6. CONTROL OF THE TSPA-LA MODEL

This section discusses control of the TSPA-LA model. The controls are applicable for model development, model testing, correction of model errors, and the production of TSPA simulations (including the compliance simulations for the License Application). The controls cover the entire life-cycle of the model, from management direction of what changes are to be made to the model, to the control of completed TSPA simulations and their results. It should be noted that these controls do not replace the QA procedures that govern work involving the TSPA-LA model, rather they provide additional guidance for implementing the requirements of the QA procedures. The controls and guidelines for this work will be documented in a controlled document for use by all TSPA analysts (*Total System Performance Assessment Model Desktop Guidelines*, currently in draft). All documentation generated in the control processes will be filed in the records system with the TSPA-LA documentation.

6.1 DESCRIPTION OF THE TSPA MODEL

The TSPA-LA model consists of four major parts, the GoldSim model file, the DLLs called by the GoldSim model file, the set of input files used by DLLs, and the database which passes input parameters to the GoldSim model file.

There is also a three-tier hierarchy of analysis cases for the TSPA-LA model: the master case, base cases, and sensitivity cases (see Figure 6.1-1). The master case is designed to simulate multiple performance assessment scenario classes. A base case is produced when the master case is run for a given scenario class case and set of simulation settings (e.g. nominal scenario class, 300 realizations, 20,000-year duration). A sensitivity case is produced when a base case is run with a change to the model (e.g., neutralization of drip shield sensitivity case).

6.2 MANAGEMENT CONTROL

The TSPA-LA model may require modification for a number of reasons. The management control of these changes is presented in this section, and illustrated in Figure 6.2-1.

New or revised AMRs being developed for the LA will utilize the FTL/ATL/PTL processes as described in Section 3. During the development of new or revised AMRs, TSPA analysts will be involved with the SMEs in defining the technical output of their AMRs for use in the TSPA-LA model. Draft information (e.g., DTNs and AMRs) will be provided for initial implementation into the TSPA-LA model. The results of the initial implementations will be reviewed by the appropriate SMEs to ensure that the implementation is consistent with the SMEs intent for the model. Any discrepancies will be addressed by changing the implementation in the TSPA-LA model and/or changing the supporting AMRs and/or DTNs prior to their being finalized.

In addition, new or revised AMRs developed for the LA will be reviewed by the TSPA Department as part of the AP-2.14Q, *Review of Technical Products and Data*, of the AMRs. Part of this review will determine whether changes to the TSPA-LA model are required and if they are within the TSPA model development scope and schedule.

Potential changes to the TSPA-LA model due to identified errors will be reviewed by the TSPA Department as part of the disposition of Technical Error Reports (TERs) per AP-15.3Q, *Control of Technical Product Errors*.

Internal TSPA-LA model changes (e.g., change in model logic to set scenario-case specific parameters) will be identified as part of TSPA-LA model development. Changes within the TSPA-LA model development scope and schedule will be approved by the TSPA Department Manager. If the changes are outside the TSPA-LA model development scope and schedule the TSPA Department Manager will elevate the issue to the Performance Assessment Strategy and Scope Manager for resolution. Management approval of changes to the TSPA-LA model will also be predicated on whether the change is necessary to comply with regulatory requirements, if final input feed date has passed for the requested change, or if the TSPA-LA model itself has been finalized or "frozen" for TSPA-LA.

Changes to the TSPA-LA model will be tracked by the TSPA Department. An example form that may be utilized to track the changes is shown in Figure 6.2-2. A similar form is included in the previously mentioned controls and guidance document under development. When the model is in the development stage, written approval from the TSPA Department Manager, TSPA Model Calculations Lead, and TSPA Configuration Management Lead is required for TSPA analysts to change/introduce new process models, model abstractions, or parameters into the TSPA-LA model. The written authorization will specify the source(s) (e.g., AMRs, DTNs, etc.) from which process models, model abstractions, or input parameters are to be taken. If only draft source(s) are available, this will be noted in the authorization.

Changes to TSPA-LA model for the purpose of performing sensitivity studies or other analyses of the TSPA-LA model also require written approval from the TSPA Department Manager, TSPA Model Calculations Lead, and TSPA Configuration Management Lead.

Another important aspect of the control of the TSPA-LA model is to ensure consistent, well-documented inputs. The supporting organizations provide abstractions, and technical product output to the TSPA-LA model. What this content is expected to be was initially determined in a scope and schedule review conducted in early 2002. The scope and schedule reviews were lead by the Performance Assessment Scope and Strategy Subproject and resulted in addition of detail to the Technical Work Plans for each Work Package containing an AMR. The detail was incorporated into revisions to the Technical Work Plans, which specified content for FEPs, ACMs, parameters and uncertainty to be supplied to the TSPA-LA model.

The detailed plan for the systematic treatment of uncertainty in support of the LA products is intimately linked to this overall strategy of placing more management emphasis and control on the development of inputs to the TSPA-LA and the LA itself. These additional product management emphasis and controls include:

- A consistent model hierarchy and structure that feeds the TSPA-LA model architecture
- A consistent treatment and documentation of model abstractions that support the TSPA-LA
- A consistent treatment and documentation of ACMs
- A consistent treatment and documentation of FEPs that are included in the TSPA-LA as well as how they have been included and where their inclusion has been documented
- A consistent evaluation of the definition and performance of the barriers and the basis for the projection of barrier performance
- A consistent evaluation of parameter uncertainty and how that uncertainty is propagated through the model hierarchy to TSPA-LA and how the significance of that uncertainty is evaluated
- A consistent documentation of how the models are integrated and information flows between the models and analyses, including roadmaps of information supporting the TSPA-LA
- A consistent basis for determining the appropriate amount of confidence required for model validation
- A consistent evaluation of what data were used to develop parameter distributions and why those data are sufficient to capture the range of possible observations.

The above emphasis determines much of the content of the AMRs that will support the TSPA-LA and the postclosure safety case to be presented in the License Application. These AMRs remain the primary supporting documentation of the TSPA-LA and the License Application Safety Case as they were in the Site Recommendation document hierarchy. Appropriately assigning this scope, FEP by FEP, model by model, and parameter by parameter into the AMRs has been accomplished in updated Technical Work Plans for each of the supporting AMRs.

The more detailed scope definitions that result from the above process yield a much more consistent and comprehensive treatment of not only parameter uncertainty but also FEP uncertainty and ACM uncertainty. It also allows for early definition of the scope and content of the TSPA-LA within the context of the *TSPA-LA Method and Approach* document as agreed to in several TSPAI KTI agreements. Finally, this more detailed scope definition will allow the AMR authors to focus on the key performance-related aspects of their models and analyses in a more risk-informed way.

6.3 PHYSICAL CONTROL OF FILES

The TSPA-LA model file and its associated input files, DLLs, and database are controlled by storing them in a set of controlled subdirectories on the TSPA file server. Read access to these subdirectories is limited to TSPA Department staff. Write access is limited to the TSPA Model Calculations Lead, the TSPA-LA Configuration Management Lead, and the System Administrator.

Input files for the TSPA-LA model will be obtained from TDMS and stored in a controlled subdirectory on the TSPA file server. A baseline list of files is established by the TSPA-LA Configuration Management Lead. Any subsequent changes to the input files are documented as changes to the baseline list and are initialed and dated by the TSPA Model Calculations Lead and the TSPA-LA Configuration Management Lead.

DLLs for the TSPA-LA model are obtained from SCM, and are installed in a controlled subdirectory on the TSPA file server by the TSPA-LA Configuration Management Lead. A baseline list of DLLs is established by the TSPA-LA Configuration Management Lead. Any subsequent changes to the DLLs are documented as changes to the baseline list and are initialed and dated by the TSPA Model Calculations Lead and the TSPA-LA Configuration Management Lead.

Input parameters (both certain and uncertain) for the TSPA-LA model are controlled by the TSPA Inputs Database. The database is stored in a controlled subdirectory on the TSPA file server.

Completed TSPA-LA model cases are stored in a controlled subdirectory on the TSPA file server. Also, any post-processed results, plots, additional calculations or documentation to support a given case or set of cases will be stored in a controlled subdirectory on the TSPA file server.

6.4 CHANGE CONTROL AND CHECKING

Approved changes to the TSPA-LA model are documented in a conceptual description of the changes, a checklist of the changes to the model, and a change log generated by the GoldSim code. The conceptual description provides an overview of the changes that are to be incorporated into the model. It also contains documentation of any development and testing work that was performed to support the change to the TSPA-LA model. The checklist documents the specific changes made to the model. The change log provides a record of what changes were actually made to the GoldSim model file. The conceptual description, checklist, change log, and TSPA-LA model file are all checked to verify that the changes are correctly implemented into the TSPA-LA model.

A change to TSPA inputs is also documented in the TSPA Inputs Database.

Checking is performed by a qualified individual (assigned by the TSPA Model Calculations Lead), usually another TSPA analyst, who was not involved in modifying the controlled model file or input file(s).

Two types of checks are done on a model; parameter-level checking and conceptual model checking. Parameter-level checking verifies that all of the changes to the model file and/or external files were done correctly. Conceptual model checking considers whether the implementation in the model correctly reproduces the conceptual model (process model or model abstraction) in the associated AMR, model, or scientific analysis.

Parameter-level checking will be documented in a checklist similar to Figure 6.4-1. The steps involved in this check include:

- Check changed/added GoldSim elements against their source information to verify that they were changed correctly.
- Verify that the input links of added elements are correct.
- Verify that the output links of added parameters are correct.
- Check that the links to and from any deleted elements have been appropriately reconnected.
- Verify (by inspecting source references for changes) that each change to an external file is correct.
- A full multiple-realization run of the model will be performed. The results of this run will be evaluated to verify that the correct changes were made to the model.

The conceptual check considers whether the changes to the model correctly reflect the conceptual model changes. The conceptual description should include a general description of the changes made to the model. Any development and testing work to support the changes should also be documented in the conceptual description. General questions that the conceptual check should answer (if applicable, if not applicable then so note) include:

- Does the modified portion of the model respond appropriately to its inputs?
- Do the model components downstream from the modifications respond appropriately?
- Are model inputs and outputs within their specified ranges?
- Can the final dose results be explained in terms of upstream parameters (e.g., waste package/drip shield failure curves, seepage flow, pH, solubilities, EBS release rates)?
- Did the modification(s) invalidate an upstream or downstream conceptual model?
- Is mass conserved within each major subsystem?
- Is energy conserved within each major subsystem?
- Can each entry in the GoldSim run log be shown to have no/negligible impact on the run?
- Is the model implemented correctly for each scenario class?

Any differences between the results of the initial and modified case should be explained and properly documented by the checker in terms of the changes made to the model.

If preliminary AMRs and DTNs are initially used to implement a LA process model/abstracting into the TSPA-LA model, an additional back-check will be made to ensure that the TSPA implementation is consistent with the final AMRs and DTNs.

6.5 MANAGING TSPA-LA MODEL INPUTS (TSPA INPUT DATABASE)

TSPA-LA model input parameters (excluding simulation settings and TSPA system parameters) will be managed by the TSPA Input Database. The database will be developed in Microsoft-Access. The database will not perform any calculations or logical evaluations, rather it strictly acts as a central storage location from which input parameters are downloaded into the GoldSim TSPA-LA model file.

Input parameters will be manually extracted from DTNs stored in the TDMS. The parameter entry forms in a DTN will be used to locate the parameters in the DTN. Input parameters which are accepted data (e.g., atomic weights, radionuclide half-lives, etc.) will be manually extracted from a controlled source. Parameters entered into the database will be checked and verified against their source.

Since the TSPA Input Database is part of the overall TSPA-LA model, it will be developed, controlled, and documented in the same manner as the other parts of the TSPA-LA model.

Figure 6.5-1 illustrates the information flow between TDMS, the TSPA file server, and the TSPA Input Database.

A set of input parameter tables based on the database inputs will be developed as part of the TSPA-LA Model Document. Appendix F contains an example table which illustrates the information to be captured.

6.6 CONTROL OF TSPA-LA MODEL RESULTS

TSPA-LA model results consist of the completed TSPA model simulation files (i.e., cases), information extracted from the model (e.g., plots, tables), and post-processed information.

The TSPA-LA model simulations are documented in a readme file that is submitted as part of the DTN for the simulations. The readme file contains descriptions of the simulations, the supporting documentation, the input files and input parameters, and the software used. A flow chart is also provided (either in the readme file or as a separate file in the DTN submission) which illustrates the relationship between the TSPA-LA master case, the TSPA-LA base cases, and the TSPA-LA sensitivity cases.

Plots of TSPA-LA model results will be documented with a checklist (format will be identified in the aforementioned Controls and Guidelines Document under development within the TSPA Department). The TSPA-LA model cases and the model elements from which results are extracted are documented in the checklist. Additional information such as axis labels, time-scales, data-set labels, etc. will also be verified via the checklist (see Figure 6.6-1 for example checklist).

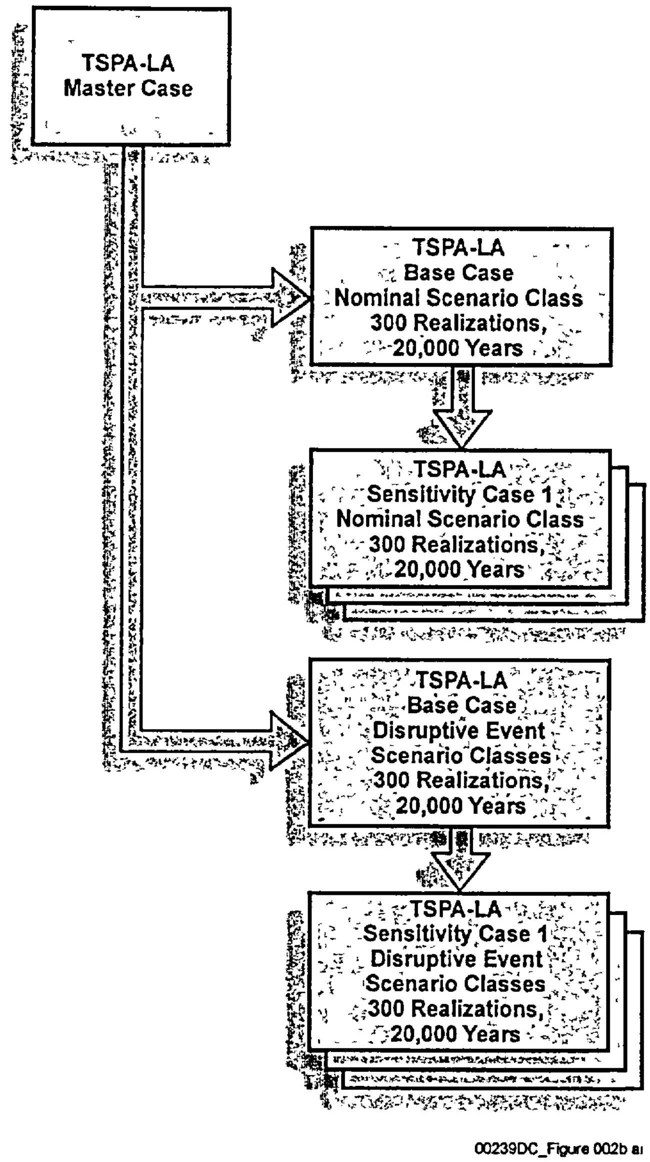


Figure 6.1-1. Example of the Relationship among the TSPA-LA Master Case, Base Cases, and Sensitivity Cases

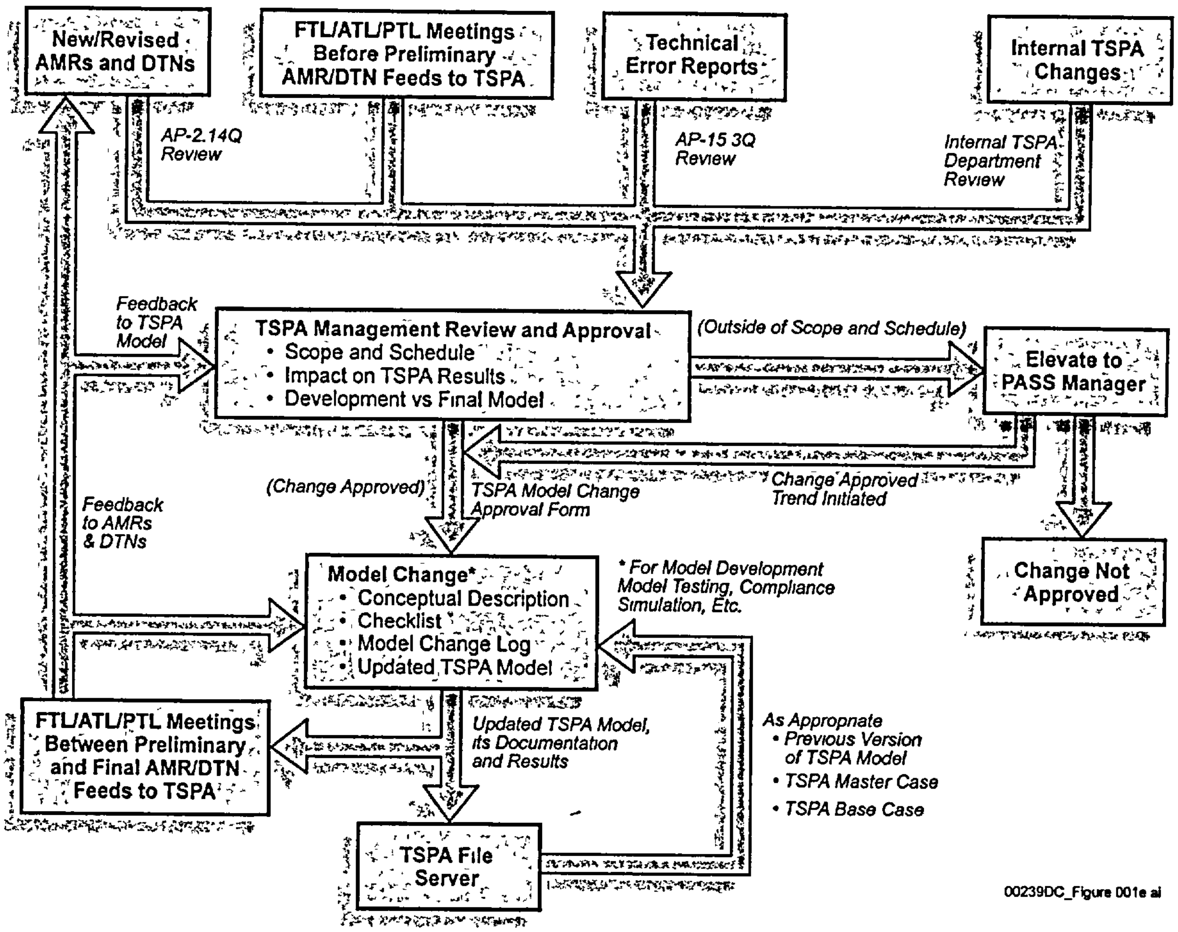


Figure 6.2-1. Flowchart Illustrating the Management Control Process for the TSPA-LA Model

TSPA Model Change Approval Form **QA: ___**

1. Change Number:
2. Basis for Proposed Changes(s)·
3. Description of Proposed Change(s):
4. Expected Date of Change:
5. Is the change after the "frozen" date for the TSPA-LA model? __________
6a Approve Change(s) ________ 6b. Disapprove Change(s) ________
7. Donald A. Kalinich, TSPA Model Calculations Group Lead Signature. Date:
8. John F. Pelletier, TSPA Configuration Management Lead Signature: Date:
9. Jerry A. McNeish, TSPA Department Manager Signature: Date:
10. Peter Swift, PASS Manager (signature required if change is after the TSPA-LA model freeze date) Signature: Date:

Figure 6.2-2. Example TSPA Model Change Approval Form

QA: ___

Case:
Starting Case:

Analyst:
Checker:

Parameter/Element/ Etc.	Location	Description of Change	Source	Checker Initials

Figure 6.4-1. Example TSPA Model Checklist

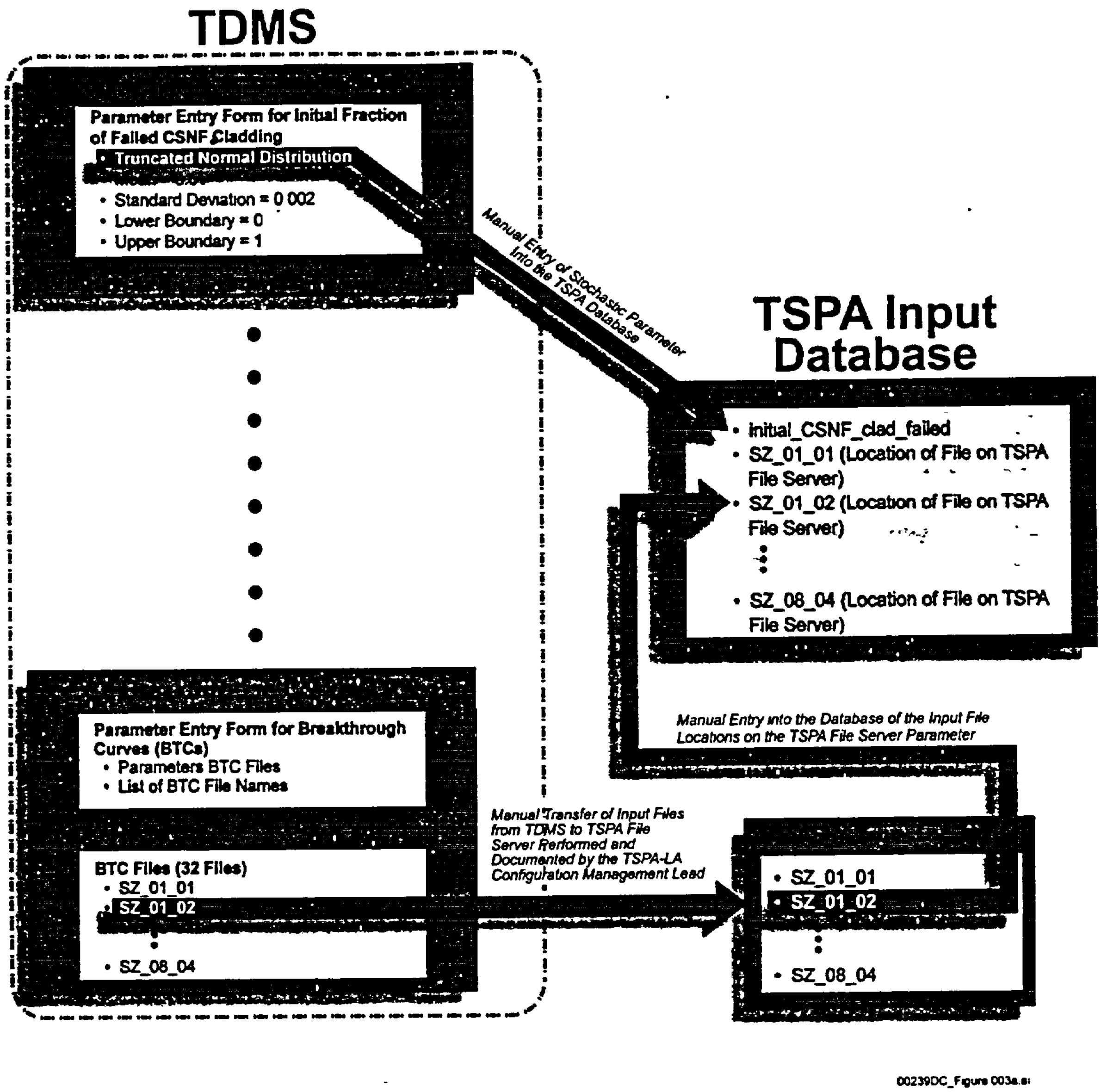


Figure 6.5-1. Illustration of Information Flow among the TDMS, TSPA File Server, and TSPA Input Database

QA: ___

Plot Name:

Analyst:
Checker:

Case	Element Plotted	Data Columns for Plot	Checker Initials

Additional items to check:

Are the time scales correct for each data set?

