstraction is considered valid and usable in TSPA calculations for any time after the temperature in the repository has decreased to well below boiling after the thermal pulse. Many of the waste degradation tests were performed at 90°C but mostly sampled at near room temperature.	Radionuclide concentrations, Ionic strength of fluid , pH	Waste form model

Table A-2. Model Abstractions Used by the TSPA–SR for the Nominal Scenario. (Continued)

PA Dept	Document Number, Short ID, DIRS Number	Document Title	Model Abstraction Type	Description of Model Abstraction	Inputs to Model	Dependent Processes
EBS	ANL-EBS-MD-000045 E0105 [DIRS: 153265]	In-Drift Precipitates/ Salts Analysis, Rev 00, ICN 02	Response Surface	This model was developed to evaluate the effects of water vaporization (evaporation) on water composition at a given location in the EBS (e.g. the drip shield surface). The presence or absence of backfill is irrelevant to the model. The output of the model that is important to the TSPA is pH, chloride concentration, ionic strength, and approx. maximum RH for dry conditions to exist. These effects are important in estimating colloid mobility and corrosion rates for the drip shield and waste package. In addition, these effects may be important in predicting spent fuel dissolution rates and radionuclide transport.	Temperature, RH, seepage flux & composition, evaporation Flux, fugacity of carbon dioxide, incoming seepage chemical composition	EBS transport model
SZ	ANL-NBS-HS-000030 S0055 [DIRS: 139440]	Input & Results Base Case SZ Flow and Transport Model TSPA, Rev 00	Probability Distribution (and also Simplified Numerical Model)	Provides radionuclide transport simulation results for the SZ site-scale model for use in TSPA calculations. The approach is to produce a set of radionuclide breakthrough curves at the accessible environment, 20 km from the repository. These breakthrough curves contain information on the radionuclide travel times through the SZ that is used in the TSPA calculations to determine the arrival times and mass of radionuclides in the biosphere. In addition, the analysis provides a simplified one-dimensional radionuclide transport model for the purpose of simulating radionuclide chains in the TSPA simulator. 1) The convolution integral method is used to determine the radionuclide mass flux at the SZ / biosphere interface. 2) The effects of climate change on radionuclide transport are incorporated by scaling the breakthrough curves simulated for present climatic conditions	Input files and groundwater flow field for radionuclide transport simulations from the final calibrated SZ site-scale flow model, uncertainty distributions for stochastic SZ transport parameters, matrix porosity and bulk density in the area of the ISM, groundwater recharge distribution at the water table under Yucca Mountain, Mean infiltration for present, glacial, and monsoonal climates.	Saturated zone transport model
SZ	ANL-NBS-MD-000011 S0050 [DIRS: 147972]	Uncertainty Distribution for Stochastic Parameters, Rev 00	Probability Distribution	Parameters for the SZ model for TSPA–SR. Specifies the important parameters to be represented stochastically and the minor parameters to be represented as constants. Constants were assessed for validity and the stochastic values were assigned bounded distributions.	Aquifer parameters: sp. Discharge, porosity, density, partitioning coefficient., dispersivity, retardation, etc.	SZ flow and transport model

Table A-2. Model Abstractions Used by the TSPA–SR for the Nominal Scenario. (Continued)