If the data sets are labeled in the data table, are they labeled properly?

Have all cases plotted been noted on the plot?

Is the name of the plot file noted on the plot?

Are the axis labels correct?

Is the legend correct?

If appropriate, is the plot disclaimer shown?

Figure 6.6-1. Example TSPA Plot Checklist

7. TSPA-LA MODEL VALIDATION

Validation of the TSPA-LA model is an important part of developing understanding and confidence in the model. It is important to note that validation refers to models, whereas verification refers to computer codes used to implement these models. Only the former is discussed in this section. Overall, the validation process is implemented and controlled by AP-SIII.10Q, *Models*.

This section provides an overview of the key aspects of the TSPA-LA model and its validation, including specific actions to be taken to enhance confidence (Section 7.1 and 7.2) and demonstrate stability and reliability of the statistical aspects of the numerical model (Section 7.3).

7.1 THE MODELING PROCESS: AN OVERVIEW

Validation of a computer model of a physical system involves a series of steps taken during and after the development of the model, designed to generate and enhance confidence in the predictions of the model. The modeling process starts from the modeler's understanding of the true physical system (the reality). A conceptual model is then formulated using simplifications, assumptions and some idealizations, and is translated into a mathematical model and subsequently to a numerical model. An appropriate computer code is selected to implement the numerical model. The inputs to the code are prepared and the code is executed to obtain the model predictions. This process is illustrated in Figure 7.1-1.

7.1.1 Conceptual, Mathematical, and Numerical Models

The first step in generating confidence in the model predictions consists of ensuring that the conceptual model captures the features of the physical system relevant to performance prediction; and that the idealizations, assumptions, and simplifications introduced result in a model that is appropriate for its intended use. In a similar way, the mathematical model should be adequate to represent the key processes in the conceptual model. The process of selection of input parameters and/or data, and the characterization of their associated uncertainties, should be documented in a way that generates confidence in the model development activity. The numerical model should include the proper level of discretization from considerations of precision, convergence, and stability (model calibration). Establishing model-to-reality conformity is the first step in validation. This conformity should be established separately for the conceptual, mathematical and numerical models. Documentation of all considerations leading to the formulation of the conceptual, mathematical, and numerical models and their calibration (in the AMRs), including the justification of assumptions, simplifications, and idealizations, should lend validity to the model formulation stage. Technical review of these models, in their formulation stage, would be considered as a step in the direction of model validation.

7.1.2 Computer Code and Associated Inputs

Converting the numerical model to a set of computer code algorithms is a process that must be transparent and traceable. Links from the numerical model to the computer code should be documented to permit easy checks on input construction. All inputs should be checked, controlled, and documented (see Sections 6.2 and 6.5). This process of checking the computer code construction and the associated inputs aids in establishing the validity of the model during the model-development stage (see AP-SIII.10Q, *Models*, Sec. 5.4.1b). Computer code verification itself, to ensure that the code implements the numerical model correctly, is controlled by AP-SI.1Q, *Software Management*.

7.1.3 Model Predictions: Corroboration with Independent Data

From a strictly computational perspective, a proper numerical model and a correct computer code should result in correct model predictions. However, it is not easy to demonstrate that a numerical model is an adequate representation of the complex physical system. To compensate for this difficulty, the final step in validation requires that the model predictions should be established as plausible and reasonable by corroboration with data from an independent source. This last step may be designated as model prediction validation.

However, the model prediction validation is not a trivial task. In the conventional modeling practice, prediction validation is achieved by comparing model predictions with experimental measurements. However, since these measurements would be impossible to obtain at the temporal and spatial scales of interest for postclosure performance, one or more of the seven alternative approaches listed in Section 5.4.1c of AP-SIII.10Q, *Models*, will be used to demonstrate prediction validation. The seven approaches are listed here for convenience:

- Comparison of model with data (not calibration)
- Comparison of results with alternative mathematical models
- Comparison with data published in refereed journals
- Peer review
- Technical review by independent reviewers
- Comparison of abstraction results to process models
- Comparison of pre-test model predictions to data collected during associated testing.

7.1.4 Different Stages of Model Validation

Based on the steps described above, the model validation activities are shown in Figure 7.1-2. These activities can be formulated as three separate stages, in the logical sequence of: (1) the input, (2) the code, and (3) the outputs of the model. Stage 1 relates to the validation of the model formulation stage including the selection of inputs and addressing the issues of convergence and stability of the model (calibration issues). Stage 2 addresses the mechanical issues of code verification and the construction of error-free inputs. Stage 3 addresses the validation based on the model outputs (predictions). Accordingly, this stage includes both the confidence-building activities recommended in AP-SIII.10Q, Sec. 5.4.1b, and the post-developmental activities by comparison with independent data as recommended in AP-SIII.10Q, Sec. 5.4.1c.

- **Stage 1: Model Formulation Validation/Calibration**–Show that the conceptual, mathematical and numerical models represent the physical system. Document the process of selection of the input parameters and/or data (and their uncertainties). Also, document the numerical model calibration activities to demonstrate the convergence and stability of the model. These steps generate confidence in the model (AP-SIII.10Q, Sec. 5.4.1b).
- **Stage 2: Computer Code and Inputs Verification**–Show that the computer code is verified thoroughly. Show that the input construction is error-free.
- **Stage 3: Model Prediction Validation**–Corroborate the model predictions with data from independent sources (AP-SIII.10Q, Sec. 5.4.1c). This stage includes confidence building activities, such as simplified test cases, as per AP-SIII.10Q, Sec. 5.4.1b. The rationale for combining some of the activities under both Sec. 5.4.1b, and Sec. 5.4.1c of AP-SIII.10Q lies in the fact that they both call for scrutiny of the model outputs. In contrast, Stage 1 scrutinizes the model inputs and model formulation.

When all the above three stages are completed, the model may be considered validated, so that its predictions could be used with confidence in assessing the performance of the physical system.

7.2 THE TSPA MODEL: VALIDATION

7.2.1 Stage 1: Model Formulation Validation/Calibration

The TSPA model is comprised of a linkage of several model components. The supporting AMRs document the validation of the underlying process models and/or abstraction models, including all the three stages cited in Section 7.1.4. In principle, each of these models is already validated before being integrated with the other models under the control of the TSPA-LA model computer code, GoldSim. It would therefore appear that the TSPA model will have *ipso facto* passed through Stage 1 (formulation of the conceptual, mathematical and numerical models) of the validation, subject possibly to a few caveats, as described below.

For example, the documentation for the process of selection of the model component input parameters and/or data, including their uncertainties, will be included in the relevant model document, and not in the TSPA-LA Model Document. However, it is conceivable that the combination of model components coupled together in the TSPA-LA model might generate conditions such that one or more model components produces output beyond the validated range documented in the model document. This will be examined as part of the TSPA model validation effort. Other conditions specific to the TSPA model, such as spatial, temporal, and stochastic discretization, convergence, and stability (see Section 7.3 and Appendix E) should also be checked as part of both development and post-development activities. These and other

TSPA model calibration activities will be documented in the TSPA-LA Model Document. Proposals for demonstrating convergence and stability of the stochastic aspects of the TSPA model are discussed in Section 7.3. A final point is that a few of the TSPA model inputs are specific to the system model, such as timestep length and others (see Section 6.5), and these will be documented in the TSPA-LA Model Document.

7.2.2 Stage 2: Computer Code and Input Verification

The purpose of this stage is to verify the suite of software codes and their associated input files as they implement the integrated TSPA model. Since all the component process models and other abstracted models will be validated for LA through all the stages (as documented in the different AMRs), Stage 2 of validation, (i.e., the code verification) has to demonstrate that all mechanical aspects of integrating the component codes are free from errors. Also, the construction of inputs within GoldSim must be shown to be error-free (see Section 6, also).

Step 1: Verification of the Integrated System Computer Code: GoldSim–The integrated system code, GoldSim, is fully verified by the code vendor, Golder Associates. It will also be qualified for use in TSPA in accordance with AP-SI.1Q, *Software Management*.

Step 2: Verification of DLLs as Single Modules in GoldSim–Some of the abstraction models within the TSPA-LA total system model will be implemented as DLLs, which are separately compiled and linked modules or subroutines that can be called by GoldSim—good examples being the waste package degradation software module WAPDEG and the UZ transport software module FEHM. The DLLs will be qualified by their developers, both from the standpoint of being correct representations of their underlying conceptual and mathematical models, and in terms of their mechanical operation as a DLL. Since the ability to properly call DLLs is a feature for which the GoldSim is qualified, DLLs qualified as previously described will, by default, be qualified to be called from within the TSPA-LA GoldSim model file.

Step 3: Verification of DLLs in the Integrated Model–There are two aspects to verification of all of the TSPA DLLs in the full TSPA-LA model. The first deals with the potential of two or more DLLs to conflict with each other in terms of memory requirements, duplicate input or output file unit numbers, etc. The second regards the potential interactions between DLLs (e.g., an output file generated by DLL "A" is used as an input file by DLL "B"). The appropriate test cases will be run and documented during model development to ensure that these types of verification issues are properly resolved.

Step 4: Verification of Inputs–Inputs to the TSPA model are controlled by the TSPA Input Database (see Section 6.5). Input parameters will be manually extracted from DTNs stored in the TDMS. The parameter entry forms in a DTN submittal will be used to locate the parameters in the DTN. Parameters entered into the TSPA Input Database will be checked and verified against their source DTNs.

Step 5: Verification of Single Model Components–The model components in the integrated TSPA model will have already been validated prior to implementation into the TSPA model.

Verification of proper implementation in the TSPA-LA model will be performed for each model component.

Step 6: Verification of Coupling between Model Components–The information transfer between connected model components will be verified. At this point, with the individual model components also validated and verified, it logically follows that the combination of coupled models are verified and validated.

7.2.3 Stage 3: Model Prediction Validation

Prior to this stage of validation, the input construction, the coupling of the model components, and the internal data transfers are all proven to be correctly handled in the TSPA model. The final phase of validation involves comparing model predictions with independently collected data.

Since, in general, the data cannot be observed on the real system (i.e., the combined natural and engineered systems modeled in the TSPA) at the times of interest (e.g., at 10,000 years after repository closure), conventional validation methods may not be applicable. One or more of the seven approaches recommended in AP-SIII.10Q, *Models,* and listed in Section 7.1.3 will be utilized for model prediction validation, as described in Section 7.2.3.2 below. Of these seven, the candidates to be used for the TSPA-LA model are: (1) comparison with alternative mathematical models, and (2) technical review by independent reviewers.

7.2.3.1 Confidence-Building Activities

Prior to the post-development validation activities using the approaches in Section 5.4.1c of AP-SIII.10Q, *Models*, a series of confidence-building activities will be performed, as indicated in Section 5.4.1b of AP-SIII.10Q, *Models*. These activities include such things as simple test cases (simplified inputs), analysis of selected deterministic realizations (e.g., a "median-like" realization), sequential "one-on" barrier analysis, and barrier neutralizations. These types of simulations help to test the different model components and their interactions within the total system model and they offer an enhanced understanding of the performance of the system and its parts, including an understanding of causal relationships, which in turn generates confidence in the entire TSPA model.

Simplified Test Cases–A sequence of simplified TSPA model components will be developed and tested within the framework of the TSPA-LA total system model. For example, at one extreme, one may consider a single waste package, with a failure resulting in a "constant" release rate of a single radionuclide, over a specified duration. The released radionuclide can be tracked through the different components (the EBS, UZ, and SZ) and mass conservation can be demonstrated. It is possible for this special case to check the model predictions with either alternative analytical solutions, or "back-of-the-envelope" calculations. Based on these results, the credibility of model predictions can be established. Table E.1-2 provides some examples of the model simulations in this category.

Single Deterministic Realizations: Median- and Higher-Dose Realizations–The compliance measure for Yucca Mountain is a mean time history of the repository performance averaged over multiple possible futures of the system performance (preamble to 10 CFR Part 63 (66 FR 55732 [156671], p. 55752)). Recognizing that cause-effect relationships are sometimes difficult to discern from such a "composite" measure of performance, several individual deterministic realizations will be evaluated to explicitly demonstrate causality in the total system model. Specifically, a single realization close in value to the median-dose time history (based on the multiple-realization runs) will be scrutinized and the releases from the components will be rationally explained. A study of the cause-and-effect relationships among key model components will be presented. This technical narrative should generate additional confidence in the TSPA model. A similar presentation will be made for a realization close in value to the 95th percentile (higher-dose) time history. The last entry in Table E.1-2 refers to this type of simulation.

Sequential One-On Barrier Simulations–These are stylized analyses that are designed to show understanding of system behavior and relative contribution of various barriers. The purpose of these analyses, similar to Electric Power Research Institute (EPRI)'s Hazard Index analyses (EPRI 2002 [158069]), is to provide rough, quantitative estimates of the importance of various barriers and processes (or combinations thereof) in reducing the potential hazard due to the emplacement of radioactive wastes at Yucca Mountain. The approach is to artificially "turn off" the function of all barriers and processes initially, and then add them back sequentially in some logical order (e.g., waste form barriers first, natural barriers second, and engineered barriers last). These studies are expected to offer an in-depth understanding of the system and thus build confidence in the validity of the TSPA-LA model.

Table E.3-1 contains examples of one set of sequential one-on barrier/FEPs simulations for the nominal scenario class. Additional one-on simulations may be run for the igneous groundwater release scenario and the seismic scenario class. Also, the barriers/FEPs could be added in a different sequence, and different treatments of the barriers/FEPs could be considered.

Barrier/Process Neutralizations–In a neutralization analysis, the fundamental idea is to examine the extent to which performance of the overall system is degraded if the ability of a given barrier to perform as expected is compromised. As such, the approach precludes reliance on complete knowledge of any one process. This increases confidence that the postclosure performance objectives, as specified in the regulations, will be met.

The TSPA-LA model will first be evaluated for the base case with all the barriers performing as expected (including their uncertainties). In the next step, each barrier is neutralized one at a time (i.e., the barrier is assumed to be absent and/or performing at very pessimistic levels). In other words, the barrier is physically in place, but its ability to retard and/or attenuate water and/or radionuclide movement is completely ignored. The performance of the neutralized system is computed and compared against that of the base case.

Examples of barrier/process neutralization simulations are provided in Table E.4-1. They would be performed for both the nominal and igneous groundwater release base cases. Barrier/process neutralization simulations may also be developed for the igneous eruptive release and seismic modeling cases. Also, different ways of neutralizing the barriers/processes could be considered, and additional processes/barriers could be considered.

As in the case of sequential one-on analyses, these studies are expected to offer an in-depth understanding of the system and thus build confidence in the validity of the TSPA-LA model.

7.2.3.2 Model Prediction Validation Approaches

This section describes in more detail some of the approaches that may be used from Section 5.4.1c of AP-SIII.10Q, *Models*—the "post-development validation activities."

Comparison with Alternative Models–The TSPA-LA model predictions may be compared directly to similar results from other well-established models, such as EPRI's IMARC model (EPRI 2002 [158069]) and NRC's TPA model (NRC 1999 [152183]), if they are updated to the TSPA-LA model inputs (as per AP-SIII.10Q, Sec. 5.4.1c). The uncertainty range for dose results from the DOE TSPA and the EPRI and/or NRC models could be compared, if the corresponding inputs are similar. The comparison is not currently applicable to the DOE TSPA-LA model (still under development), but could be made with a precursor model such as the TSPA-SR or TSPA-FEIS model that may have formed the basis for either a published EPRI model or a published NRC model. A cdf, pdf, or box plot for dose from these various models could be compared. A reasonable overlap may be considered to provide further evidence of the validity and/or robustness of the DOE TSPA model predictions. In order to use such a comparison based on the TSPA-SR or TSPA-FEIS models, for validation of the TSPA-LA model, it would be necessary to evaluate how much had changed from the earlier TSPA model to the TSPA-LA model, to see how much significance could be placed in this comparison.

Technical Review–Another method of validation is to subject the model predictions to an intense scientific review (technical review per AP-2.14Q), where the reviewers study the model and its predictions critically and identify any "implausible" results or loop-holes in the analysis and offer suggestions to correct those situations. This type of careful scientific scrutiny will be used as a validation methodology.

It should be mentioned that the TSPA-SR method, which is a precursor to the TSPA-LA, has been subjected to a peer review by an OECD/NEA-IAEA International Review Team (OECD and IAEA, 2002 [158098]). To quote from their findings:

> "...the TSPA-SR methodology is soundly based and has been implemented in a competent manner...Overall the IRT considers that the implemented performance assessment approach provides an adequate basis for supporting a statement on likely compliance within the regulatory period of 10,000 years..."

The International Review Team also recommended a number of improvements and changes to result in more confidence and robustness in the TSPA model. Given the favorable review by an international review panel, this should generate confidence in the validity of the TSPA-LA model, which will evolve from the TSPA-SR model.

7.3 STABILITY AND RELIABILITY OF TSPA MODEL RESULTS

In TSPA-LA, Latin hypercube sampling (LHS) (McKay et al. 1979 [127905]) will be used in the propagation of uncertainty. This sampling technique has been selected, as in past TSPAs, because of the efficient manner in which it stratifies across the range of each uncertain variable and the observed stability of uncertainty and sensitivity analysis results obtained in past applications of LHS in performance assessments for complex systems (McKay et al. 1979 [127905]; Iman and Helton 1991 [159039]; Helton 1999 [159042]). Here, stability relates to how much variability takes place in the outcome of interest as the model results are repeatedly calculated with different samples. Theoretical results indicate that, under certain conditions, LHS does indeed exhibit better statistical convergence properties than random sampling (McKay et al. 1979 [127905]; Stein 1987 [159060]). However, these results are difficult to apply in practice. As a result, a practical method of assessing the stability of results obtained with LHS is needed.

The main issue regarding stability of the TSPA model results is whether enough Monte Carlo runs have been performed to adequately quantify the uncertainty in the dose estimates. The OECD-IAEA International Review Team expressed concern on this issue (OECD and IAEA 2002 [158098]). The NRC identified the stability of the TSPA model results as a Key Technical Issue (KTI) agreement item (i.e., TSPAI 4.03 (Meserve 2001 [156977]), as described in Appendix B). Section 4.2.1.4 of the *Yucca Mountain Review Plan* (CNWRA 2002 [158449]) specifically mentions the stability of the TSPA-LA model results as an acceptance criteria, stating:

> "A sufficient number of realizations has been obtained, for each scenario class, using the total system performance assessment code, to ensure that the results of the calculations are statistically stable."

Another concept associated with the probabilistic model calculations is the reliability, or confidence, in the mean dose estimates. The stability and reliability of the TSPA-LA results, produced to demonstrate regulatory compliance, are important to validation and confidence building (as per AP-SIII.10Q, Section 5.4.1b) and are the subject of the discussion presented in this section. For the purposes of this discussion of statistical convergence of TSPA-LA model results, the following definitions will be used:

- **Stability** – refers to the sensitivity of expected dose to sample size, and is therefore a reflection of the "accuracy" of the Monte Carlo simulation methodology.

- **Reliability** – refers to the uncertainty in estimates of the expected dose, and is therefore a reflection of the "precision" of the Monte Carlo simulation methodology.

The stability question can be answered by running the model multiple times with a different number of realizations each time, and examining the convergence behavior of the expected dose. The reliability question can be answered by computing the confidence intervals for the estimated value of expected dose.

The exact approach to be used for investigating stability and reliability of the TSPA-LA model has not been finalized. However, some of the techniques under consideration are described in the following sections. These techniques are drawn from previous TSPA studies, other radioactive waste performance assessment programs (e.g., Waste Isolation Pilot Plant (WIPP), Atomic Energy of Canada, Ltd (AECL)), as well as the probabilistic risk analysis literature.

7.3.1 Tests for Stability

As noted earlier, stability refers to the sensitivity of model results to sample size. Quantification of the stability of model results involves carrying out multiple model runs with a different number of realizations each time, and examining how the computed outcomes appear to converge on some constant value. Note that this is the value that would have been obtained with an infinite number of realizations. However, practical considerations allow only a finite number of realizations to be used – hence the need to deal with the issue of stability or statistical convergence.

Approaches proposed for evaluating the stability of model results involve graphical comparisons of model output at various sample sizes, performing statistical tests to evaluate if the expected dose obtained with two different sample sizes are the same or different, and performing statistical tests to evaluate if the distributions of dose obtained with two different sample sizes are the same or different. These approaches are briefly summarized below.