PA Dept	Document Number, Short ID, DIRS Number	Document Title	Model Abstraction Type	Description of Model Abstraction	Inputs to Model	Dependent Processes
TH	ANL-NBS-HS-000029 N0125 [DIRS: 123916]	Abstraction of Drift Scale Coupled Processes, Rev 00	Probability Distribution	This AMR is an abstraction of data and a comparative analysis. An abstraction method for the THC water chemistry and gas-phase composition in the host rock adjacent to the emplacement drift wall is provided. Also included is an analysis of different geochemical systems and how they impact the TH predictions of the THC process-level model. Finally, it provides a detailed evaluation of the thermal hydrologic performance of a geologic repository obtained from process-level models that either include or do not include reactive transport process (TH-only, THC, edge cooling, etc…) that result in response to heat addition. It is concluded that either process model, THC or TH-only, are equally valid in determining the TH response of a geologic system subjected to heat addition by repository decay heat. On the other hand, if the TSPA abstraction input requires the water and gas composition in the near-field host rock, the drift-scale THC model is appropriate.	Temp., liquid saturation, air/water fluxes, ion & gas concentrations	Various process-level models
UZ	ANL-NBS-HS-000023 U0125 [DIRS: 153104]	Abstraction of Flow Fields for RIP, Rev 00 ICN 01	Probability Distribution	Post-processes 18 “base case” UZ site-scale flow fields from TOUGH-2. In addition, four flow fields that are used for future full-glacial climates are processed. Flow fields processed for used in TSPA particle tracking calculations. Infiltration rates were extracted from the four full-glacial-climate flow fields for use in seepage abstraction models in the TSPA.	TOUGH2 output	UZ transport - FEHM

Table A-2. Model Abstractions Used by the TSPA–SR for the Nominal Scenario. (Continued)

PA Dept	Document Number, Short ID, DIRS Number	Document Title	Model Abstraction Type	Description of Model Abstraction	Inputs to Model	Dependent Processes
UZ	ANL-NBS-HS-000026 U0065 [DIRS: 141418]	Particle Tracking Model and Abstraction of Transport Process, Rev 00	Simplified Numerical Model	A particle-tracking algorithm is developed that incorporates the transport processes determined to be relevant in the site characterization program, including advection, dispersion, sorption, and matrix diffusion. In addition, new model development was required to allow for finite spacing between fractures in the matrix-diffusion model, multiple-species transport with decay/ingrowth, and the integration with the TOUGH2 and GoldSim applications. These capabilities were incorporated into the current version of FEHM. This version of the code can be used to perform the UZ transport calculations for TSPA–SR as long as the limits on the model are recognized and parameters are chosen accordingly.	Mean fracture aperture and spacing, variance in aperture, moisture retention curves, cumulative probabilities for colloid transport between one matrix and another calculated from interpolation of pore volume data from Yucca Mountain Hydrologic Samples, probabilities for constants and retardation factors from C-wells microsphere data.	UZ transport
UZ	ANL-NBS-MD-000005 U0120 [DIRS: 154291]	Abstraction of Drift Seepage, Rev 01	Probability Distribution	Results of seepage process-model simulations for a large number of cases were synthesized, and distributions representing the uncertainty and spatial variability of seepage into drifts as a function of percolation flux were derived.	Rock properties, drift & waste package geometry, fluxes, gamma parameter and residual liquid fracture saturations for the base, low, and high infiltration cases, infiltration flow fields plus gamma parameters and residual liquid fracture saturations for fault zones for the base, low, and high glacial-transition	WAPDEG & EBS transport models
WF	ANL-EBS-MD-000015 F0055 [DIRS: 136060]	CSNF Waste Form Degradation: Summary Abstraction	Simplified Numerical Models	Provides a current summary of data and updated models for commercial spent nuclear fuel (CSNF) intrinsic (forward) dissolution (high water-flow) rates. Bounding models that apply to all UO_2-based spent fuel expected to be disposed in a repository.	CSNF dissolution rates	

Table A-2. Model Abstractions Used by the TSPA–SR for the Nominal Scenario. (Continued)