(a) Graphical comparison - The simplest test for stability involves examining a graph of the computed model outcome (e.g., expected dose) versus sample size. Alternatively, for time-dependent problems, the model outcomes for different sample sizes can be overlain on the same graph to facilitate a comparative analysis. This is the approach followed in TSPA-SR, where a visual examination of results was performed to assess whether an adequate number of realizations was performed. Specific percentiles (e.g., 5th, 50th, 95th percentiles) of the output data were calculated for a suite of model runs and compared. The suite of model runs included 300-, 500-, and 1000-run simulations of the nominal TSPA model. In addition, several 300-run simulations were performed with different random seed numbers for the LHS sampling. As pointed by the NRC and others (e.g., KTI agreement TSPAI 4.03 (Meserve 2001 [156977]); OECD and IAEA 2002 [158098]) such simple tests need to be supplemented by quantitative measures to define the adequacy of the number of model runs in the TSPA calculations.

(b) Testing for difference in mean - The difference in mean doses obtained from samples of two different sizes can be tested for statistical significance. The difference in the mean dose can be small, but can be significant, if the sample size is large. Similarly, the difference can be large, but not significant, if the sample size is small. A quantity that measures the significance of the difference of means is based on the standard error (sample standard deviation divided by the square root of the sample size). The standard error measures the accuracy with which the sample mean estimates the "true" mean. In this approach, a Student-t is computed based on the standard error of the difference of the means (Press et al. 1992 [103316]) and the significance of the difference is evaluated, using the t distribution. An appropriate level of significance (e.g., 1% or 5%) is chosen to ensure that the means are not significantly different. A significant difference between the means suggests that the smaller sample size, and possibly the larger sample size as well, is providing an inadequate estimate of the mean.

(c) Testing for difference in distributions: In order to assess if two different distributions are statistically alike, i.e., there is no significant shift in the magnitude of the values of the distributions (i.e., larger or smaller values), a statistical ranking test may be performed. One such test is the Wilcoxon Rank Sum test (Walpole et al. 1998 [152180])). In order to apply the Wilcoxon Rank Sum test to evaluate the similarities between two distributions (e.g., 300-run vs. 1000-run simulations at a particular output time), the two data distributions are combined and ranked from lowest to highest values. Next, the rankings from one of the two distributions are summed. The rank sum is then used in a mathematical formulation to compute a Z statistic, which is compared to a tabulated Z statistic for an assumed significance level to determine if the distributions are statistically different or alike.

The two tests described above for verifying whether the means are similar and whether the distributions are similar can also be used in conjunction with the methods described in the next section (for estimating the confidence in estimates of the mean) to provide a consistency check on the identification of the smallest sample size that appears to produce statistically stable estimates of the expected dose.

7.3.2 Tests for Reliability

To assess the reliability, or confidence, in the mean dose results, it is appropriate to calculate confidence intervals about the mean. Uncertainty in the mean of a distribution, which is caused by the use of a finite sample size can be represented by a sampling distribution (Cullen and Frey, 1999 [107797]). A variety of methods are available for characterizing uncertainty in the sample mean of a distribution, each based on a different assumption regarding the sampling distribution. Some of these methods are discussed next, and address KTI agreement TSPAI 4.05 (Meserve 2001 [156977]).

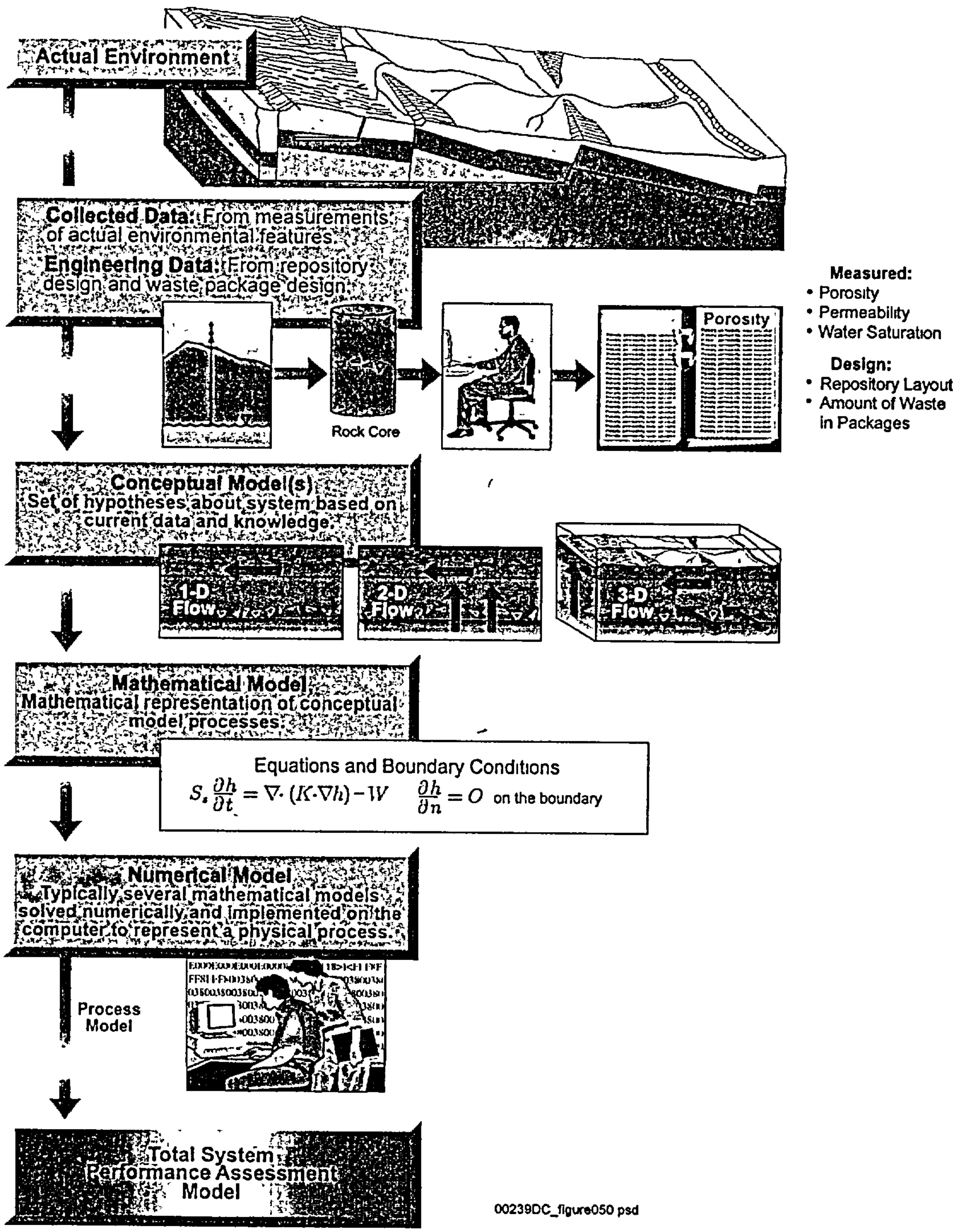
(a) Central limit theorem – A well-known result from statistics, the central limit theorem, states that if the sample size, n, is reasonably large, no matter what the distribution of x, the sample mean will be approximately normal (Benjamin and Cornell, 1970 [110221]). Once the mean and its standard deviation have been computed, estimates of reliability (such as 95% confidence intervals) can be obtained using the properties of the normal distribution.

(b) Sub-sample analysis – In this approach, the sample set is divided into a smaller number of sub-samples, and the mean computed for each of these sub-samples. Thus, an approximation of the sampling distribution of the mean is created. Next, the mean of the means, and the standard deviation of the means, is used in conjunction with the properties of the t-distribution to obtain the 95% (or any other desired) confidence interval. Such an approach was used in the 1994 AECL performance assessments to determine the confidence associated with the expected dose at selected points in time (Goodwin et al. 1994 [124152], Section A.3.5). It should be pointed out that a random sampling scheme was used in the AECL performance assessment study, as compared to the LHS scheme to be used in TSPA-LA.

(c) Replicated sampling – A replicated sampling procedure developed in the NRC's high level waste program at SNL provides an effective approach to estimating the potential sampling error in quantities derived from LHS (Iman 1982 [146012]). With this procedure, the LHS is repeatedly generated with different random seeds. These samples are used to produce a sequence of values for the expected dose, from which its mean and standard error are computed. Confidence intervals for the expected dose can then be estimated with the *t*-distribution. The appropriate value for the number of replicates cannot be known with assurance before an analysis because the size and location of the resultant confidence interval will depend on both the mean and standard error. For example, a much wider confidence interval might be acceptable if the expected dose was much less than a regulatory outcome of concern than would be the case if it was close to a regulatory outcome of concern. In practice, a reasonable computational strategy is to start with a small number of replicates (e.g., 3-5), and then add additional replicates if the initial confidence interval is too close to an outcome of concern.

(d) Bootstrap – Bootstrap simulation is a numerical procedure for simulating the sampling distribution and estimating its mean, standard deviation and confidence intervals associated with such quantities. Cullen and Frey (1999 [107797]) describe the percentile-bootstrap method, known as bootstrap-*p*, to estimate confidence intervals for the mean of a distribution. Given a data of sample size *n*, the general approach in bootstrap simulation is to: (1) assume a distribution which describes the quantity of interest, (2) perform *r* replications of the data set by randomly drawing, with replacement, *n* values, (3) calculate *r* values of the statistics of interest. In step 1, parametric models such as normal or log-normal distributions can be used to fit to the data, or the empirical distribution can be sampled by assuming that the data can be described by a cumulative distribution that is piecewise linear between each data point, or the actual data set itself can be resampled. Furthermore, confidence intervals for the mean can be readily obtained from the *r* values that form an approximation of its sampling distribution.

(e) Non-parametric bounds – When the underlying population distribution is not normal and a small sample of the distribution is available, then the normal distribution may not be a good approximation of the sampling distribution of the mean. A non-parametric method that has been used to compute confidence intervals, which does not require that the data are normally distributed, is the Tchebycheff inequality. Here, the confidence intervals around the mean are taken to be plus or minus some multiple of the standard error. However, the Tchebycheff method produces significantly larger estimates of the confidence limits as compared to the normal distribution. An improvement on the Tchebycheff inequality was developed by Guttman (Woo 1989 [159073]). The multipliers for the Guttman inequality method are larger than the normal bound coefficients, but significantly smaller than the Tchebycheff coefficients. For instance, at a 95% confidence bound these multipliers for the normal, Guttman, and Tchebycheff methods are 1.96, 2.68, and 4.47, respectively. The Guttman inequality can be used to provide bounds on the confidence limits generated with such methods as the bootstrap or replicated sampling which attempt to recreate the sampling distribution.



Source: DOE 1998 [100550], Figure O-2

Figure 7.1-1. Generalized Performance Assessment Approach

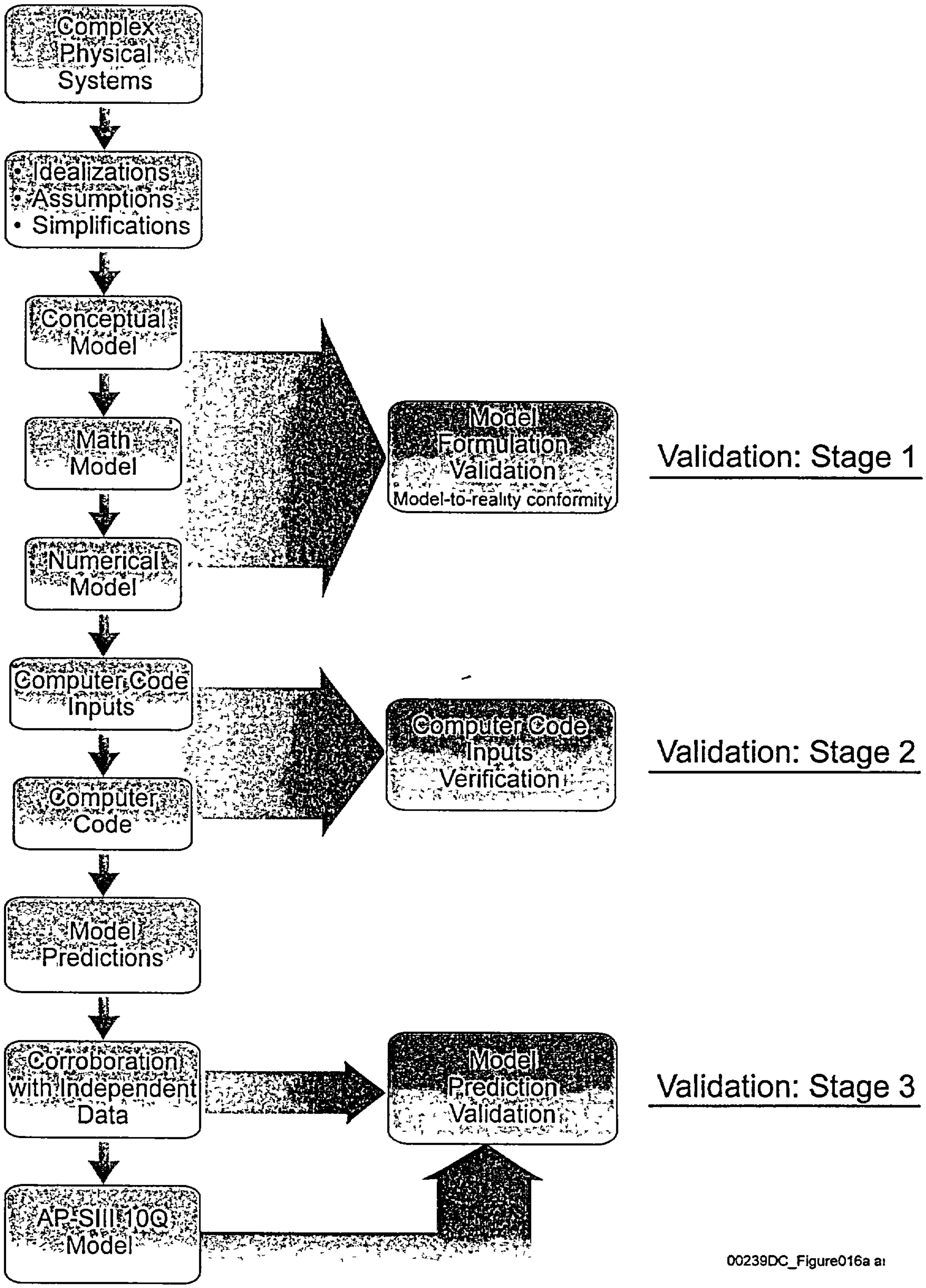


Figure 7.1-2. Model Validation Stages

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8. TSPA-LA ANALYSES

The analysis of the TSPA-LA will cover three broad topics. It will describe the uncertainties inherent in the model and how they are manifested in the results. This approach is described in Section 8.1. It will evaluate the sensitivity of the model through a variety of techniques. This approach is described in Section 8.2. The analyses will also support the development of a description of barriers and their capabilities from the perspective of the TSPA-LA model. This aspect, which is also important to satisfying the 10 CFR Part 63 requirements, is presented in Section 8.3. These analyses will be documented in detail in the TSPA-LA Analysis Document, a draft outline for which is provided in Appendix D.

8.1 APPROACH TO UNCERTAINTY ANALYSES

The probabilistic framework underlying the TSPA-LA calculations is based on the regulatory requirements described in Section 1.3. Briefly, multiple calculations will be carried out for each of the scenario classes described in Section 4, using sampled values of parameters representing the expected uncertainty range, to calculate the expected dose required for compliance analysis as per 10 CFR Part 63. The suite of simulations that will form this calculation set are presented in Appendix E. In this section, the focus is on the approach for describing the base-case simulation results. The base-case simulations are probabilistic calculations, carried out separately for each of the nominal, igneous and seismic scenarios classes. These simulations will be carried out in two steps: (a) covering the 0 to 10,000 year regulatory time period with results to be documented in the License Application, and (b) covering the 0 to 20,000 year period to demonstrate that the model results have no major changes after the regulatory time period. The methodology for interpreting results of these simulations is described below.

8.1.1 Nominal Scenario Class

The nominal scenario class contains a single modeling case that is composed of the set of expected FEPs, as determined by a formal FEP screening procedure described in Section 3.2.2. The nominal scenario class for TSPA incorporates the important effects and system perturbations caused by climate change and repository heating that are projected to occur over the 10,000-year compliance period.

The principal model components of the TSPA-LA, listed in the general order information is passed from model to model (as shown in Figure 5-2), include:

- Unsaturated zone flow
- Engineered barrier system environment
- Waste package and drip shield degradation
- Waste form degradation and mobilization
- Engineered barrier system flow and transport
- Unsaturated zone transport

- Saturated zone flow and transport
- Biosphere.

The nominal scenario class exercises these component models to describe the anticipated sequence of processes that are expected to occur during the lifetime of the proposed repository. A more detailed description of the processes included in the nominal scenario class can be found in Section 5.1.

Results of the nominal scenario class will be analyzed at the total-system and the subsystem level. Analyses of total system results will be based on the expected dose metric, and will include analysis of one or more of the following:

- Time history plots of the expected dose, along with running 5^{th}, 50^{th}, and 95^{th} percentile curves. Dose-time history from all of the individual realizations will also be presented in the form of a "horsetail plot"
- Key radionuclides and their contributions to expected dose
- Side-by-side histogram of dose at selected times, showing the temporal evolution of dose distribution and the frequency of extreme outcomes
- Side-by-side histogram of time to reach specified dose, showing the performance of the system in comparison to regulatory dose and time limits.

Analyses of subsystem results will be based, among other things, on metrics related to the integrity of engineered components and will include analysis of one or more of the following:

- Cumulative drip shield failures
- Cumulative waste package failures
- Waste package opening area
- Water flow rates into drift, through the drip shield and into waste package
- Fractional cladding failures.

Additional subsystem metrics include those related to the movement of radionuclides through the system, such as:

- Mean release rates for a variety of key radionuclides representing different combinations of sorption potential and solubility characteristics. These results may be presented for the waste form, the waste package, EBS, UZ, and SZ subsystems.
- EBS release rates may be further analyzed in terms of release process (e.g., advective versus diffusive) and waste types (e.g., CSNF and codisposal waste).
- UZ and SZ releases may be further analyzed in terms of spatial discretization (e.g., infiltration bins) and spatial location (e.g., mass collection regions).

Figures 8.1.1-1 through 8.1.1-12 present illustrations of how the performance of the total system and various subsystems will be represented to highlight the various metrics discussed above. These analyses will be carried out in terms of the expected value of the appropriate metric. In addition, the spread around the mean for each of the metrics will be presented at selected times in the form of side-by-side box plots to indicate the uncertainty in projected outcomes. Figures 8.1.1-1 through 8.1.1-12 should not be construed as depictions of actual performance projections, rather they show illustrative examples of how the system response will be graphically presented.

8.1.2 Igneous Scenario Class

The volcanic eruption and igneous intrusion groundwater transport modeling cases are the two igneous activity modeling cases considered for TSPA-LA. These two modeling cases were described in Section 4 and are briefly recounted below.

The volcanic eruption modeling case will consider the direct transport of waste to the ground surface from the repository in a volcanic eruption. This modeling case will begin with an eruptive event, which will be characterized in the TSPA by both its probability and its physical properties such as energy and volume of the eruption, composition of the magma, and properties of the pyroclastic ash (Figure 5.3-1). Interactions of the eruption with the proposed repository will be described in terms of the damage to the EBS and the waste package. Characteristics of the waste form in the eruptive environment will be described in terms of waste particle size. Atmospheric transport of waste in the volcanic ash plume begins with entrainment of waste particles in the pyroclastic eruption and will be affected by wind speed and direction. The manner and details in which waste dispersion will be handled for the eruptive event are currently under review. The final detailed approach will be discussed in the appropriate AMR.

BDCFs will be developed for exposure pathways relevant to atmospheric deposition of contaminated ash, rather than for the groundwater pathways considered for nominal performance. As a final step, the volcanic eruption BDCFs will be used to determine radiation doses resulting from exposure to contaminated volcanic ash 18 km from the proposed repository.

The igneous intrusion groundwater transport modeling case will consider an igneous intrusion that travels down the drifts and remains underground. Although the intrusion damages waste packages and other components of the EBS, FEPs analyses have concluded that it does not significantly alter the long-term flow of water through the mountain (CRWMS M&O 2000 [151553], Section 6.2.16). As shown in Figure 5.3-2, the igneous intrusion groundwater transport model will use information about the probability of intrusion, the characteristics of the intrusion, and the response of the proposed repository to calculate damage to waste packages. Groundwater transport away from the damaged packages will be calculated using the nominal scenario class models, and doses to humans from contaminated groundwater are determined using nominal BDCFs.

Results of the igneous scenario class will be analyzed at the total-system and the subsystem level. Presentation of these results will be similar to the structure presented previously for the nominal scenario class. However, not all elements will need to be presented by virtue of the disruptive nature of the scenario class, which could eliminate certain barriers and/or transport pathways.

8.1.3 Seismic Scenario Class

The seismic scenario class considers seismic hazards that occur near the repository. Although the subsequent ground motion and fault displacement (if screened in) at the repository horizon damages waste packages and other components of the EBS, ongoing FEPs analyses indicate that these seismic hazards will not significantly alter the long-term flow of water through the mountain. This modeling case begins with a ground-motion event, which will be characterized in the TSPA-LA by its mean annual frequency and amplitude (see also Sections 4.3 and 5.3.2). This seismic hazard may cause damage to drip shields, waste packages, and cladding. Radionuclides are then released from damaged waste packages and subsequently transported by the groundwater to the biosphere. Groundwater transport away from the damaged packages will be calculated using the nominal scenario class models, and doses to humans from contaminated groundwater are determined using nominal BDCFs.

Results of the seismic scenario class will be analyzed at the total-system and the subsystem level. Presentation of these results will be similar to the structure presented previously for the nominal scenario class. However, not all elements will need to be presented by virtue of the disruptive nature of the scenario, which could eliminate certain barriers and/or transport pathways.

8.1.4 Combined Results

For compliance demonstration purposes, it is necessary to produce a quantitative result suitable for comparison with the regulatory limit. This requires that the probabilistic calculations of the expected annual dose histories for the nominal and disruptive scenario classes be combined through a probability weighting method, where the contribution of each scenario class to the expected dose is the product of the dose from that scenario class and its probability (the probabilities being as indicated in Table 4-1). This expected annual dose includes the likely performance of the disposal system (the nominal scenario class) and the consequences of unlikely events (disruptive scenario classes).

The probabilistic framework employed for the TSPA-LA calculations will produce multiple histories of annual dose for the nominal scenario class and each of the disruptive scenario classes. A Monte Carlo simulation technique will be used to incorporate uncertainty and variability in the model input parameters by using different vectors of sampled values for each realization. Therefore, results for each modeled scenario will include a separate dose history for each sampled vector. Dose histories for each input vector will be combined to produce a conditional mean dose history for each scenario. The use of the term "conditional" indicates that these are the mean doses expected if the chosen scenario conditions were certain to occur. Because the scenario probabilities partition the probability space, the conditional mean dose histories must be weighted by the scenario probabilities and summed to give the overall expected annual dose history.

8.1.5 Groundwater Protection Analyses

An analysis of groundwater protection will be conducted in accordance with the regulations at 10 CFR 63.331, 63.332, and 63.342. This analysis will consider likely features, events, and processes, i.e., those estimated to have a probability greater than one chance in 10,000 of occurring within 10,000 years of disposal. The analyses may consider some unlikely features, events, or processes, but in no case will they consider features, events, or processes not included in the nominal scenario class (e.g., igneous or seismic scenario classes). 10 CFR 63.331 sets limits on radionuclides in the representative volume of groundwater at the accessible environment for the first 10,000 years after repository closure. The limits for contamination within a representative volume of 3,000 acre-ft of groundwater are defined in terms of activity concentration per unit volume and dose, depending on radionuclide or type of radiation emitted.

Concentration Limits-There are two concentration limits defined. The combined activity concentration limit for radium-226 and radium-228 is 5 picocuries per liter. The gross alpha activity (including radium-226 but excluding radon and uranium) is 15 picocuries per liter. Both of these limits include contribution from natural background radiation sources (10 CFR 63.331) at the location of the RMEI.

In assessing compliance against these standards, TSPA will where possible, use the calculated concentration of the appropriate radionuclides. For those radionuclides included by the standard but not tracked explicitly in the TSPA model, it will be assumed that all progeny are in secular equilibrium with their tracked predecessor to determine their contributions to total activity concentration.

Dose Limit-The dose limit is defined as the total annual dose from the combined beta and photon emitting radionuclides. The limit defined by the standard is 4 mrem (0.04 mSv) per year to the whole body or any organ, based on drinking 2 liters of water per day from the representative volume (10 CFR 63.331). The representative groundwater volume is that which would be withdrawn annually from an aquifer containing less than 10,000 mg/L of total dissolved solids, and centered on the highest concentration in the plume of contamination at the same location as the RMEI (10 CFR 63.332).

TSPA-LA will calculate the concentrations of the contributing radionuclides in the representative volume in a manner consistent with the method used to demonstrate compliance with the groundwater protection standard in 10 CFR 63.311.

In determining compliance with the 4 mrem per year dose limit, the radionuclide dependent parameters will be dose conversion factors (committed dose equivalent per unit intake of a radionuclide) for the whole body and individual organs. These dose conversion factors for the ingestion pathway are provided in Table 2.2 of Federal Guidance Report No. 11 (Eckerman et al. 1988 [101069]). The algorithm used to calculate either the whole body dose or any organ dose is given by

$$D_i = \sum_{all\ j} D_{ij} \qquad \text{Eq. 8.1-1}$$

where

D_i is the annual dose (mrem/year) to whole body ($i=0$) or organ i from drinking two liters of water per day from the representative volume.

D_{ij} is the annual dose (mrem/year) from radionuclide j to whole body ($i=0$) or organ i from drinking two liters of water per day from the representative volume and is given by Eq. 8.1-2:

$$D_{ij} = w \times d \times DCF_{ij} \times C_j \qquad \text{Eq. 8.1-2}$$

where

w is the daily intake of drinking water prescribed in 10 CFR 63.312 (2 liters/day)

d is the number of days in a year (365.25 days/year)

DCF_{ij} is the dose conversion factor from Federal Guidance Report No. 11 (Eckerman et al. 1988 [101069]) for ingestion of radionuclide j for the whole body or individual organ i (mrem/Bq)

C_j is the concentration (Bq/liter) of radionuclide j in the representative volume of groundwater calculated by TSPA as prescribed by 10 CFR 63.332.

Based on Equations 8.1-1 and 8.1-2, the dose limit in Table 1 of 10 CFR 63.331 is

$$D_i \leq 4 \text{ mrem/yr, for all } i \qquad \text{Eq. 8.1-3}$$

TSPA will calculate the annual dose to the whole body and individual organs from the beta and photon emitting radionuclides tracked by TSPA and their decay products. For the radionuclides not tracked by TSPA but included in the groundwater protection standard, it will be assumed that all progeny are in secular equilibrium with their tracked predecessor in order to determine their contributions to annual dose.

8.2 APPROACH TO SENSITIVITY ANALYSES

The TSPA-LA model represents the behavior of a complex system with hundreds of parameters. Many of the parameters are uncertain and/or variable, and their interaction with one another can also be complex and/or highly nonlinear. It is difficult to obtain an understanding of exactly how the model works and what the critical uncertainties and sensitivities are from a simple evaluation of model results. To this end, sensitivity analysis provides a useful and structured framework for unraveling the results of probabilistic performance assessments by examining the sensitivity of the TSPA-LA model results to the uncertainties and assumptions in model inputs.

Sensitivity analysis, in its simplest sense, involves quantification of the change in model output corresponding to a change in one or more of the model inputs. In the context of probabilistic models, however, sensitivity analysis takes on a more specific definition, namely, identification of those input parameters (and their associated uncertainties) that have the greatest influence on the spread or variance of the model results (Helton 1993 [100452]). This is sometimes referred to as global sensitivity analysis or uncertainty importance analysis to distinguish it from the classical (local) sensitivity analysis measures typically obtained as partial derivatives of the output with respect to inputs of interest.

The contribution to output uncertainty (variance) by an input is a function of both the uncertainty of the input variable and the sensitivity of the output to that particular input. In general, input variables identified as important in global sensitivity analysis have both characteristics; they demonstrate significant variance and are characterized by large sensitivity coefficients. Conversely, variables which do not show up as important per these metrics are either restricted to a small range in the probabilistic analysis, and/or are variables to which the model outcome does not have a high sensitivity.

In the context of TSPA-LA, the goal of sensitivity analysis is to answer questions such as:

- Which uncertain variables have the greatest impact on the overall uncertainty (spread) in probabilistic model outcomes?
- How can significant input-output relationships be identified if the association between input-output pairs is nonlinear and nonmonotonic?
- Which are the key factors controlling the separation of model outcomes into higher-dose and lower-dose producing realizations?

TSPA-LA will use regression-based analyses, entropy-based analyses, and classification-tree-based analyses to answer these questions, respectively. Details of each of these methods are described in the following sections. The analyses will be carried out using results from the probabilistic TSPA-LA model calculations at a fixed point in time (e.g., at the time corresponding to the peak of the mean dose during the regulatory period). The sampled inputs corresponding to each of the realizations will be treated as independent variables and the computed outputs will be treated as dependent variables. The outputs can either be total system-level performance measures, such as annual dose rate to a RMEI, or they can be subsystem-level performance measures, such as cumulative radionuclide mass flux at the water table.

8.2.1 Regression-Based Analyses

The goal of regression-based analyses is to build a multivariate linear regression model between the output and the uncertain inputs in order to identify the strength of association between various input-output pairs (Helton 1993 [100452]). To this end, the variables are first rank transformed to linearize any underlying nonlinear trends and facilitate the application of linear regression tools. In the surrogate input-output model, the output variable is represented as a weighted linear sum of the uncertain inputs. The unknown weights (regression coefficients) are generally determined using a stepwise regression procedure as described below.

In the stepwise regression approach, a sequence of regression models is constructed starting with a single selected input parameter (usually the parameter that explains the largest amount of variance in the output). One additional input variable is included at each successive step (usually the parameter that explains the next-largest amount of variance). The process continues until all of the input variables that explain statistically significant amounts of variance in the output have been included in the model. This approach avoids having to treat all of the independent uncertain variables simultaneously in a single model.

The relative importance of the uncertain inputs is expressed in terms of the standardized regression coefficient (SRC). This is obtained by multiplying the value of the regression coefficient for a variable by its standard deviation and normalizing it by the standard deviation of the output. The larger the absolute value of the SRC, the more important is the contribution of the variable to the overall spread of the output. The SRCs can also be interpreted as regression coefficients that would be obtained from a regression analysis with the input and output variables normalized to zero mean and unit standard deviation. In general, the importance ranking deduced from the order of entry into the regression model is the same as that obtained from the absolute value of the SRC (or alternatively, from the absolute value of the rank correlation coefficient), especially if the input variables are uncorrelated or weakly correlated.

A more robust indicator of importance, particularly when the input variables are correlated, is the R^2-loss, which represents the reduction in the goodness-of-fit of the current regression model if the variable of concern is dropped from the regression model (RamaRao et al. 1998 [100487]). A large value of R^2-loss (i.e., a large decrease in explanatory power) indicates that the removed variable explained a large proportion of the variance in the output and, therefore, the variable is an important component of the model.

8.2.2 Entropy-Based Analyses

The information-theoretic concept of entropy is a useful metric for the characterization of uncertainty (or information) in the univariate case, and redundancy (or mutual information) in the multivariate case (Press et al. 1992 [103316]). Because mutual information is a natural measure of input variable relevance, it has been used as an indicator of variable importance in many areas of science such as language, speech and image processing, analyses of nonlinear systems, delay estimation in time series, neural network-based modeling and biomedical applications.

The following theoretical discussion is based on Press et al. (1992 [103316]). Let the input variable x and the output variable y have multiple possible states. For continuous variables, these could be taken as deciles (i.e., a total of ten states) or quintiles (i.e., a total of five states). This information can be compactly organized in terms of a contingency table–a table whose rows are labeled by the values of the independent variable, x, and whose columns are labeled by the values of the dependent variable, y. The entries of the contingency table are nonnegative integers giving the number of observed events for each combination of row and column.

The mutual entropy (information) between x and y, which measures the reduction in uncertainty of y due to knowledge of x (or vice versa), is defined as the difference between the sum of the individual entropies of x and y, and the joint entropy of x and y. Expressions for these entropies can be found in Press et al. (1992 [103316]), and involve simply counting the number of occurrences of various states of x alone, y alone and xy together.

Once the contingency table has been constructed, several measures of association can be calculated. One such useful measure is the R-statistic (Granger and Lin 1994 [159077]) which takes values in the range [0,1]. R is zero if x and y are independent, and is unity if there is an exact nonlinear relationship between x and y. It can also be shown that if x and y have a bivariate normal distribution, then the R-statistic is identical to the absolute value of the correlation coefficient between x and y.

The contingency table can also be visualized using a "bubble plot," where the entries of the contingency table are shown as bubbles of varying sizes. Here, the contingency table is organized such that the quintiles (or deciles) of the independent variable (input) increase from left to right, and that of the dependent variable (output) increase from top to bottom. The size of the bubble indicates how many observations fall in each quintile-quintile (or decile-decile) box.

The entropy-based measure R-statistic can thus be recognized as a very general tool for quantifying the strength of an association. It is applicable to both linear/nonlinear and monotonic/nonmonotonic relationships, whereas the regression-based measures discussed earlier are restricted to linear and monotonic associations only.

As an example, a bubble plot for an important variable identified on the basis of the R-statistic is presented in Figure 8.2.2-1. A V-shaped pattern is revealed in this figure, indicating that the highest quintile dose values correspond to those in the middle of the input distribution. This nonmonotonic association, although evident in a scatter plot (Figure 8.2.2-2), would have been difficult to identify using regression analyses because these are restricted to examining only monotonic relationships.

8.2.3 Classification-Tree-Based Analysis

Although regression modeling is routinely used for identifying key drivers of uncertainty for the entire output, specialized approaches may be required for examining small subsets (e.g., top and bottom deciles) of the output. To this end, classification tree analysis (Breiman et al. 1998 [151294]) can provide useful insights into what variable or variables are most important in determining whether outputs fall in one or the other (extreme) category. Traditional applications of classification trees have primarily been in the fields of medical decision making and data mining for social sciences.

A binary decision tree is at the heart of classification tree analysis. The decision tree is generated by recursively finding the variable splits that best separate the output into groups where a single category dominates. For each successive fork of the binary decision tree, the algorithm searches through the variables one by one to find the purest split within each variable. The splits are then compared among all the variables to find the best split for that fork. The process is repeated until all groups contain a single category (as far as practicable). In general, the variables that are chosen by the algorithm for the first several splits are most important, with less important variables involved in the splitting near the terminal end of the tree.

The tree-building methodology used in TSPA-SR and also planned for TSPA-LA is based on a probability model approach (Venables and Ripley 2001 [159088]). Classifiers at each node are selected based on an overall maximum reduction in deviance, for all possible binary splits over all the input variables. The classification tree is built by successively taking the maximum reduction in deviance over all the allowed splits of the leaves to determine the next split.

Termination occurs when the number of cases at a node drops below a set minimum, or when the maximum possible reduction in deviance for splitting a particular node drops below a set minimum.

The use of classification trees in sensitivity analysis involves several steps beyond the basic tree construction. After the tree is built, the nodes are evaluated as to their relative contribution in determining important variables. The earliest splits contribute most to the reduction in deviance and are considered to be most important in the classification process. The later splits may be marginally important, or may simply fall in the range of statistical "noise." Usually, an attempt is made to "prune" the tree (i.e., reduce the number of splits) to the point where only a handful of variables are left which can be used to classify the majority of the outputs. Pruning is usually accomplished by increasing the minimum reduction in deviance necessary for node splitting and then rebuilding the tree.

If two or three variables are identified as holding most of the explanatory (or classification) power in the model, the results can be further visualized through the use of a partition plot. A partition plot is a scatter plot of the two most important input variables, with the categorical outcomes defined by unique symbols. One horizontal and one vertical line show the location of the splits for the input variables. The main utility of a partition plot is to display the clustering of outcomes (if any) in the parameter space. This helps provide a visual interpretation of the decision rules generated by the classification tree algorithm.

The binary classification tree approach outlined above (and the tree based model in general) has several advantages when compared to linear and additive models:

- Tree-based models are adept at capturing non-additive behavior. Because the output from TSPA-LA analyses come from complex nonlinear models of physical processes, not being restricted to simple additive input-output models is a distinct advantage over conventional linear regression based sensitivity analyses.
- Tree-based models can handle more general (i.e., other than of a particular multiplicative form) interactions between predictor variables.
- Tree-based models are invariant to monotonic transformations of the input variables.

As an example, a classification tree is presented in Figure 8.2.3-1, where only four variables are needed to perfectly categorize the model outcomes into high and low groups (i.e., dose in the top and bottom 10 percentiles). A visual interpretation of the key decision rules generated by the classification tree algorithm is provided by the partition plot shown in Figure 8.2.3-2. High values for both variables leads to high doses, and conversely, low values for at least one of these two variables leads to low doses. Such insight about the interaction of two important variables and how they affect the model outcome is typically missing from standard input-output scatter plots or tables of regression analysis results.

8.2.4 Implementation Issues

Regression-based measures of uncertainty importance are well-known in the sensitivity analysis literature. However, the applicability of these techniques is restricted to conditions where nonmonotonic patterns and possible variable interactions do not influence the input-output relationship. Entropy-based measures, on the other hand, have a broader applicability for identifying significant input-output patterns, monotonic or otherwise.

Classification trees are a useful tool for identifying key variables affecting extreme outcomes in probabilistic model results. When supplemented with a two-variable decision tree and/or a partition plot, the separation of extreme outcomes in the uncertain parameter space is easy to visualize and explain. The power of classification trees lies in handling nonlinear and non-additive behavior, albeit for monotonic input-output models.

The methods discussed in this section are limited to those that utilize only the sampled input values and computed model outcomes from a Monte Carlo simulation experiment, and do not require new simulations. However, if additional model calculations do not entail significant computational expense, then two other uncertainty importance analysis techniques may be utilized. The Morris method (Morris 1991 [159078]) uses an efficient sampling scheme to evaluate the sensitivity of model output to an uncertain input at various points in the parameter space and rank the variables accordingly. In the Fourier Amplitude Sensitivity Test, or FAST (Saltelli et al. 1999 [159079]), the overall variance is decomposed into terms representing first-order (individual variable) and higher-order (variable interaction) contributions as the basis for importance ranking.

Finally, it should be noted that there is no single "perfect" technique for uncertainty importance analyses. One or more techniques may be necessary, and/or appropriate, depending on the nature of input-output relationship. To that end, the following step-wise procedure will be utilized in TSPA-LA:

- Carry out stepwise linear rank regression analysis to identify key contributors to output variance.
- Check for significant nonmonotonic input-output patterns using entropy analysis.
- Use classification tree analysis to determine how key variables affect extreme model outcomes.

8.3 APPROACH TO SUPPORT THE MULTIPLE BARRIER ANALYSES

The discussion of the TSPA-LA analyses so far has concentrated on the demonstration of compliance with the individual protection performance objective at 10 CFR 63.113(b). In addition, this discussion has addressed the analyses to be conducted for the groundwater protection objective at 10 CFR 63.113(c). What has not been discussed so far is the role these TSPA-LA analyses will play in supporting the multiple barrier requirements at 10 CFR 63.115. These requirements call for DOE to:

- Identify those design features of the engineered barrier system and natural features of the geologic system that are considered barriers important to waste isolation
- Describe the capability of the barriers, identified as important to waste isolation, to isolate waste, taking into account uncertainties in characterizing and modeling the behavior of the barriers.
- Provide the technical basis for the description of the capability of the barriers, identified as important to waste isolation, to isolate waste. The technical basis for each barrier's capability shall be based on and consistent wit the technical basis for the performance assessments used to demonstrate compliance with 10 CFR 63.113(b) and (c).

Each of these requirements is discussed in the following.

8.3.1 Description of Barriers

The definitions in 10 CFR 63.2 clarify the requirement to identify the barriers considered important to waste isolation. The term "barrier" means "any material, structure or feature that prevents or substantially reduces the rate of movement of water or radionuclides from a proposed repository to the accessible environment, or prevents the release of or substantially reduces the release rate of radionuclides from the waste". Further, 10 CFR 63.2 defines "barrier important to waste isolation" as "those natural and engineered barriers whose function is to provide a reasonable expectation that high-level waste can be disposed of without exceeding the requirements of 10 CFR 63.113(a) and (b). "

The barriers important to waste isolation at Yucca Mountain are broadly categorized as natural barriers (associated with the geologic and hydrologic setting) and engineered barriers. The engineered barriers complement the natural barriers by prolonging the containment of radionuclides within the repository and limiting their eventual release.

The natural barriers important to waste isolation consist of the following:

- Surficial soils and topography, which limit water infiltration
- Unsaturated zone rock units above the repository horizon, which limit water flux into repository drifts
- Unsaturated zone rock units below the repository horizon, which limit radionuclide transport
- Volcanic tuffs and alluvial deposits below the water table, which limit radionuclide transport in the saturated zone.

The engineered barriers important to waste isolation consist of the following:

- The drip shield, which protects the waste package from rock fall and limits the water contacting the waste package and water available for advective transport through the waste package and the invert

- The waste package, which limits the water contacting the waste form
- Cladding on spent fuel, which limits the water contacting the CSNF portion of the waste form
- The waste form that limits the rate of release of radionuclides to the water that contacts the waste
- The drift invert which limits the rate of release of radionuclides to the natural barriers.

8.3.2 Description of Barrier Capability

The complete description of the capabilities of barriers important to waste isolation will focus on the capabilities of these barriers to limit movement of water or radionuclides. This description will include model and parameter uncertainties in the discussion of the capability to limit movement of water or radionuclides. It will discuss the changes in barrier capability over the 10,000 year compliance period and the effects of spatial variability in preventing or substantially delaying movement of water or radionuclides. This approach addresses KTI agreements TSPAI 1.01, and TSPAI 1.02.

The level of information provided in the description of barrier capabilities will be commensurate with the relative importance of these barriers in meeting the individual protection requirement of 10 CFR 63.113(b). Accordingly, this description will relate the capabilities of the barriers to limit the movement of water or radionuclides to the TSPA analyses to address individual protection. For the most part, this discussion will be based on the physical arguments that underlie the TSPA results. In addition, the description will include, as appropriate, quantitative analyses that include: (1) intermediate performance analyses, and (2) pinch-point analyses. The pinch-point analyses are a specific form of the intermediate performance analyses, with the only metrics of interest being those related to the reduction in mass at several discrete locations. The intermediate performance analyses, as proposed, are more general and include model subcomponent characteristics as performance measures.

Intermediate Performance Analyses-This approach to evaluating the contribution that different barriers provide to the overall performance of the repository system involves analyzing the intermediate performance of the total system as the system evolves over time. Here, intermediate performance refers to the functioning of individual subcomponents of the TSPA-LA model, rather than on the behavior of the entire waste disposal system. This approach describes the results of the system's temporal and spatial evolution and the uncertainty in this evolution. Thus, the intermediate performance analyses involve examining the internal workings of the reference case simulation for the nominal scenario class. Performance measures of interest include such characteristics of the TSPA-LA model as percolation flux, seepage percentage as a function of percolation flux, time to first breach of drip shield and waste package, fraction of fuel intact, groundwater breakthrough times, etc. Examining the intermediate results provides insight into how different components contribute to total system performance. These results, which will be derived directly from the TSPA-LA model (and not from any "extreme scenario" or "degraded barrier" simulation), will enable uncertainty in barrier characteristics and barrier interdependence to be taken into account. The intermediate performance analyses as described here build upon the type of subsystem analyses discussed in detail for the nominal scenario class in Section 8.1.1.

Pinch-Point Analyses-The pinch-point analysis approach is based on the processing of output from TSPA calculations at subsystem boundaries, or "pinch-points". These are locations where mass or energy is being transferred from one modeling domain (or subsystem or barrier) to another. Because the engineered and natural barriers seek to isolate waste from the environment by attenuating the movement of radionuclides, thus reducing the amount of mass released, two metrics related to the reduction in mass are proposed to measure the effectiveness of different barriers for waste isolation. These barrier effectiveness measures provide an indication of how the contaminants are distributed throughout the system, as well as an understanding of how the barriers are acting together to provide waste isolation.

The first metric quantifies the absolute mass reduction within each barrier (i.e., how much mass is retained in each barrier as a fraction of the initial inventory). Figure 8.3.2-1 provides a visual assessment of such a metric for a single nuclide, technetium-99, in an evaluation of the Canadian repository program (Goodwin et al. 1994 [124152], Figure 6-7). Figure 8.3.2-1 shows how technetium-99 is retained within different barriers and isolated from the biosphere at two different points in time: 10,000 years and 100,000 years. However, this definition of barrier effectiveness factor tends to understate the importance of downstream barriers, which receive a small fraction of the initial inventory. Therefore, a second barrier effectiveness factor is proposed to quantify the relative mass reduction in each barrier. Here the inflowing mass for the barrier is used as the normalizing factor (for the amount of mass retained within the barrier) as opposed to the initial inventory.