PA Dept	Document Number, Short ID, DIRS Number	Document Title	Model Abstraction Type	Description of Model Abstraction	Inputs to Model	Dependent Processes
WF	ANL-EBS-MD-000037 F0170 [DIRS: 154620]	In-Package Chemistry Abstraction, Rev 01	Probability Distribution	The chemical parameter pH was used as a "key" parameter where response surfaces were generated with pH as a function of the independent parameters, water flux, WP corrosion rate, and fuel exposure for CSNF packages, for co-disposal packages a distribution of pH was generated. Relationships were formulated between pH and total carbonate and pH and Eh such that for any set of independent parameters the pH, total carbonate, and Eh could be directly calculated.	ionic strength, pH, CO_3, Fl, Cl	Waste form model, WAPDEG
WF	ANL-WIS-MD-000004 F0065 [DIRS: 155609]	DSNF and Other Waste Form Degradation Abstraction, Rev 01, ICN 01	Probability Distribution	Degradation models of DOE owned spent nuclear fuel (DSNF) and the immobilized ceramic plutonium (PU) disposition waste forms are selected for application in the proposed monitored geologic repository (MGR) post-closure TSPA.	Data, information, and models for the degradation of DSNF and Pu disposition waste forms were obtained from laboratory experiments, DOE reports, NSNFP reports, and OCRWM AMRs.	Waste Form model
WF	ANL-WIS-MD-000006 F0015 [DIRS: 150561]	Inventory Abstraction, Rev 00, ICN 02	Response Surfaces	This analysis interprets the results of a series of relative dose calculations and recommends sets of radionuclides that should be modeled in the TSPA–SR and TSPA–FEIS. The recommendations of the sets of radionuclides to model are based on two timeframes (100 years after closure to 10,000 years and 10,000 to 1,000,000 years). The goal was to identify the minimal set of radionuclides that would contribute 95 percent of the dose. The exposure scenarios considered are direct, nominal, and human intrusion.	Radionuclide physical parameters	Waste Form model

Table A-2. Model Abstractions Used by the TSPA–SR for the Nominal Scenario. (Continued)

PA Dept	Document Number, Short ID, DIRS Number	Document Title	Model Abstraction Type	Description of Model Abstraction	Inputs to Model	Dependent Processes
WF	ANL-WIS-MD-000010 F0095 [DIRS: 155455]	Summary of Dissolved Concentration Limits, Rev 01	Probability Distribution	Solubility limits for 14 elements were derived. Three radioisotope solubilities were abstracted as a function of in-package chemistry dependent on temperature, pH, and CO_2 concentration. Three radionuclide solubilities (actinium, curium, and samarium) were set equal to that of americium. Four additional radioisotope solubilities were defined by probability distributions (plutonium, lead, protactinium, and nickel). The solubilities of the remaining screened-in radioisotopes were set at bounding values.	Physical parameters of 14 elements, Eh, pH, other ion concentrations	Waste form model
WF	ANL-WIS-MD-000012 F0115 [DIRS: 153933]	Waste Form Colloid-Associated Concentrations Limits: Abstraction and Summary, Rev 00, ICN 01	Functions	A model is developed for GoldSim to calculate colloid concentration as a function of ionic strength, as well as for determining the stability of smectite and iron-(hydr)oxide colloids as a function of both ionic strength and pH. The abstraction employs bounding relationships that are closely tied to the colloid generation and characterization experimental programs conducted at ANL and LANL.	Inputs are radionuclide concentration, pH, ionic strength, colloid stability parameters and functions and mass of colloids.	Waste form model
WF	ANL-WIS-MD-000018 (no short ID) [DIRS: 144167]	In-Package Source Term Abstraction, Rev 00	Functions	An analysis is presented such that the time term in the rind calculation is no longer time since time zero (or absolute time); instead, the time term is the length of the time since the wasteform became available for degradation. This represents a more appropriate method for calculating rind volume in terms of how waste packages fail at different times over the life of the repository. This method also accounts for rate of cladding failure for CSNF packages for determining exposed mass. The volume of water in the rind for each wasteform type in a waste package at any time step is a function of the fraction of exposed wasteform multiplied by the volume of rods, the porosity, and the water saturation of the wasteform.	Length of time since the wasteform became available for degradation; volume of the rods, porosity; water saturation of the wasteform	Waste form model
WP	ANL-EBS-MD-000003 W0035 [DIRS: 144229]	General and Localized Corrosion of WP Outer Barrier, Rev 00	Functions	Addresses the development of models to account for the degradation of the outer barrier of the waste package. A combination of functions in a decision tree	Temperature RH, electrolytes, pH, oxidants, physical constants	WAPDEG