As described above, the pinch point analyses can help quantify the capabilities of barriers to radionuclide transport. Capabilities of barriers to restrict water movement (i.e., those above the repository) can be made in terms of average flux across the repository or on a per-package basis, (i.e., how the precipitation flux gets transformed into a smaller quantity contacting the packages).

8.3.3 Technical Basis for Describing Barrier Capability

The technical basis for the description of the capabilities of the barriers important to waste isolation is required to be consistent with the technical basis for the performance assessments used to demonstrate compliance with 10 CFR 63.113(b) and (c). As planned for TSPA-LA, in all cases, the technical basis for both the TSPA-LA model and the multiple barrier analysis will be the same set of AMRs. This will be the case regardless of whether the description of barrier capabilities is based on physical arguments (where the conceptual basis for TSPA-LA models and multiple barrier analysis will be consistent), or intermediate performance and pinch-point analysis (where the mathematical basis for TSPA-LA models and multiple barrier analysis will be consistent). In this sense, the technical basis for the multiple barrier analysis will not only be consistent with the performance assessments, it will be the same.

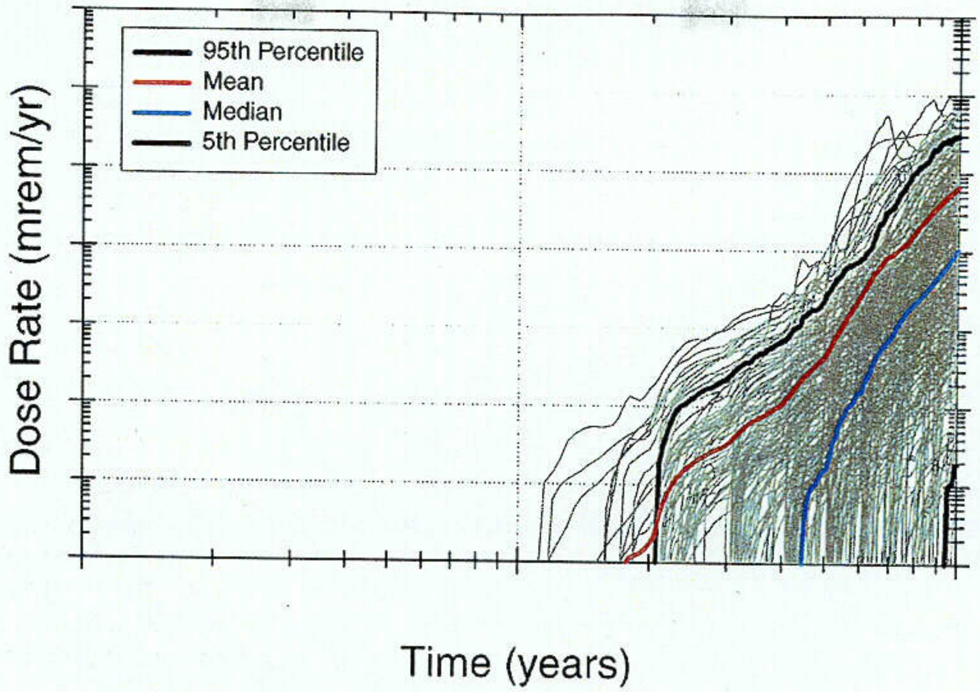


Figure 8.1.1-1. Example of an Expected Dose Time History, along with Running 5th, 50th and 95th Percentile Curves

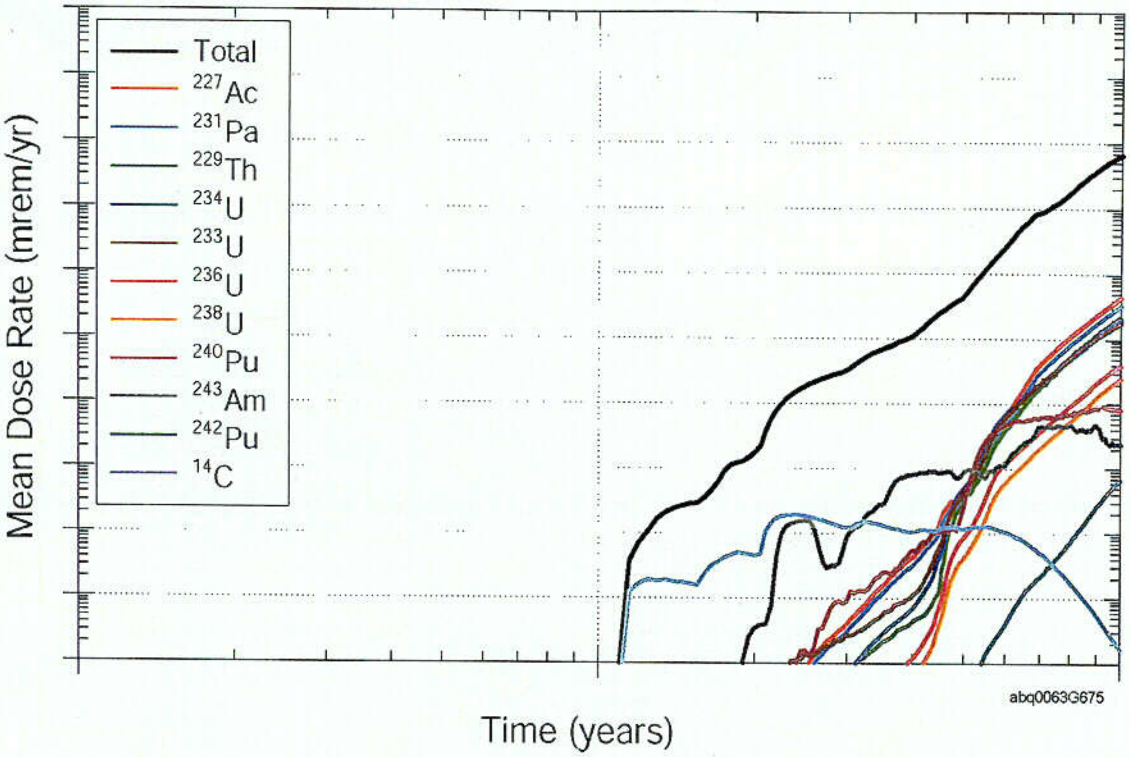


Figure 8.1.1-2. Example of Key Radionuclides and their Contributions to Expected Dose

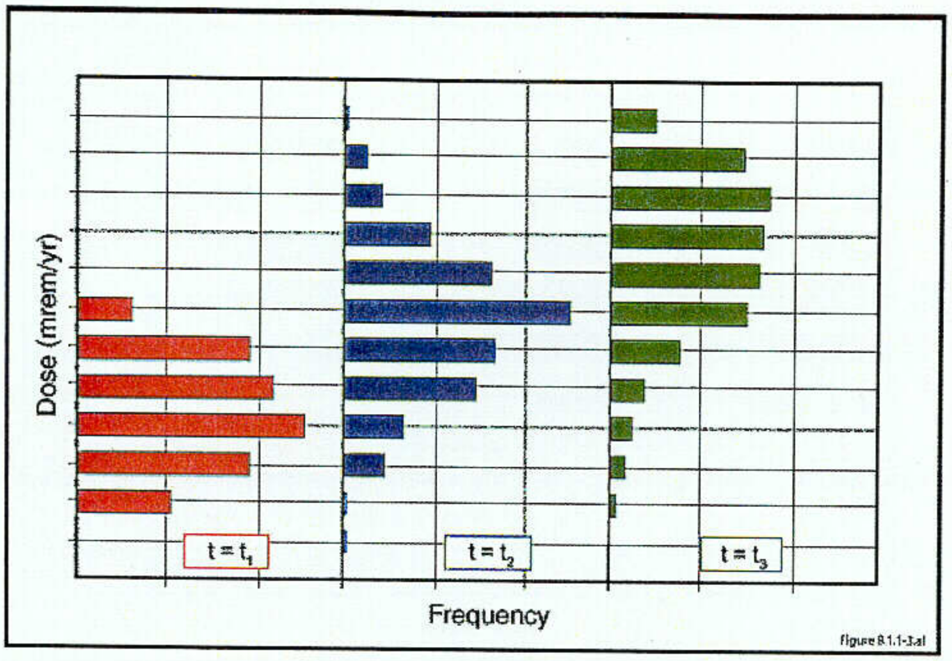


Figure 8.1.1-3. Example of Side-by-Side Histogram of Dose at Selected Times

C03

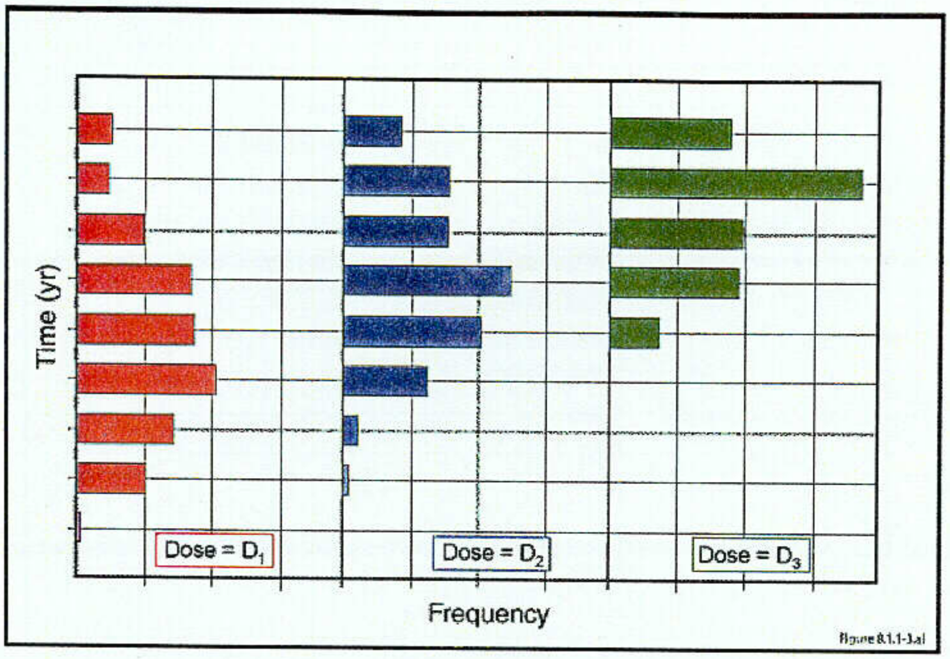


Figure 8.1.1-4. Example of Side-by-Side Histogram of Time to Reach Specified Dose

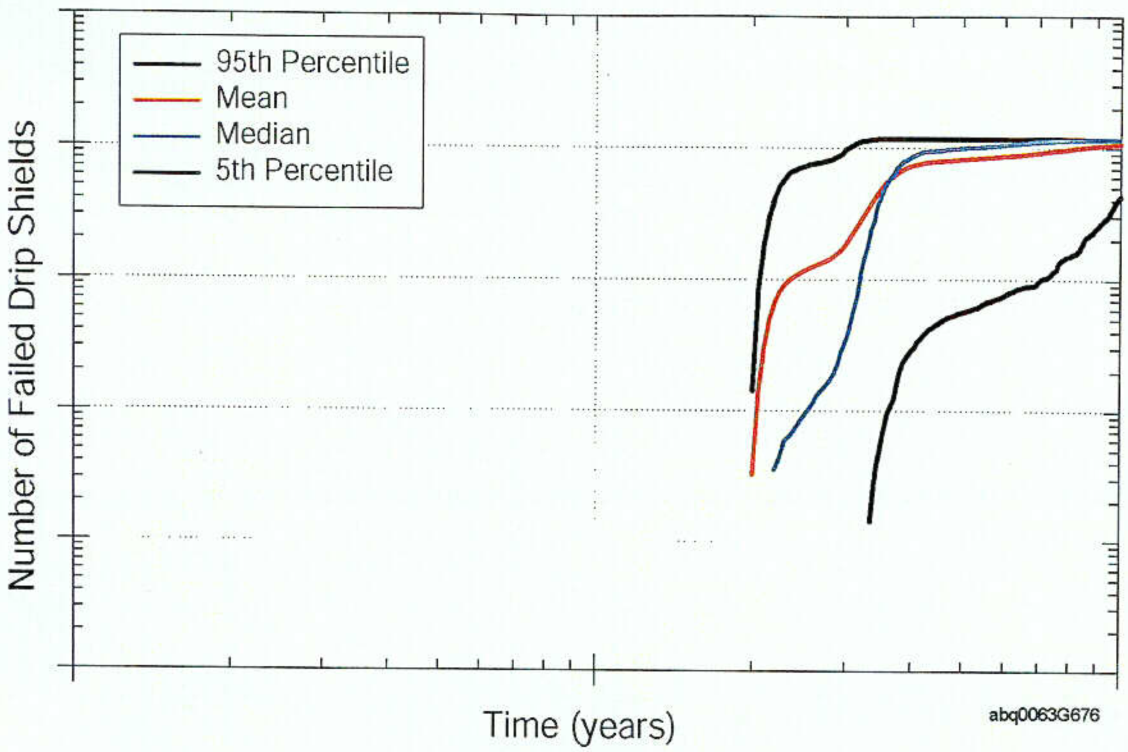


Figure 8.1.1-5. Example of Cumulative Drip Shield Failures

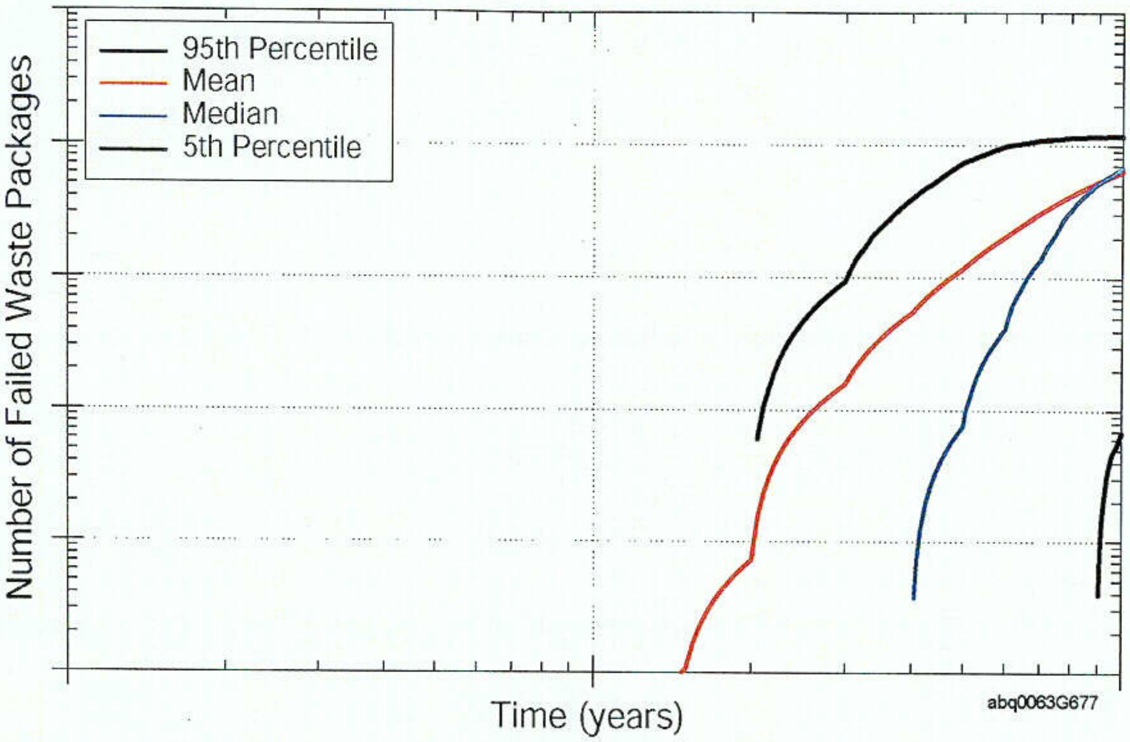


Figure 8.1.1-6. Example of Cumulative Waste Package Failures

C06

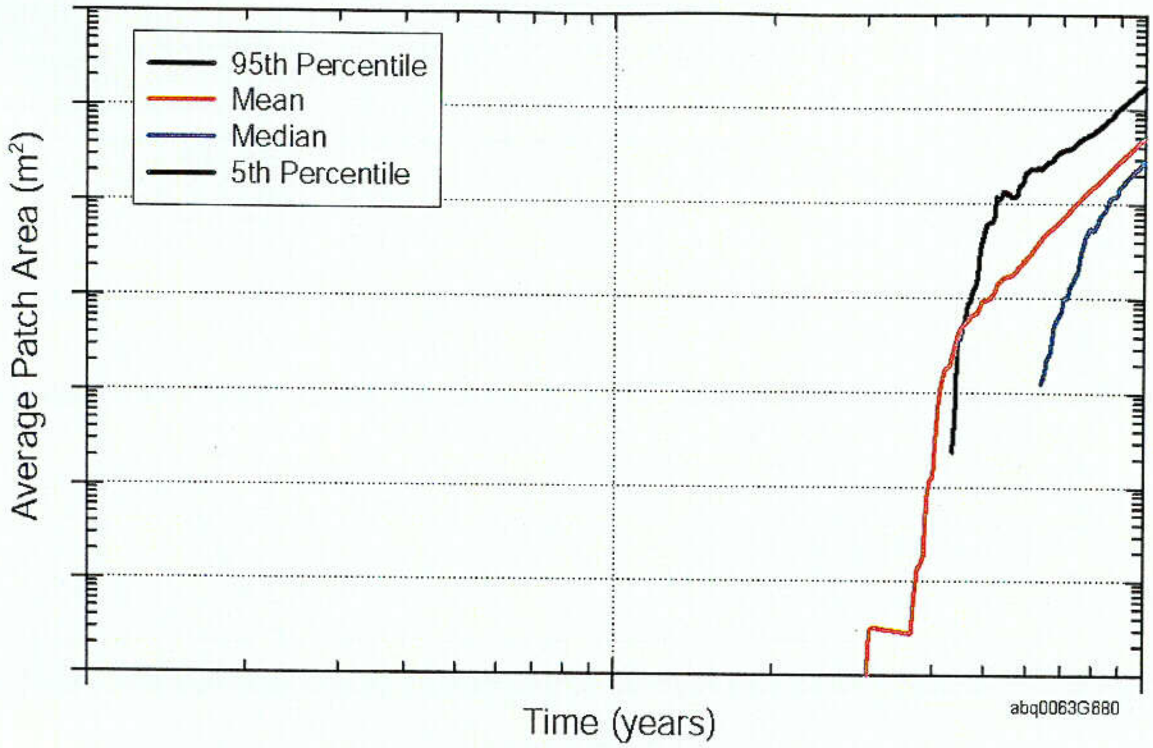


Figure 8.1.1-7. Example of Waste Package Opening Area

C07

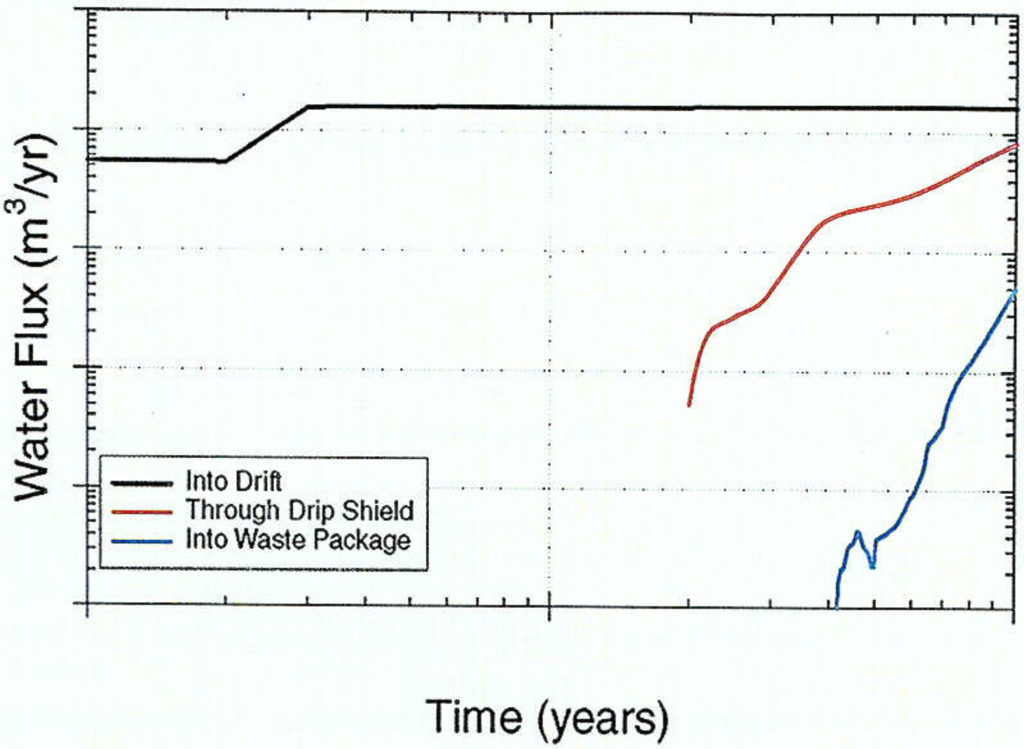


Figure 8.1.1-8. Example of Water Flow Rates into Drift, Through the Drip Shield and into Waste Package

C08

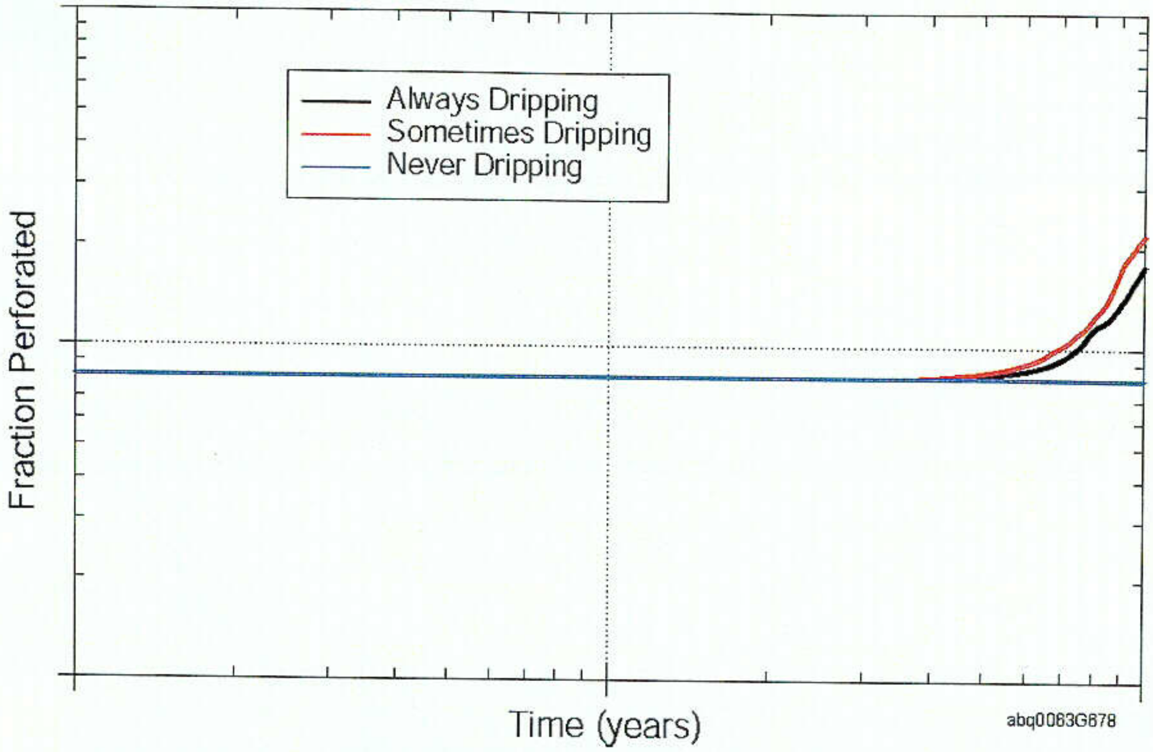


Figure 8.1.1-9. Example of Fractional Cladding Failures

C09

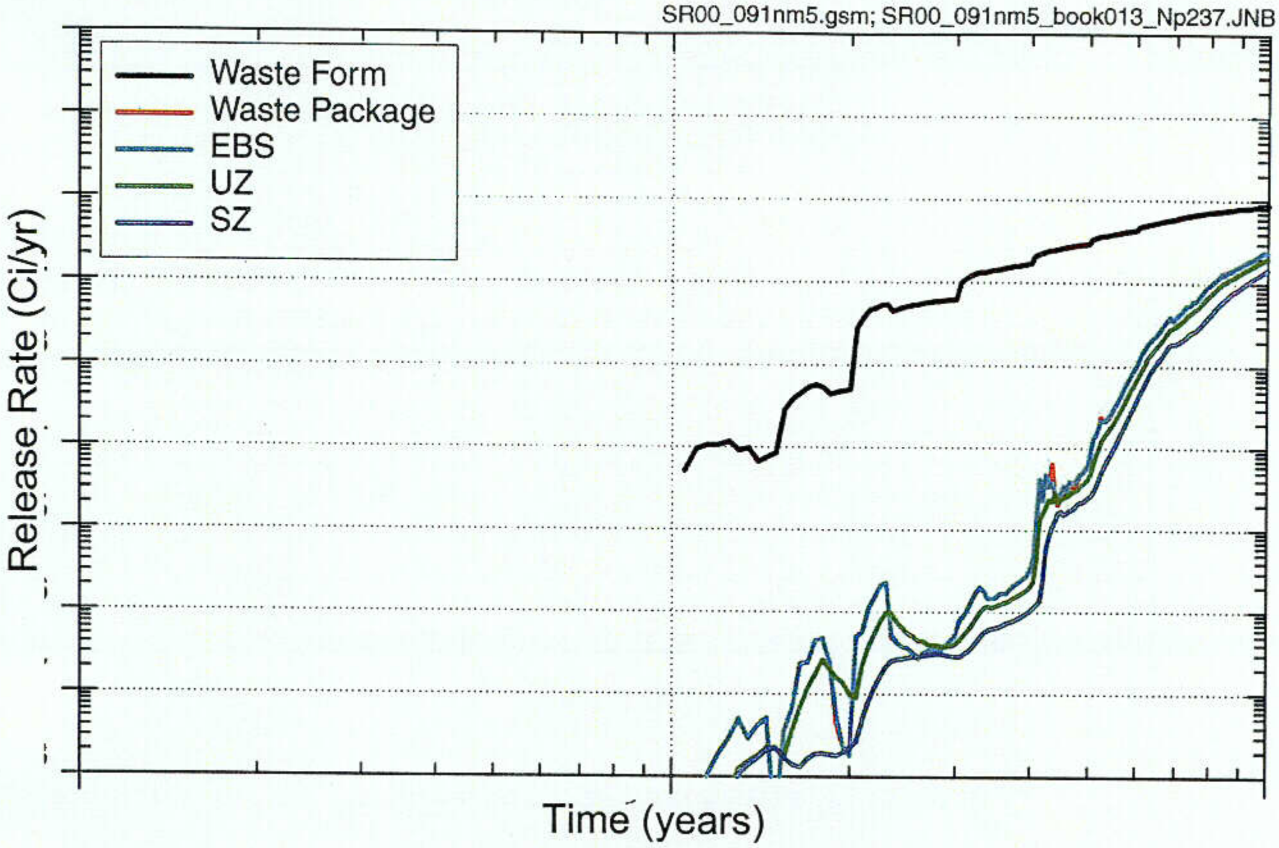
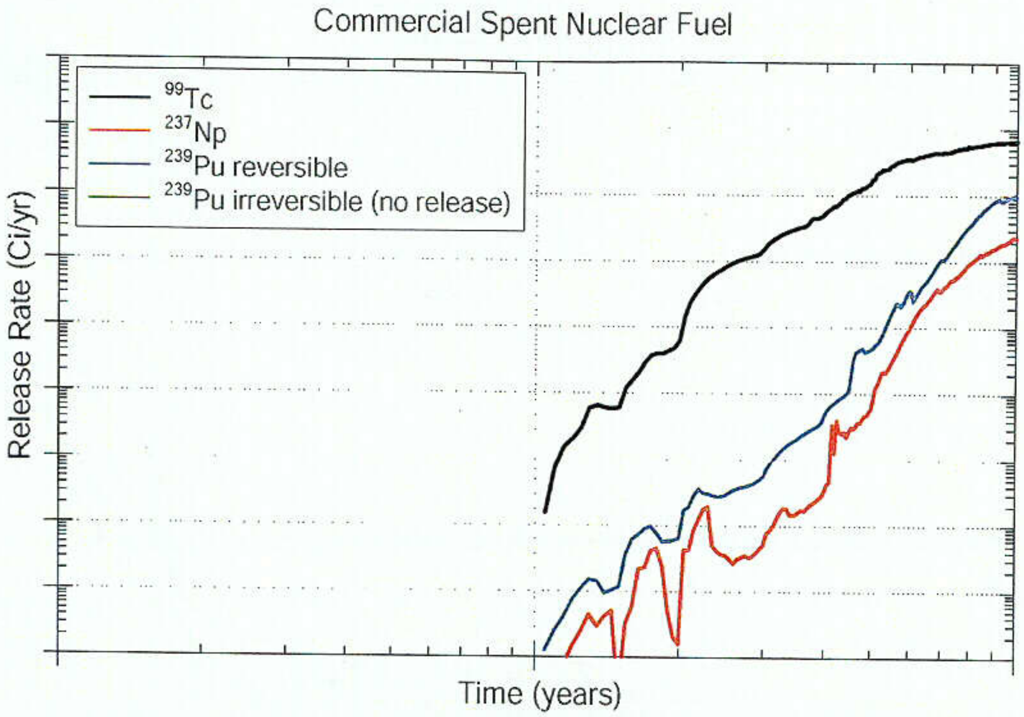


Figure 8.1.1-10. Example of Mean Release Rates for a Key Radionuclide

C10



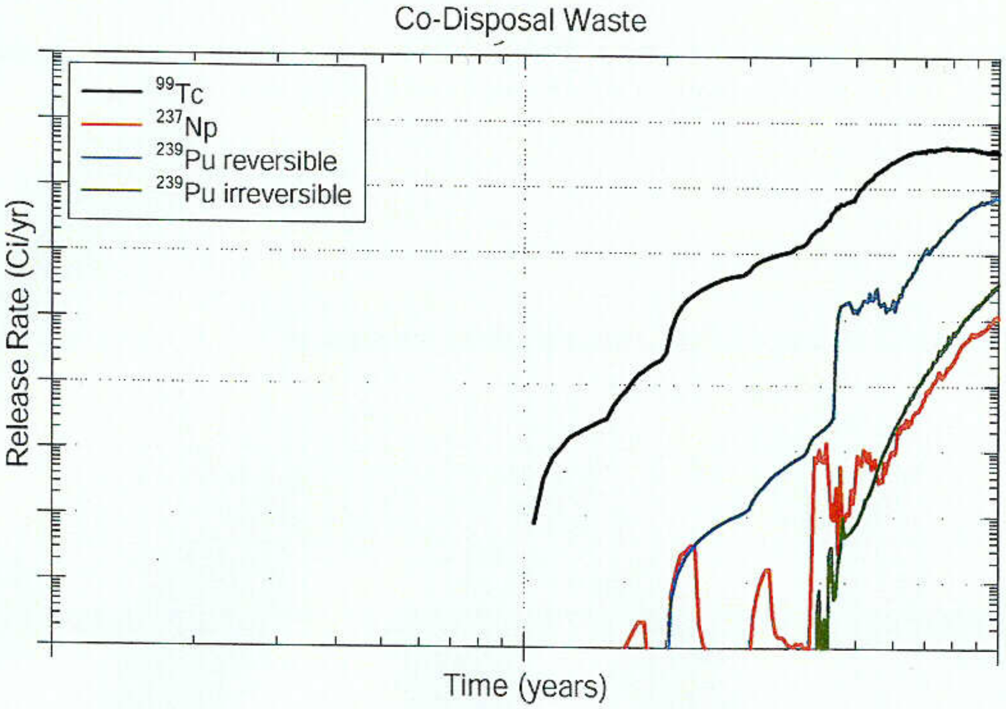


Figure 8.1.1-11. Example of EBS Release Rates from Different Waste Types

C11

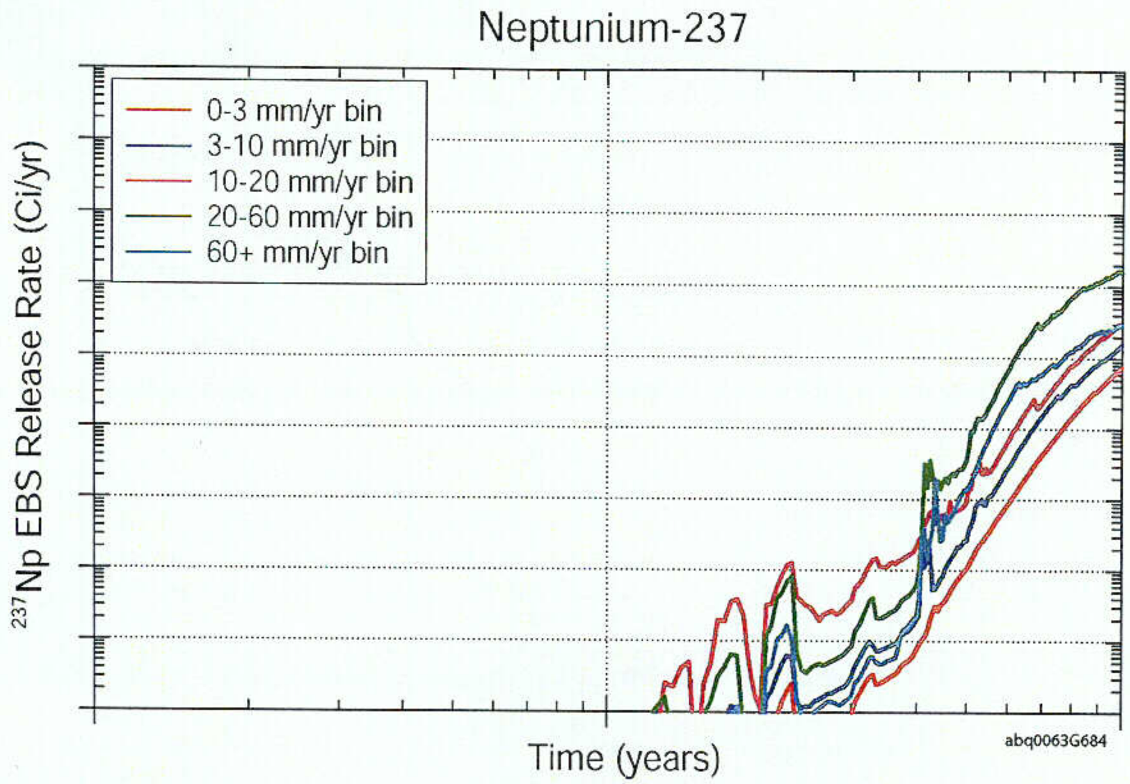


Figure 8.1.1-12. Example of UZ Release from Different Infiltration Bins

C12

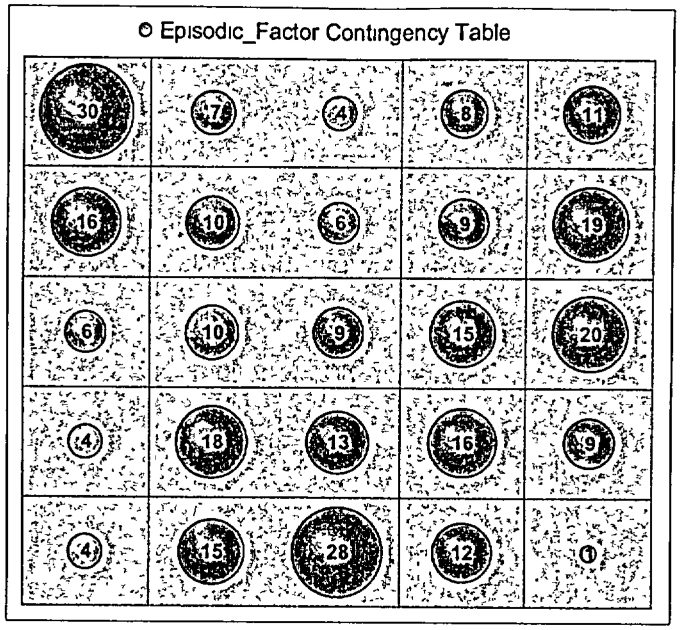


Figure 8.2.2-1. Example Bubble Plot Showing Episodic Factor Quintiles (x-axis) vs Dose Quintiles (y-axis)

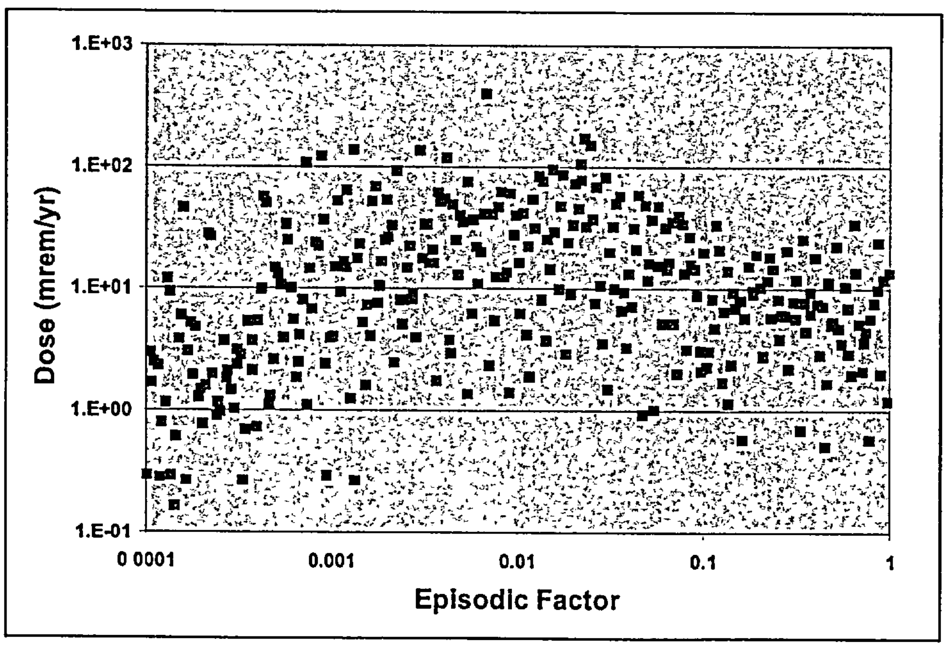


Figure 8.2.2-2. Example Scatter Plot for Two Variables

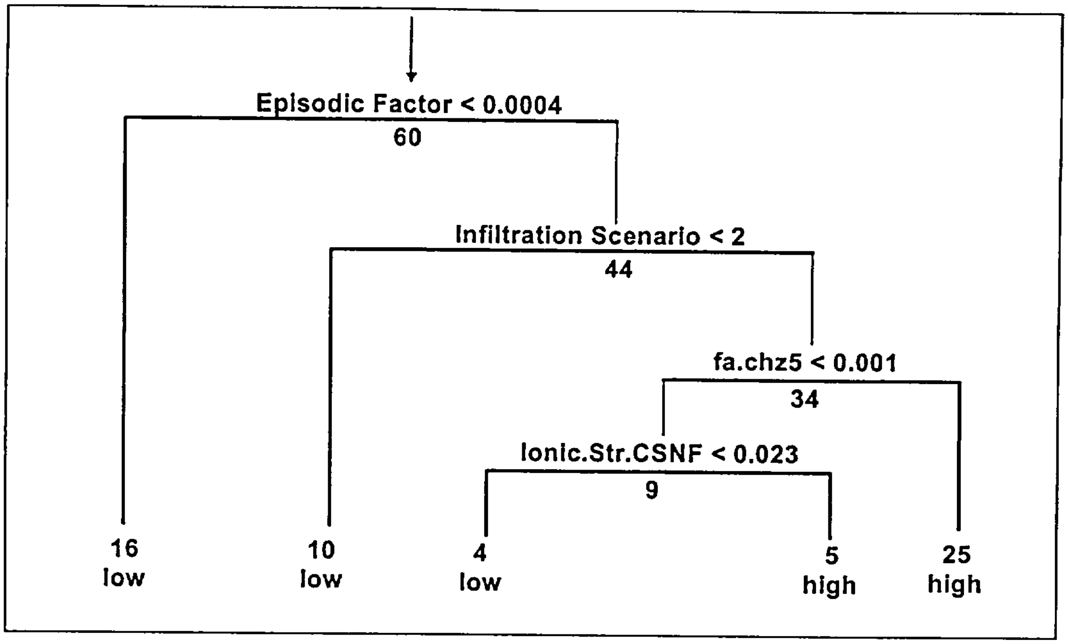


Figure 8.2.3-1. Example Classification Tree Showing Decision Rules for Separating High-dose and Low-dose Producing Realizations

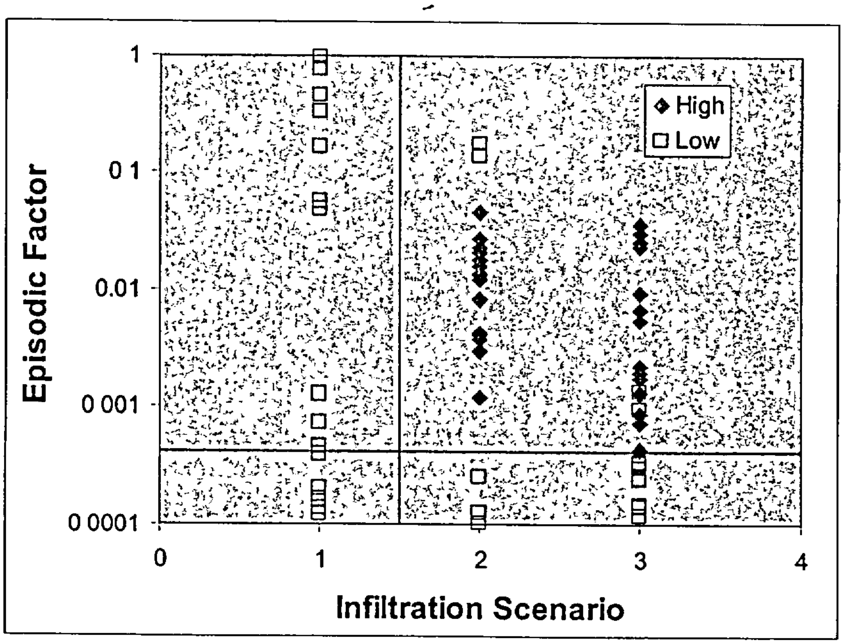
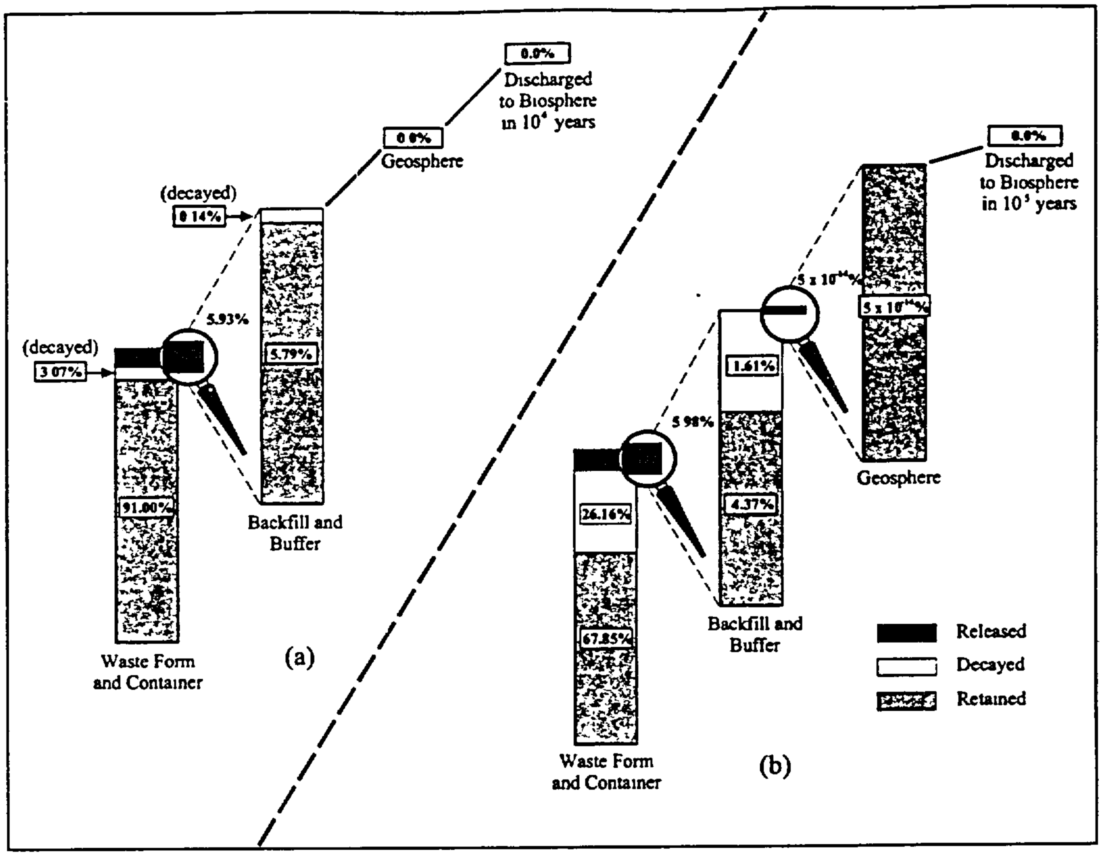


Figure 8.2.3-2. Example Partition Plot Showing Clustering of High- and Low-Outcomes in the Parameter Space of the Two Most Important Variables



Source: Goodwin et al. 1994 [124152], Figure 6-7

Figure 8.3.2-1. Graphical Depiction of Barrier Effectiveness Showing Distribution of Tc-99 in the Disposal System after (a) 10,000 Years and (b) 100,000 Years

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9. SUMMARY

The TSPA-LA methods and approach are based on NRC requirements and Office of Civilian Radioactive Waste Management (OCWRM) project Administrative Procedures. A brief summary of the approach, traceability, transparency, and analyses used to satisfy the *Yucca Mountain Review Plan* (CNWRA 2002 [158449]) acceptance criteria follows.