Table A-2. Model Abstractions Used by the TSPA–SR for the Nominal Scenario. (Continued)

PA Dept	Document Number, Short ID, DIRS Number	Document Title	Model Abstraction Type	Description of Model Abstraction	Inputs to Model	Dependent Processes
WP	ANL-EBS-PA-000003 W0040 [DIRS: 147648]	Abstraction of Models for Pitting & Crevice Corrosion Drip Shield/Waste Package, Rev 00	Functions	Abstraction analyses consider localized corrosion of the waste package outer barrier (Alloy 22) and drip shield (Titanium grade 7). The analyses consider 1) initiation thresholds for pitting and crevice corrosion both in the presence and absence of dripping water and their uncertainty and variability under repository conditions and 2) penetration rates as a function of time, temperature, and other exposure conditions both in the presence and absence of dripping water, and the uncertainty and variability of the penetration rate under repository conditions.	Temperature, pH, and the log of chloride concentration, corrosion potential and critical potential measurements of Alloy 22 and Titanium grade 7, solution compositions for simulated dilute, concentrated, acidified, saturated, and basic saturated water.	WAPDEG
WP	ANL-EBS-PA-000004 W0045 [DIRS: 151549]	Stress Corrosion Cracking of Drip Shield and Waste Package Outer Barrier and Hydrogen Induced Corrosion of Drip Shield, Rev 00 ICN 01	Functions (and also Probability Distribution)	The abstractions developed are: 1) stress and stress intensity factor profiles as a function of depth, 2) threshold stress intensity factor, 3) threshold stress to initiate crack growth, 4) parameters A and *n* of the Slip Dissolution model, 5) incipient crack density and size used with the Slip Dissolution Model, and 6) probability for the occurrence and size of manufacturing defects in the closure lid welds. Major efforts of the abstraction were given to develop an approach to represent uncertainty and variability of the model parameters.	Stress, stress intensity profiles as a function of depth, threshold stress, incipient crack densities, crack growth model, model parameters for outer shell flat and extended closure lid weld regions	WAPDEG
WP	ANL-EBS-PA-000005 W0120 [DIRS: 135968]	Abstraction of Models for Stainless Steel Structural Material Degradation, Rev 00	Functions	General and localized corrosion of the waste package inner barrier (316NG) is analyzed. Potential-based localized corrosion initiation threshold functions for 316NG stainless steel (based on data collected for 316L stainless steel) were derived from the functional dependence of experimentally obtained electrochemical potential data on absolute temperature, pH, and the base 10 logarithm of chloride ion concentration. It was concluded that localized corrosion initiation is probable at neutral pHs, temperatures below 380K, and chloride concentrations in the range of 10^{-4} to 10 mol/L.	Solution temperatures ranging from 30 to 120°C, chloride ion concentrations between 67 and 154,000 mg/L, and pH values between 2.7 and 10.2	None Identified

Table A-2. Model Abstractions Used by the TSPA–SR for the Nominal Scenario. (Continued)

PA Dept	Document Number, Short ID, DIRS Number	Document Title	Model Abstraction Type	Description of Model Abstraction	Inputs to Model	Dependent Processes
WP	ANL-WIS-MD-000007 F0155 [DIRS: 151662]	Clad Degradation - Summary and Abstraction, REV 00 ICN 01	Functions; (and also Probability Distribution)	This analysis describes the postulated condition of commercial Zircaloy clad fuel after it is placed in the YMP site as a function of time. Provides correlations, parameters, and data tables for use in the TSPA–SR.	Uses data, formulas, etc. from several other AMRs related to cladding degradation.	Waste Form model
WP	ANL-WIS-PA-000001 E0095 [DIRS: 155638]	EBS Radionuclide Transport Abstraction, Rev 00 ICN 02	Simplified Numerical Model	This AMR provides the algorithms for transporting radionuclides using the flow geometry and radionuclide concentrations determined by other elements of the TSPA–SR model. In particular, this model is used to quantify the time-dependent radionuclide releases from a failed waste package and their subsequent transport through the EBS to the emplacement drift wall/UZ interface.	Drift & waste package dimensions , properties, and construction, properties of water	EBS Transport model

Table A-3. Scientific Analysis Abstractions Used in the TSPA–SR for the Nominal Scenario.