9.1 SUMMARY OF APPROACH

The approach to be used for development, control, analysis and documentation of the TSPA-LA model is similar to what has been done for previous TSPA iterations. Of increased importance for TSPA-LA, compared to other TSPAs, is the need to meet the requirements of 10 CFR Part 63, and the acceptance criteria of the *Yucca Mountain Review Plan* (CNWRA 2002 [158449]), and to maintain appropriate configuration control over the information, software, models, and documentation. Processes and procedures are in place within the TSPA Department as well as in the supplying organizations, for the appropriate configuration control.

The process for developing inputs (parameters, abstractions, alternative conceptual models, and uncertainty) for the TSPA is integrated across the Performance Assessment Project, as well as with other suppliers (e.g., National Spent Nuclear Fuel Program, Naval Reactors). This effort will provide for consistent, defensible inputs to the TSPA-LA model. Also, the process will follow the enhanced FEPs development approach to develop the FEPs ultimately utilized in the TSPA. Scenario development has led to the definition of two scenario classes: nominal scenario class, and disruptive event scenario class. The disruptive event igneous scenario class will have two modeling cases: volcanic eruption modeling case, and igneous intrusive modeling case. The disruptive event seismic scenario class will be a class by itself. The stylized human intrusion analysis will be treated separately from the scenario classes, primarily because the event as defined in 10 CFR Part 63.321 is not expected to occur in the regulatory time period (10,000 years).

The probabilistic simulations of the total system will be evaluated to determine the key factors contributing to the dose at 18 km. Current plans are to analyze simulations up to 20,000 years, and to utilize 300 realizations per analysis. These plans may be modified for various reasons as the analyses progress.

The documentation suite for the TSPA-LA will include the TSPA-LA Model Document, the TSPA-LA Analysis Document, and the corresponding sections in the LA itself. The latter may be simply extracts or simple syntheses of the foundation TSPA-LA documents. In addition, a large volume of supporting documents will be directly referenced from the TSPA-LA documents including model reports, analysis reports, design documents, and calculation documents (see Appendix G for planned document hierarchy).

9.2 SUMMARY OF TRANSPARENCY AND TRACEABILITY

An overall objective of any integrated performance assessment, but in particular total system performance assessments of proposed nuclear waste repositories, is to provide a "transparent and traceable" analysis that allows the reader the opportunity to understand the basic assumptions and their scientific basis in such a way that he or she may understand and test the accuracy and reproducibility of the conclusions. AP-SIII.10Q, *Models*, has defined transparency as the attribute of producing documents that are sufficiently detailed as to purpose, method, assumptions, inputs, conclusions, references, and units, such that a person technically qualified in the subject can understand the documents and ensure their adequacy without recourse to the originator. AP-SIII.10Q, *Models*, has defined traceability as the ability to trace the history, application, or location of an item, data, or sample using recorded documentation.

Throughout the TSPA-LA documentation, the underlying data, assumptions, models, and analyses will be discussed with appropriate conceptual drawings and integration graphics to illustrate the role of the model component, the technical basis of the model component, and the information flow from or to each model component. In addition, interim results will be presented both at the TSPA system level and the subsystem level to illustrate how information (in terms of mass, water, energy, activity) flows from one part of the system to the next in the integrated total system model. Also, the hierarchy of all analysis and model reports that support the final information feed to the TSPA-LA model will be presented.

The defensibility of the analyses and models that support the TSPA-LA model is contained in the relevant AMRs. It is the AMRs that provide the fundamental scientific underpinning, and the associated assumptions and conservatisms necessary for a defensible, yet reasonably cautious analysis of expected performance.

It is beyond the scope of the TSPA documentation to summarize the depth and breadth of the information contained in the analysis model reports that form the basis for the TSPA-LA. The individual models are based on appropriate site-specific information, analog data, and relevant literature data sources that have been integrated by the principal scientific investigators to provide a reasonable and defensible characterization of each individual process relevant to postclosure performance. Quantifiable uncertainty in the individual model component was also included as appropriate.

In addition to the analysis and model reports providing a traceable chain of references for the defensibility of the scientific bases for the TSPA-LA, they will also provide a hierarchy of data tracking numbers. The sources and hierarchy of data sets used as input to the TSPA-LA model will be summarized in the TSPA-LA Analysis Document, with additional detail in the TSPA-LA Model Document. The status of each data set used as input to the TSPA-LA model can be ascertained by tracing the data set and all its predecessors using the TDMS and DIRS databases. This capability allows the DOE and NRC to track the status of all data sets used in the development of the postclosure safety case.

The data, analyses, and models used as the technical basis for the TSPA-LA, as well as the assumptions, uncertainty, and variability that go along with these data, analyses, and models will be traceable back to their source documents and data sets. This traceability allows all interested reviewers to examine the defensibility of the individual model components and reach their own conclusions regarding their scientific adequacy.

9.3 SUMMARY OF UNCERTAINTY TREATMENT IN TSPA-LA ANALYSES

TSPAs are, by their very nature, uncertain projections of the possible behavior of the individual model components describing the relevant processes affecting the containment and isolation of radioactive wastes from the biosphere. This uncertainty is explicitly included in the models and resulting analyses in the form of discrete probability distributions that encompass the range of possible outcomes.

There remains uncertainty in the individual process models and their abstraction into the TSPA-LA model. Much of this uncertainty will be quantified and included in the TSPA-LA model. The TSPA-LA results will reflect this quantified uncertainty.

In addition to the quantified uncertainty in the TSPA-LA model, there may also be unquantified uncertainty that will be represented by using an appropriately realistic representation of a particular model. These representations (which may be necessarily conservative) result when there is insufficient information available or significant complexity exists that is not amenable to quantified uncertainty. Elicitation approaches could be used if it was desired to quantify the uncertainty in these conservative judgments.

9.4 SUMMARY OF HOW THE APPROACH SATISFIES YUCCA MOUNTAIN REVIEW PLAN ACCEPTANCE CRITERIA

The methods and approach presented in this document for the TSPA-LA will develop a TSPA-LA model and analyses that will satisfy the *Yucca Mountain Review Plan* (CNWRA 2002 [158449]) acceptance criteria for postclosure repository safety. The *Yucca Mountain Review Plan* (CNWRA 2002 [158449]) requires that the NRC review the barriers important to waste isolation. The TSPA-LA approach to the multiple barrier analysis was briefly described in Section 8.3. The intent is to briefly describe the barriers, and provide some evaluation of their capabilities as to their effect on water and radionuclide movement from the repository.

The scenario analysis approach is another significant part of the *Yucca Mountain Review Plan* (CNWRA 2002 [158449]) acceptance criteria. Both nominal and disruptive scenario classes have been defined, and will be analyzed in the TSPA-LA. The approach to this selection of scenarios has been discussed, along with the approach to ensure appropriate identification and screening of the FEPs relevant to the Yucca Mountain site. The FEPs, as well as the concomitant parameters, abstractions, alternative conceptual models, and associated uncertainty, will be defined and developed utilizing the new integrated approach discussed in Section 3. This approach brings together the necessary SMEs and TSPA personnel to develop consistent, traceable inputs for the TSPA-LA model.

The *Yucca Mountain Review Plan* (CNWRA 2002 [158449]) requires traceability of the inputs to the TSPA-LA. The controls of the process of testing, developing, and analyzing the TSPA-LA model that contribute to the overall traceability of the analyses are described in Section 6.

Detailed consideration of all *Yucca Mountain Review Plan* (CNWRA 2002 [158449]) acceptance criteria has been incorporated into the planning of the TSPA-LA, including the supporting PA and Design organizations. This effort is designed to lead to an integrated safety assessment of the repository, that is defensible, traceable, and readily transparent to the technical reviewers of the analysis.

10. REFERENCES

The following is a list of the references cited in this document, Column 1 represents the unique six digit DIRS number, which is placed in the text following the callout (e.g., (BSC 2001 [154659])). The purpose of these numbers is to assist the reader in locating a specific reference. The reference list is ordered numerically by the DIRS number.

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10.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

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153202 AP-SV.1Q, Rev. 0, ICN 2. Control of the Electronic Management of Information. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20000831.0065.

153493 AP-SIII.1Q, Rev. 0, ICN 1. *Scientific Notebooks.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20000516.0002.

154534 AP-2.21Q, Rev. 1, ICN 0, BSCN 001. Quality Determinations and Planning for Scientific, Engineering, and Regulatory Compliance Activities. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20010212.0018.

155216 66 FR 32074. 40 CFR Part 197, Public Health and Environmental Radiation Protection Standards for Yucca Mountain, NV; Final Rule. Readily available.

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156671 66 FR 55732. Disposal of High-Level Radioactive Wastes in a Proposed Geologic Repository at Yucca Mountain, NV. Final Rule 10 CFR Part 63. Readily available.

157282 AP-3.15Q, Rev. 3, ICN 1. *Managing Technical Product Inputs.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020102.0204.

158907 AP-SI.1Q, Rev. 3, ICN 4. Software Management. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020520.0283.

158908 AP-SIII.10Q, Rev. 0, ICN 2. Models. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020506.0911.

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159045 AP-3.11Q, Rev. 3, ICN 2. *Technical Reports.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020701.0189.

159254 AP-15.3Q, Rev. 0, ICN 0. Control of Technical Product Errors. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020212.0254.

159255 AP-SIII.3Q, Rev. 1, ICN 2. Submittal and Incorporation of Data to the Technical Data Management System. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020701.0177.

159475 DOE (U.S. Department of Energy) 2002. *Quality Assurance Requirements and Description.* DOE/RW-0333P, Rev. 12. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020819.0387.

159604 AP-2.27Q, Rev 0, ICN 0. *Planning For Science Activities.* Washington, DC: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020701.0184.

159727 AP-ENG-004, Rev. 1, ICN 0. *Resolution of Differing Professional Opinion.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20020516.0093

APPENDIX A

ACRONYMS

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APPENDIX A ACRONYMS

ACM	alternative conceptual model
AECL	Atomic Energy of Canada, Ltd
AMR	analysis model report
AP	Administrative Procedure
ATL	Abstraction Team Lead
BDCF	biosphere dose conversion factor
BIO	biosphere
BSC	Bechtel SAIC Company, LLC
BTC	break-through curve
CDF	cumulative distribution function
CFR	Code of Federal Regulations
CNWRA	Center for Nuclear Waste Regulatory Analyses
CRWMS	Civilian Radioactive Waste Management System
CSNF	commercial spent nuclear fuel
DE	disruptive events
DIRS	Document Input Reference System
DLL	dynamically linked library
DOE	U.S. Department of Energy
DSNF	DOE spent nuclear fuel
DTN	data tracking number
DS	Drip Shield
EBS	engineered barrier system
EPA	U.S. Environmental Protection Agency
EPRI	Electric Power Research Institute
FAST	Fourier Amplitude Sensitivity Test
FEHM	finite element, heat and mass transfer code
FEIS	Final Environmental Impact Statement
FEP	feature, event, or process
FR	Federal Register

ACRONYMS (Continued)

FTL	FEP Team Lead
HLW	high-level radioactive waste
HTOM	higher-temperature operating mode
IAEA	International Atomic Energy Agency
KTI	Key Technical Issue
LA	License Application
LHS	Latin Hypercube Sampling
LTOM	lower-temperature operating mode
M&O	Management and Operating Contractor
MSTH	multi-scale thermal-hydrologic
NEA	Nuclear Energy Agency
NRC	U.S. Nuclear Regulatory Commission
OECD	Organisation for Economic Co-operation and Development
PA	Performance Assessment
PASS	Performance Assessment Strategy and Scope
PDF	probability distribution function
PMR	process model report
PSHA	probabilistic seismic hazard analysis
PTL	Parameter Team Lead
QA	Quality Assurance
RH	relative humidity
RMEI	reasonably maximally exposed individual
SCC	stress corrosion cracking
SCM	Software Configuration Management
SME	subject matter expert
SR	Site Recommendation
SRC	standardized regression coefficient
SSPA	Supplemental Science and Performance Analysis

ACRONYMS (Concluded)

STN	software tracking number
SZ	saturated zone
TBD	to be determined
TDMS	Technical Data Management System
TER	Technical Error Report
THC	thermal-hydrologic-chemical
TSPA	Total System Performance Assessment
TSPAI	Total System Performance Assessment Integration
UZ	Unsaturated Zone
VA	Viability Assessment
WAPDEG	Waste Package Degradation code
WF	Waste Form
WP	Waste Package
YMP	Yucca Mountain Project

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APPENDIX B

NRC/DOE KTI AGREEMENTS ADDRESSED IN THIS DOCUMENT

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APPENDIX B NRC/DOE KTI AGREEMENTS ADDRESSED IN THIS DOCUMENT

Several TSPAI KTI agreements are addressed in this document, including TSPAI 1.01, 1.02, 4.01, 4.03, and 4.05 (Meserve 2001 [156977]). The agreements and the location of the discussion in this document are provided below.

TSPAI 1.01–DOE will provide enhanced descriptive treatment for presenting barrier capabilities in the final approach for demonstrating multiple barriers. DOE will also provide discussion of the capabilities of individual barriers, in light of existing parameter uncertainty (e.g., in barrier and system characteristics) and model uncertainty. This agreement is addressed in Section 8.3.

TSPAI 1.02–DOE will provide a discussion of the following in documentation of barrier capabilities and the corresponding technical bases: (1) parameter uncertainty, (2) model uncertainty (i.e., the effect of viable alternative conceptual models), (3) spatial and temporal variability in the performance of the barriers, (4) independent and interdependent capabilities of the barriers (e.g., including a differentiation of the capabilities of barriers performing similar functions), and (5) barrier effectiveness with regard to individual radionuclides. DOE will also analyze and document barrier capabilities, in light of existing data and analyses of the performance of the repository system. This agreement is addressed in Section 8.3.

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. This agreement is addressed in Section 3.3.

TSPAI 4.03–DOE will document the method that will be used to demonstrate that the overall results of the TSPA are stable. DOE will provide documentation that submodels (including submodels used to develop input parameters and transfer functions) are also numerically stable. DOE will address in the method the stability of the results with respect to the number of realizations. DOE will describe in the method the statistical measures that will be used to support the argument of stability. The results of the analyses will be provided in the TSPA (or other appropriate documentation) for any potential license application. This agreement is addressed in Section 7.3.

TSPAI 4.05–DOE will document the process used to develop confidence in the TSPA models. The detailed process is currently documented in the model development procedures that are being evaluated for process improvement in response to the model validation corrective action report (CAR-BSC-01-C-001). This agreement is mentioned in Section 7.3.

APPENDIX C

TSPA-LA MODEL DOCUMENT OUTLINE

APPENDIX C TSPA-LA MODEL DOCUMENT OUTLINE

1. PURPOSE

2. QUALITY ASSURANCE

3. USE OF SOFTWARE
   - 3.1 GOLDSIM
   - 3.2 SEEPAGE_LA
   - 3.3 PREWAP_LA
   - 3.4 WAPDEG
   - 3.5 GVP
   - 3.6. MFD
   - 3.7 SCCD
   - 3.8 Patch_Fail_Lag
   - 3.9 FEHM
   - 3.10 SZ_Convolute
   - 3.11 ASHPLUME
   - 3.12 IGNEOUS_ERUPTIVE

4. INPUTS
   - 4.1 DATA AND PARAMETERS
   - 4.2 CRITERIA
   - 4.3 CODES AND STANDARDS
   - 4.4 TSPA INPUT DATABASE
     - 4.4.1 UZ Flow
     - 4.4.2 EBS Environment
     - 4.4.3 Waste Package and Drip Shield Degradation
     - 4.4.4 Waste Form Degradation and Mobilization
     - 4.4.5 Engineered Barrier System Flow and Transport
     - 4.4.6 UZ Transport
     - 4.4.7 SZ Flow and Transport
     - 4.4.8 Biosphere
     - 4.4.9 Igneous Scenario Class
     - 4.4.10 Seismic Scenario Class

5. ASSUMPTIONS
   - 5.1 INTRODUCTION
   - 5.2 TSPA-LA MODEL ASSUMPTIONS
   - 5.3 ASSUMPTIONS FROM INPUTS TO THE TSPA-LA MODEL
     - 5.3.1 Unsaturated Zone Flow
     - 5.3.2 EBS Environment
     - 5.3.3 Waste Package and Drip Shield Degradation
     - 5.3.4 Waste Form Degradation and Mobilization
     - 5.3.5 Engineered Barrier System Flow and Transport
     - 5.3.6 Unsaturated Zone Transport

7. VALIDATION/CONFIDENCE BUILDING
   - 7.1 MODEL VALIDATION STRATEGY
   - 7.2 DISCRETIZATION TEST SIMULATIONS (See Table E.1-1)
   - 7.3 PROCESS TESTING SIMULATIONS (See Table E.1-2)
     - 7.3.1 Subsystem Validation
     - 7.3.2 System Validation
       - 7.3.2.1 Verification of Coupling
       - 7.3.2.2 Comparison with Other Simple Analyses
       - 7.3.2.3 Neutralization Analysis
       - 7.3.2.4 One-On Analysis

8. CONCLUSIONS

9. INPUTS AND REFERENCES
   - 9.1 DOCUMENTS CITED
   - 9.2 CODES, STANDARDS, AND REGULATIONS
   - 9.3 DATA, LISTED BY DATA TRACKING NUMBER

10. ATTACHMENTS

A ACRONYMS/GLOSSARY

B SUMMARY OF SCREENING DECISIONS AND BASIS INFORMATION CONTAINED IN THE YUCCA MOUNTAIN PROJECT AND FEATURES, EVENTS, AND PROCESSES DATABASE

C TRACEABILITY FOR MODEL AND DATA

D DATA TRACKING INFORMATION FOR TOTAL SYSTEM PERFORMANCE ASSESSMENT-LICENSE APPLICATION ANALYSES

E SUMMARY AND RESPONSE TO REVIEW COMMENTS ON PREVIOUS YUCCA MOUNTAIN TSPA ITERATIONS

F MATHEMATICAL BASIS FOR MODELS

G LISTING OF ALTERNATIVE CONCEPTUAL MODELS

Note: The individual submodel sections (e.g., 6.2.x.y) will have a brief overview similar to that in the TSPA-SR Model AMR, and then text that points the reader to Section 4 for inputs, the appropriate Section 5 subsection for assumptions, and to container(s) in a GoldSim Dashboard file (able to browse using the GoldSim Player software) where the details of the model will be discussed.

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APPENDIX D

TSPA-LA ANALYSIS DOCUMENT OUTLINE

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APPENDIX D TSPA-LA ANALYSIS DOCUMENT OUTLINE

1. PURPOSE
   -Sections 1.1 to 1.3 of TSPA-SR
   -Sections 1.6 to 1.7 of TSPA-SR

2. QUALITY ASSURANCE

3. USE OF SOFTWARE
   -list all software and status

4. INPUTS

4.1 DATA AND PARAMETERS
-list data/parameters. Significant referencing to Model Document.
4.2 CRITERIA
4.3 CODES AND STANDARDS

5. ASSUMPTIONS

6. SCIENTIFIC ANALYSIS DISCUSSION
   -Section 2 through 2.1.2 of TSPA-SR
6.1 METHOD
-Section 2.2.4 through 2.2.5.2, and 2.2.5.5 of TSPA-SR
6.2 ANALYSES - NOMINAL SCENARIO CLASS
-Section 4.1 of TSPA-SR
6.3 ANALYSES – IGNEOUS SCENARIO CLASS
-Section 4.2 of TSPA-SR
6.4 ANALYSES – SEISMIC SCENARIO CLASS
6.5 ANALYSES – COMBINED SCENARIO CLASSES
-Section 4.3 of TSPA-SR
6.6 SENSITIVITY ANALYSES
-uncertainty importance analyses – Section 5.1 from TSPA-SR
6.7 ANALYSES – GROUNDWATER PROTECTION

7. CONCLUSIONS

8. REFERENCES
8.1 DOCUMENTS CITED
8.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES
8.3 SOURCE DATA, LISTED BY DATA TRACKING NUMBER

9. ATTACHMENTS

ATTACHMENT A ACRONYMS/GLOSSARY

ATTACHMENT B ALTERNATIVE CONCEPTUAL MODEL DESCRIPTION SUMMARY

Note: Where TSPA-SR sections are identified, the TSPA-LA will have similar sections to the content in that particular section of the TSPA-SR.