PA Dept	Document Number, Short ID, DIRS Number	Document Title	Abstraction Type	Description of Abstraction	Inputs to Abstraction	Dependent processes
EBS	ANL-EBS-MD-000046 E0010 [DIRS: 151563]	Physical & Chemical Environmental Abstraction Model, Rev 00 ICN 01	Parameter Reduction	Provides an overall conceptualization of the physical and chemical environment in the emplacement drift. It includes the physical components of the EBS. The intended use of this descriptive conceptualization is to assist the Performance Assessment Department in modeling the physical and chemical environment within a repository drift. The TSPA may use P/CE abstracted parameters and models to specify groundwater compositions and microbial masses for potential application at the outer surfaces of the drip shield and waste package and in the invert.		WAPDEG, Waste form model, EBS transport model
EBS	ANL-EBS-MD-000040 E0035 [DIRS: 129278]	In-Drift Gas Flux & Composition. Rev 00	Parameter Reduction	Abstraction in the sense that results provide justification to limit parameters/events considered. The scope of the document is to evaluate the need to consider possible changes to the in-drift gases, particularly CO_2, O_2, N_2 and steam (H_20) in future performance assessments based on the conceptual framework for -in-drift gas flux and composition discussed in the report. The conceptual analysis and mass balance calculations presented suggest that in-drift gas flux and composition will not be strongly affected by interactions with in-drift and near-drift materials.	The data and parameters are taken from other AMRs and YMP documents. Masses and compositions of the various metals and alloys included in the repository, gas influx into the drifts	WAPDEG

Table A-3. Scientific Analysis Abstractions Used in the TSPA–SR for the Nominal Scenario. (Continued)

PA Dept	Document Number, Short ID, DIRS Number	Document Title	Abstraction Type	Description of Abstraction	Inputs to Abstraction	Dependent processes
UZ	ANL-NBS-HS-000020 T0090 [DIRS: 151953]	Fault Displacement Effects in the Unsaturated Zone. Rev 01	Parameter Reduction	An abstraction in the sense that results provide justification to limit parameters/events considered. The purpose of the analysis is to evaluate the potential for changes to the hydrogeologic system caused by fault displacement to affect radionuclide transport in the UZ at Yucca Mountain. Results suggest that transport between the potential repository and the water table is only weakly coupled to changes in fracture aperture. Overall, insignificant changes in transport behavior are found for large changes in fracture aperture. The analysis concludes that the effects of fault displacement on UZ transport can be excluded from models for TSPA.	Data and parameter inputs for UZ flow calculations using TOUGH2 presented in this analysis are contained in the AMR titled “UZ Flow Models and Submodels”	UZ Flow and Transport

Table A-4. Uncertain Parameters used for TSPA–FEIS.

TSPA Component Model	Parameter Type or Name	Number of Parameters Used	Descriptions or Use
System	BIN Probabilities	12	Used in selecting bins for various parameters including: low, mean, and high infiltration scenario and for SS clad waste fuel packages for low, mean, and high infiltration scenarios. These are used for both low thermal and high thermal operating modes (LTOM and HTOM).
System	Random Values (Rand-Env, , Rand-Env_SS)	2	Random generator used for selecting the environment for placing waste packages and for placing SS clad fuel packages.
System	Rand_Fuel_Type	1	Random generator used for selecting the fuel type for human intrusion and juvenile failure scenarios
Waste Package	Gaussian Variance Partitioning Parameters (*xx*_GVP_*xxxx*)	6	Parameter for the fraction of the original distributions variance due to uncertainty for the Ti-7 Drip Shield and for Alloy 22
Waste Package	Gaussian Variance Partitioning Parameters (*xx*_GVP_*xxxx*)	6	Parameter for the cumulative probability used to sample the median of the variability distributions from the uncertainty distribution for the Ti-7 Drip Shield and for Alloy 22
Waste Package	Gaussian Variance Partitioning Parameters (*xx*_GVP_*xxxx*)	6	Parameter for the fraction of the original distributions variance due to uncertainty for Ti-7 Drip Shield and for Alloy 22
Waste Package	Variance Input (VarShar_*xxxx*)	6	WAPDEG variance input for Package-Package for Alloy 22 inner and outer barrier and Ti-7; for No Drip and Drip general corrosion conditions
Waste Package	Variance Input (VarShar_*xxxx)*	4	WAPDEG variance input for Package-Package for Alloy 22 inner and outer barrier; for In Package general corrosion and pitting corrosion conditions
Waste Package	Variance Input (VarShar_*xxxx*)	4	WAPDEG variance input for Package-Package and Patch-Patch for Alloy 22 inner and outer barrier; for Drip pitting corrosion.
Waste Package	Variance Input (VarShar_*xxxx*)	2	WAPDEG variance input for Patch-Patch for Alloy 22 inner and outer barrier ; for In-Package pitting corrosion
Waste Package	Variance Input (VarShar_*xxxx*)	4	WAPDEG variance input for Package-Package and for Patch-Patch for Alloy-22 inner and outer barrier; for Stress Corrosion Cracking
Waste Package	Variance Input (VarShar_*xxxx*)	2	WAPDEG variance input for Package-Package for Alloy-22 inner barrier; for stress threshold
Waste Package	Variance Input (VarShar_*xxxx)*	2	WAPDEG variance input. Aging multiplier for Package-Package for Alloy-22 inner and outer barrier;
Waste Package	Variance Input (VarShar_*xxxx*)	4	WAPDEG variance input. MIC multiplier and RH Threshold for MIC conditions, for Alloy-22 inner and outer barrier;

Table A-4. Uncertain Parameters used for TSPA–FEIS. (Continued)

TSPA Component Model	Parameter Type or Name	Number of Parameters Used	Descriptions or Use
Waste Package	Outer Lid (OL) and Inner Lid (ML) Parameters (*xxxx*_OL) or (*xxxx*_ML)	14	Parameters for describing the outer and inner lids including: non-detection probability, uncertain deviation from median yield strength for inner lid, location of non-detection probability for the outer lid. Chi-square distribution for stress profile uncertainty magnitude of the stress profile uncertainty Variation from the mean, fraction of defects capable of propagation by SCC, fraction of outer surface-breaking flaws, fraction of surface-breaking defects, fraction of expected yield stress for assigning stress threshold
Waste Package	Crack Growth Exponent (nib or nob)	2	Crack growth exponent for slip dissolution in the inner and outer barriers
Waste Package	Early Failure	1	Number of early failed waste packages
Waste Package	General corrosion terms (Anchor T[C] and B)	2	Temperature at which general corrosion CDF is applied, and the general corrosion slope term
Waste Form Cladding	Cladding Failure Parameters	4	Parameters used to reflect cladding failure process including: percent of cladding stress crack corrosion failures, a cladding uncertainty term for CSNF dissolution rates, cladding unzipping velocity uncertainty, and cladding local corrosion rate uncertainty
Waste Form Cladding	Rod Failure Parameters	8	Parameters to represent the fraction or rods perforated from creep as a function of peak WP surface temperatures (includes 5 parameters for the bins used). Also includes parameters for Early Failure packages, for stainless steel clad fuel packages, and for percentage of initial rod failures
Waste Form	Activation Energies (Ea_high, Ea-Low)	2	Activation energies at high and low pH in high-level glass waste (HLW)
Waste Form	Effective Dissolution Rate (log_Keff_high, log_Keff -low)	2	Logarithms of the effective dissolution rates at high and low pH in HLW
Waste Form	pH Dependence Coefficient (mew-high, mew-low)	2	pH dependence coefficient at high pH and at low pH
Waste Form	Gap_distribution	1	Uncertainty in CSNF gap fraction
Unsaturated Zone	Kd (*xx*-Devit, *xx*-Vitric, *xx*-Zeol)	35	Kd for various radionuclides in devitrified, vitrified, and zeolitic units. Radionuclides include: Am, Cs, I, Np, Pa, Pu, Sr, Tc, Th, U
Unsaturated Zone	Kc (Kc_*xx*_gw_Colloid)	2	Kc for various colloids including: Am and Pu
Unsaturated Zone	Matrix Diffusion (Md_Anions\r\n and Md_Cations\r\n)	2	Coefficients for anion and cation matrix diffusion
Unsaturated Zone	Fracture Aperture (fa_*xxxx*)	41	Fracture aperture for various geologic units and grid locations
Seepage	Seepage Flow Factors	8	Parameters to describe seepage flow including: episodic flow factor, flow focus factor, seepage uncertainty, seepage flow rate standard deviation, seepage mean flow rate, seepage faction, and two random seeds used in various libraries.
In-Drift	CO_2	1	Parameter used to reflect uncertainty of high/low uncertainty in CO_2

Table A-4. Uncertain Parameters used for TSPA–FEIS. (Continued)

TSPA Component Model	Parameter Type or Name	Number of Parameters Used	Descriptions or Use
Chemistry	CO2_Stochastic		
Waste Form In-Package Chemistry	pH (pH_Random, pH_IPC_Uncert_CSNF)	2	Parameter used to sample between low and high corrosion rate pH values, and to reflect uncertainty of in-package pH for CSNF.
Waste Form n-Package Chemistry	pH (pH_(*Waste)*_IPC_#)	6	Parameter to reflect in-package pH for a given waste type (*Waste* being either CSNF or CDSP) for three time periods
Waste Form In-Package Chemistry	Ionic Strength (Ionic_Str_(*Waste)*_IPC_#)	5	Parameter to reflect in-package ionic strength for a given waste type (*Waste* being either CSNF or CDSP) for three time periods
EBS Transport	Kd of Corrosion Products (Kd_*Rn*_CP)	7	Kd for corrosion products for Am, I, Np, Pu, Tc, Th, and U.
EBS Transport	Uncertainty Factors (*xx_xx_xx*_Uncert)	3	Parameters used to address uncertainties in waste package flux split, drip shield flux split, and invert diffusion coefficient.
EBS Transport	Corrosion Rates (*xx*_Corrosion_Rate)	2	Parameters for stainless steel corrosion rate and for carbon steel corrosion rate
EBS Transport	In-package dimensional factors	5	Parameters for in-package diffusion including: breached thickness of waste package, rod path length, diffusion path length for stress-corrosion cracking, diffusion path length for when general corrosion patches are present, and the surface area factor
Saturated Zone	Location of radionuclide source (SCR*x*#)	8	Parameters defining the north-south and east-west locations of radionuclide sources in source regions 1 through 4
Saturated Zone	Alluvium Uncertainty Zone (FPLAN, FPLAW)	2	Parameters to determine the northern and western boundaries of the alluvium uncertainty zones
Saturated Zone	Flow Parameters	9	Parameters to describe flow conditions including: effective porosity in the valley fill hydrogeologic unit and the alluvial uncertainty zone, effective porosity of the undifferentiated valley fill hydrogeologic unit, flowing interval spacing and flow interval porosity in the fractured volcanic hydrogeologic units, parameter for determining the groundwater flux case and for determining the horizontal anisotropy case, and the longitudinal dispersivity and effective diffusion coefficient in the fractured volcanic hydrogeologic units, and alluvium density
Saturated Zone	Sorption Coefficients (KDRN#)	8	Sorption coefficients for radionuclide tracking
Saturated Zone	Sorption Coefficients (KD*RnUnit)*	7	Sorption coefficients for various radionuclides (*Rn)* including Tc, U, I, and Np in various geologic units (*Unit*) including alluvium units and fractured volcanic units; and for the strongly sorbing radionuclides for the reversible sorption model of colloid-facilitated transport
Saturated Zone	Colloidal Transport Parameters (KC-*Rn*-GW-Colloid)	5	Kc parameters for various radionuclides (*Rn*) including Am, Pu for equilibrium colloid-facilitated radionuclide transport, and the Kc for Plutonium. Also colloid retardation factors in the alluvium units and fractured volcanic units for the irreversible sorption model of colloid-facilitated transport
Waste Form Colloid Transport	Kd	7	Kd for various colloids including: Am reversible, Am Fe-OH, Pu-FE-OH, Am groundwater, Pu groundwater, Am waste form, Pu waste form
Waste Form Solubility	Waste Form Solubilities (Solubilitiy_*Rn*_Secondary _Phase)	5	Waste form solubilities for various radionuclides (*Rn*) for secondary phase including: Am, Np, Pu, Th, and U

Table A-4. Uncertain Parameters used for TSPA–FEIS. (Continued)

TSPA Component Model	Parameter Type or Name	Number of Parameters Used	Descriptions or Use
EBS Solubility	Invert Solubilities (Solubilitiy_*Rn*_Invert_Sec_Phase)	3	Invert solubilities for various radionuclides for secondary phase including: Am, Np, U
Waste Form Solubility	Solubilities and Solubility Uncertainties (Solubility_(*Rn*) and (*Rn*)_Uncert)	4	Solubilities for various radionuclides and to reflect solubility uncertainties including: Pa. Pu, Tc, Th
Waste Form Solubility	Concentration factor for Np (Log_Fc)	1	Concentration factor for NP solubility calculations
Biosphere	Groundwater BDCFs (BDCF_*Rn*)	21	BDCFs for groundwater exposure pathway for a variety of radionuclides (*Rn*) including:Ac^{227}, Am^{241}, Am^{234}, C^{14}, Cs^{137}, I^{129}, Pb^{210}, Pu^{238}, Pu^{239}, Pu^{240}, Pu^{242}, Ra^{226}, Sr^{90}, Tc^{99}, Th^{229}, Th^{230}, U^{232}, U^{233}, U^{234}, U^{236}, U^{238} (100% correlation)
Biosphere	Direct Release BDCFs (BDCF_Ash_*Rn*)	17	BDCFs for groundwater exposure pathway for a variety of radionuclides (*Rn*) including: Ac^{227}, Am^{241}, Am^{234}, Cs^{137}, Pa^{231}, Pb^{210}, Pu^{238}, Pu^{239}, Pu^{240}, Pu^{242}, Ra^{226}, Sr^{90}, Th^{229}, Th^{230}, U^{232}, U^{233}, and U^{234} (100% correlation)
Biosphere	Groundwater Usage (R1, R2)	2	Parameters to describe groundwater usage
Human Intrusion	Infiltration Flux (Borehole_*(state)*_Infiltration)	3	Parameters to describe borehole flux for three infiltration states: high, low, and mean infiltration
Human Intrusion	Input Region	1	A parameter for selecting the SZ input region for putting mass into the SZ system.
Igneous	Probability and Timing	2	Parameters to reflect distribution of igneous event probability and the time of occurrence for the indirect intrusive event,
Igneous	Number of Waste Package Parameters	7	Parameters to describe the interaction of the igneous intrusion and the repository. Used to describe factors such as: the number of drifts intersected per vent, the number of vents hitting waste packages, the number of waste packages hit per vent, number of Zone 1 + Zone 2 packages, the number of Zone 1 packages,
Igneous	Eruptive Event Parameters	8	Parameters used to describe the eruptive event and subsequent ash dispersion. These include: power of the igneous event, initial eruptive velocity, eruptive volume, ash mean particle diameter, ash median particle diameter standard deviation, ash dispersion controlling constant, wind speed, and soil removal factor.