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APPENDIX E

TSPA-LA SIMULATION LIST

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APPENDIX E TSPA-LA SIMULATION LIST

E.1 TESTING SIMULATIONS (VALIDATION AND CONFIDENCE BUILDING)

The initial simulations to be performed will be those involving testing. Testing simulations are broken into discretization testing and process testing. Discretization testing (see Table E.1-1) is broken into three major areas: spatial discretization (supports the determination of the number of source term groups), temporal discretization (time step size(s) related to numerical convergence and resolution of peaks), stochastic discretization (number of realizations, and random number seed). These analyses will be documented in the TSPA-LA Model Document.

Table E.1-1. Discretization Test Simulations

Discretization Test Simulations	Nominal	Igneous Groundwater Release	Volcanic Eruptive Release	Seismic
Temporal discretization coarser time steps finer time steps	0 – 10,000 yr	0 – 10,000 yr	0 – 10,000 yr	0 – 10,000 yr
Spatial discretization fewer source term groups additional source term groups	0 – 10,000 yr	0 – 10,000 yr	n/a*	0 – 10,000 yr
Stochastic discretization Number of realizations 300 realizations 500 realizations 1000 realizations 2000 realizations	0 – 10,000 yr	0 – 10,000 yr	0 – 10,000 yr	0 – 10,000 yr
Stochastic discretization Random number seed five or more replicates for "x" number of realizations	0 – 10,000 yr	0 – 10,000 yr	0 – 10,000 yr	0 – 10,000 yr

Note. * The dose rate from the igneous eruptive release modeling case is not a function of the number of waste package groups

Once the appropriate time step size, number of source term groups, number of realizations, and random number seed have been determined, process testing simulations will be run. These tests will demonstrate the correct performance of the submodels that make up the TSPA model. These analyses will also be documented in the TSPA-LA Model Document.

Table E.1-2. Examples of Process Testing Simulations

Model	Description
Simplified Model	Put all waste packages in a single source term group. Use a simplified WP failure curve. Apply one constant seepage flow rate. Fix chemical parameters (e.g., pH, I, etc.) to constant values.
Full Model	Continuous Release Apply a continuous radionuclide release rate to the WP, invert, UZ, or SZ.
Full Model	Pulse Release Apply a pulse radionuclide release rate to the WP, invert, UZ, or SZ.
Submodel Tests	Exercise a submodel over its range of inputs.
Single Realization	Run a single realization whose behavior is representative of the median, 5th, and/or 95th percentile dose rate curve. Save all simulation results so that the mechanistic behavior of the model can be examined.

The simulations listed in Table E.1-2 would be run for all of the base cases where applicable. Also, the above are only a subset of the process testing that will be done; additional process testing simulations may be developed, and different variations of the tests could be considered.

E.2 BASE CASE SIMULATIONS

Base case simulations will be run for each TSPA scenario class (e.g., nominal, igneous groundwater release, igneous eruptive release, seismic). A base case simulation with a duration of the regulatory time period (10,000 years) will be run for each scenario class, as will a simulation with a duration to 20,000 years to demonstrate that the model results have no major changes after the regulatory time period (see Table E.2-1). These analyses will be documented in the TSPA-LA Analysis Document, and the 10,000 year results are expected to be documented in the License Application itself.

Table E.2-1. Base Case Simulations

Scenario Class	Duration
Nominal	0 – 10,000 years 0 – 20,000 years
Igneous Groundwater Release	0 – 10,000 years 0 – 20,000 years
Volcanic Eruptive Release	0 – 10,000 years 0 – 20,000 years
Seismic	0 – 10,000 years 0 – 20,000 years

E.3 SEQUENTIAL ONE-ON BARRIER/PROCESS SIMULATIONS

Table E.3-1 contains an example of one set of sequential one-on barrier/process simulations for the nominal scenario class. Additional simulations may be run for igneous/groundwater release modeling case and the seismic scenario class. Also, the barriers/processes could be added in a variety of different orders, different treatments of the barriers/processes could be considered, and additional processes/barriers could be considered. These analyses will be documented in the TSPA-LA Model Document.

Table E.3-1. Example of a Nominal Case Set of Sequential One-On Barrier/Process Simulations

Process Addition	Description
3,000 acre-feet	The assumption is that radionuclides cannot reach humans or biosphere without first being buffered by the 3000 acre-feet volume. For this case, assume infinite solubilities with entire inventory dissolved in 3000 acre-feet volume. Waste is assumed to be in powder form.
partial waste-form	Waste is now assumed to be in rod and glass-log form and sitting bare on the surface of the mountain (or at the repository level, but with the top of the mountain removed). But now the waste dissolves slowly according to the CSNF and codisposal degradation rates, but with infinite solubility and maximum colloids.
full waste-form	Add solubility/concentration limits for dissolved, irreversible, and reversible radionuclides.
precipitation/climate	Limited transport rate to the 3000 acre-feet biosphere (i.e., limited by the rate of advection at the precipitation rate).
infiltration/surficial soil barrier/decay heat	Soil layer and evapo-transpiration limit water ingress to the mountain.
seepage	Further limitation of flux of water contacting waste due to presence of drifts and fracture-matrix heterogeneity in the TSw.
UZ barrier	Add unsaturated zone flow and transport.
SZ barrier	Add saturated zone flow and transport.
cladding barrier	Add cladding as a barrier.
drip shield barrier	Add drip shields
invert barrier	Add invert, including its corrosion products.
waste package barrier	Add waste packages.

E.4 BARRIER/PROCESS NEUTRALIZATION

Table E.4-1 contains examples of barrier/process neutralization simulations. They would be performed for both the nominal and igneous groundwater release base cases by modifying the TSPA model. Barrier/process neutralization simulations may be developed for the volcanic eruptive release modeling case and seismic scenario class. Also, different ways of "neutralizing" the barriers/processes could be considered, and additional processes/barriers could be considered. Combinations of barriers may also be neutralized (e.g., two or more at a time rather than just one at a time). These analyses will be documented in the TSPA-LA Model Document.

Table E.4-1. Examples of Barrier/Process Neutralization Simulations

Barrier	Barrier/Process to be Modified
Waste Package	Neutralize the waste package
Drip Shield	Neutralize the drip shield
Engineered Barrier System	Neutralize the invert
Unsaturated Zone	Neutralize seepage
Waste Form	Neutralize solubility
Engineered Barrier System/Waste Package	Neutralize EBS and WP K_ds
Unsaturated Zone	Neutralize the UZ
Saturated Zone	Neutralize the SZ

E.5 DSNF AND NAVAL FUEL SENSITIVITY SIMULATIONS

Table E.5-1 contains examples of DSNF and Naval fuel sensitivity simulations. They would be performed for both the nominal and igneous groundwater release base cases. Simulations may also be developed for the igneous eruptive release modeling case and seismic scenario class. The current categorization of DSNF would result in 10 additional sensitivity analyses using the TSPA model. These analyses will be documented in the TSPA-LA Analysis Document.

Table E.5-1. Examples of DSNF and Naval Fuel Sensitivity Simulations

Fuel Type	Base Case Inventory Replacement
Naval	fuel source term release rate[1]
DSNF	inventory type 2 – Pu/U alloy
DSNF	inventory type 3 – Pu/U carbide
DSNF	inventory type 4 – MOX/Pu oxide
DSNF	inventory type 5 – Th/U carbide
DSNF	inventory type 6 – Th/U oxide
DSNF	inventory type 7 – Uranium metal
DSNF	inventory type 8 – Uranium oxide
DSNF	inventory type 9 – Al-based SNF
DSNF	inventory type 10 – U Nitride SNF
DSNF	inventory type 11 – U-Zirconium hydride

1 The naval fuel source term will be supplied by Naval Reactors and documented in a classified report. An unclassified summary will be provided to the DOE.

APPENDIX F

EXAMPLE TSPA-LA INPUT PARAMETER TABLE

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APPENDIX F EXAMPLE TSPA-LA INPUT PARAMETER TABLE

Tables of input parameters for the TSPA-LA model will be produced as part of the TSPA-LA Model Document. Table F-1 provides an example which illustrates the information that will be captured in these tables. Note that the information in this table is illustrative and may not reflect the final input parameters and/or sources used in the TSPA-LA model.

Table F-1. Seepage Input Parameters to the TSPA-LA Model (example)

Input Parameter	Description	Location	Abstraction Source	DTN Source	Uncertain/ Constant
Episodic_Factor	episodic factor	\TSPA_Model\Engineered_Barrier _System\Drift_Seepage\Seepage_ DLL_Inputs\	ANL-NBS-MD-000005, REV02 DRAFT	TBD	uncertain
Flow_Focus_Factor_Distribution	flow focus factor	\TSPA_Model\Engineered_Barrier _System\Drift_Seepage\Seepage_ DLL_Inputs\	ANL-NBS-MD-000005, REV02 DRAFT	TBD	uncertain
mean seepage flow rate	mean seepage flow rate distribution as a function of percolation flux	input file: SeepFlowMean.dat	ANL-NBS-MD-000005, REV02 DRAFT	TBD	uncertain
Seep_Uncertainty	seepage uncertainty for seepage fraction, mean seepage flow rate, and seepage flow rate std. dev.	\TSPA_Model\Engineered_Barrier _System\Drift_Seepage\Seepage_ DLL_Inputs\	ANL-NBS-MD-000005, REV02 DRAFT	TBD	uncertain
seepage flow rate std.dev.	seepage flow rate standard deviation distribution as a function of percolation flux	input file: SeepFlowSD.dat	ANL-NBS-MD-000005, REV02 DRAFT	TBD	uncertain
seepage fraction	seepage fraction distribution as a fuction of percolation flux	input file: SeepFrac.dat	ANL-NBS-MD-000005, REV02 DRAFT	TBD	uncertain
percolation flux	Percolation flux time-history 5 m from the crown of the drift. A set of percolation flux time-histories is provided for each infiltration scenario (low, mean, high) and for each infiltration bin that exist in a given infiltration scenario.	input files: CSNF_HT_high_pf_bin2.txt CSNF_HT_high_pf_bin3.txt CSNF_HT_high_pf_bin4.txt CSNF_HT_high_pf_bin5.txt CSNF_HT_low_pf_bin1.txt CSNF_HT_low_pf_bin2.txt CSNF_HT_mean_pf_bin2.txt CSNF_HT_mean_pf_bin3.txt CSNF_HT_mean_pf_bin4.txt CSNF_LT2_high_pf_bin2.txt CSNF_LT2_high_pf_bin3.txt CSNF_LT2_high_pf_bin4.txt CSNF_LT2_high_pf_bin5.txt CSNF_LT2_low_pf_bin1.txt CSNF_LT2_low_pf_bin2.txt CSNF_LT2_mean_pf_bin2.txt CSNF_LT2_mean_pf_bin3.txt CSNF_LT2_mean_pf_bin4.txt HLW_HT_high_pf_bin2.txt HLW_HT_high_pf_bin3.txt	ANL-EBS-MD-00049, REV01 DRAFT	TBD	constant

Table F-1. Seepage Input Parameters to the TSPA-LA Model (example) (Continued)

Input Parameter	Description	Location	Abstraction Source	DTN Source	Uncertain/ Constant
percolation flux	Percolation flux time-history 5 m from the crown of the drift. A set of percolation flux time-histories is provided for each infiltration scenario (low, mean, high) and for each infiltration bin that exist in a given infiltration scenario.	HLW_HT_high_pf_bin4.txt HLW_HT_high_pf_bin5.txt HLW_HT_low_pf_bin1.txt HLW_HT_low_pf_bin2.txt HLW_HT_mean_pf_bin2.txt HLW_HT_mean_pf_bin3.txt HLW_HT_mean_pf_bin4.txt HLW_LT2_high_pf_bin2.txt HLW_LT2_high_pf_bin3.txt HLW_LT2_high_pf_bin4.txt HLW_LT2_high_pf_bin5.txt HLW_LT2_low_pf_bin1.txt HLW_LT2_low_pf_bin2.txt HLW_LT2_mean_pf_bin2.txt HLW_LT2_mean_pf_bin3.txt HLW_LT2_mean_pf_bin4.txt	ANL-EBS-MD-00049, REV01 DRAFT	TBD	constant

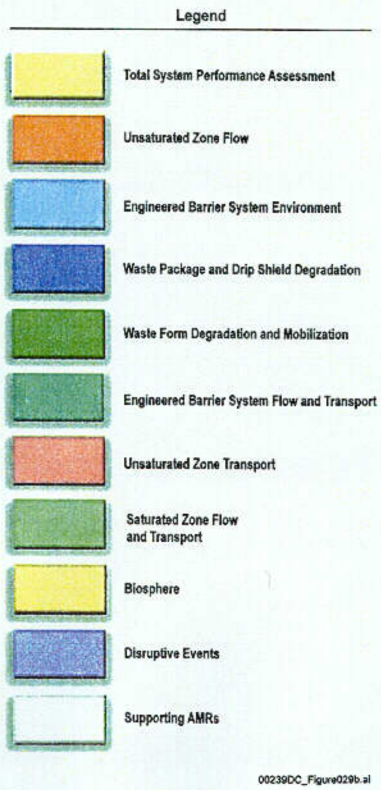
APPENDIX G

TSPA-LA DOCUMENT HIERARCHY

APPENDIX G TSPA-LA DOCUMENT HIERARCHY

The TSPA-LA will rely on numerous supporting documents for information and abstractions. A representation of the primary supporting documents for the following components is presented in the figures of this appendix (Figures G-1 through G-10): 1) UZ flow, 2) EBS environment, 3) waste package and drip shield degradation, 4) waste form degradation and mobilization, 5) EBS flow and transport, 6) UZ transport, 7) SZ flow and transport, 8) biosphere, 9) disruptive events igneous scenario class, and 10) disruptive events seismic scenario class. The document hierarchy is evolving, so these diagrams are intended to be illustrative and provide a general view of the main documents supporting TSPA-LA. Since the documentation is only proposed and is currently under development, the document identifiers are listed where available, but no DIRS are linked to this appendix. The Legend for the figures is shown below. Table G-1 presents a listing of some of the key documents that are expected to support TSPA-LA.

Note that the diagrams presented in this appendix reflect how information flows among the documentation that supports the development of each TSPA model component. The information flow presented in this context is generally not the same as the information flow between models in the TSPA model as depicted in Figure 5.1-1. In the former case, the information flow supports model development and analyses, whereas in the latter case, information flow enables model implementation. Also, note that the design and data feeds are not included on these diagrams. Finally, note that the "supporting AMR" boxes indicate documents that don't directly provide inputs to the TSPA model for that particular component. They may directly feed TSPA in another component.



C13

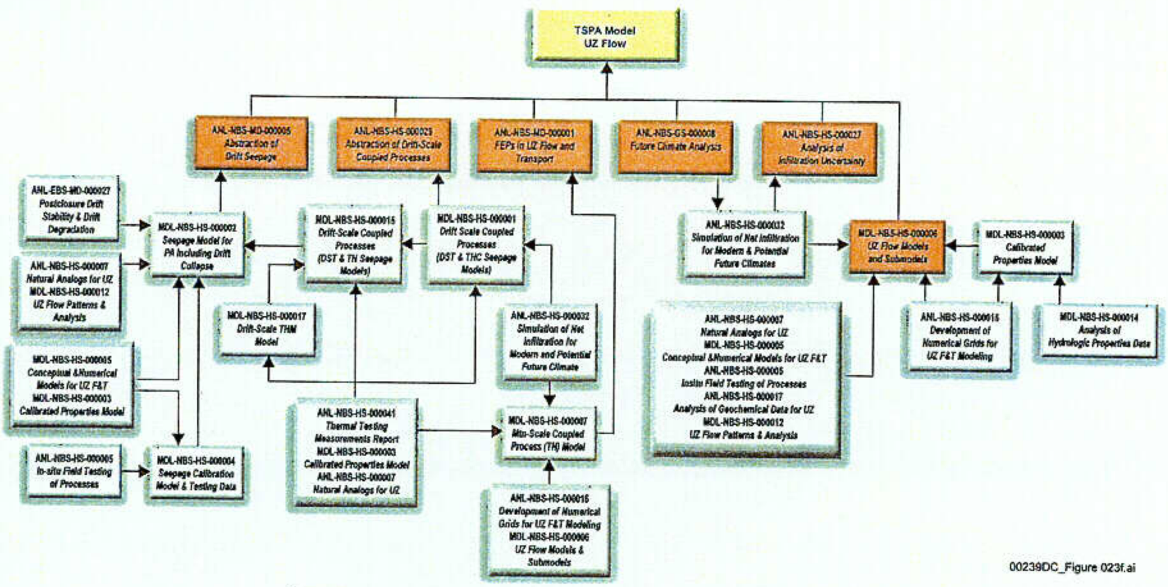
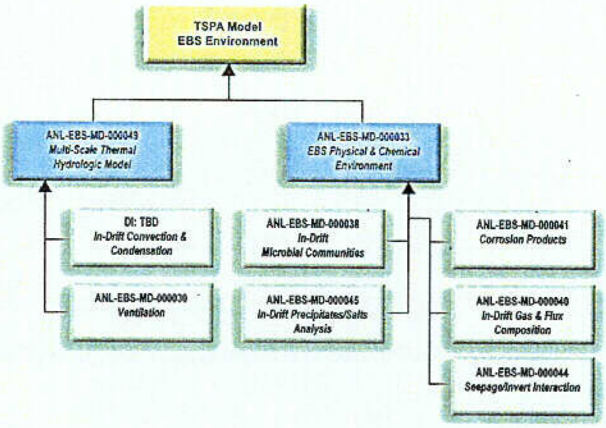


Figure G-1. Unsaturated Zone Flow Document Hierarchy



00239DC_Figure 021e.ai

Figure G-2. EBS Environment Document Hierarchy

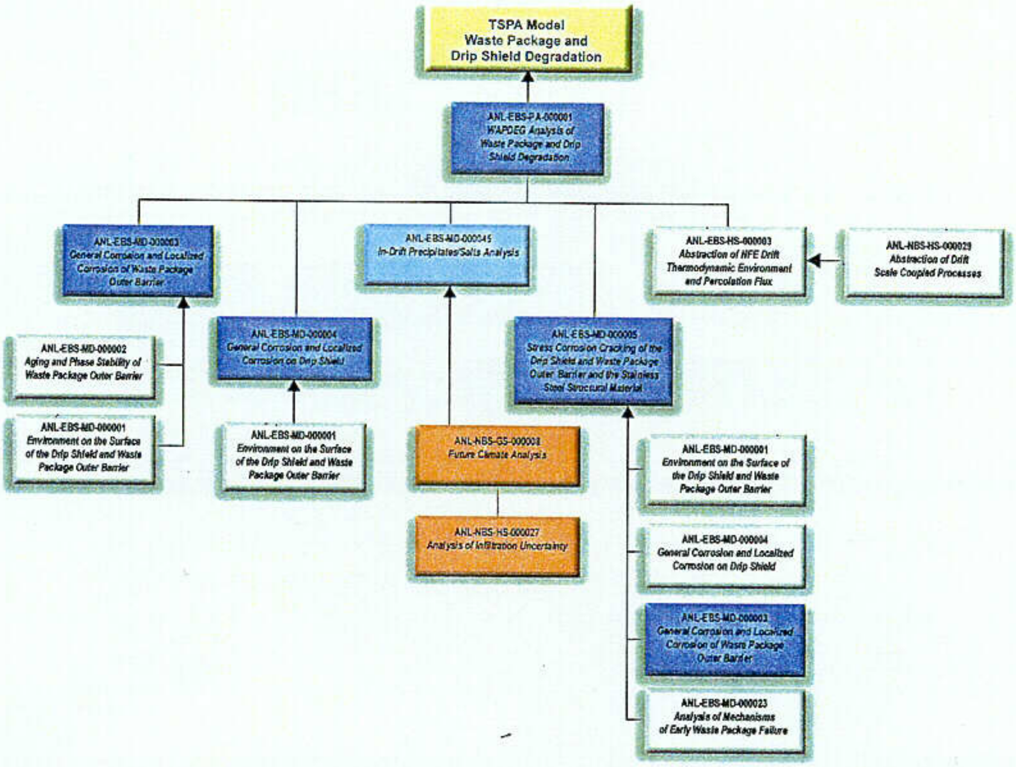


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Figure G-3. Waste Package and Drip Shield Degradation Document Hierarchy

C16

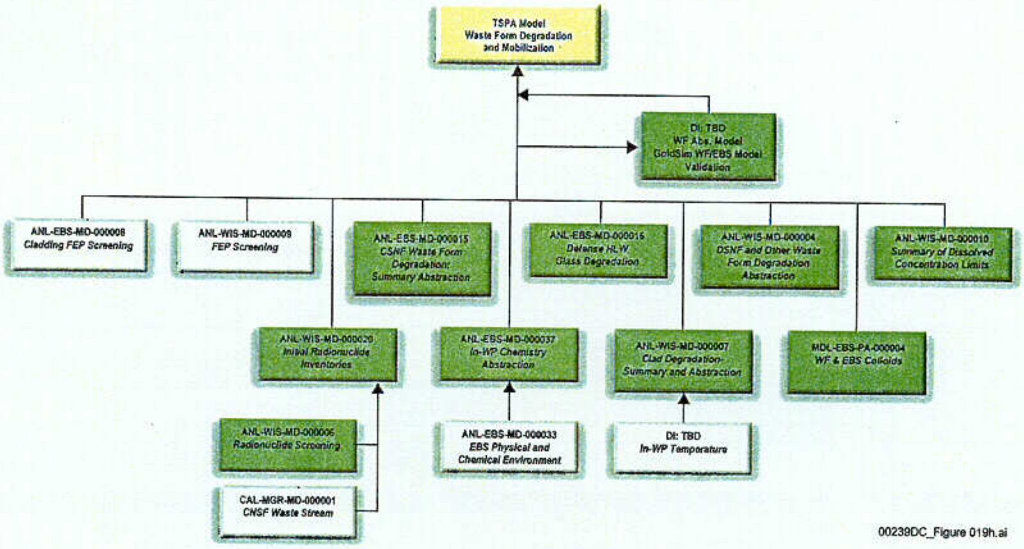

Figure G-4. Waste Form Degradation and Mobilization Document Hierarchy

C17

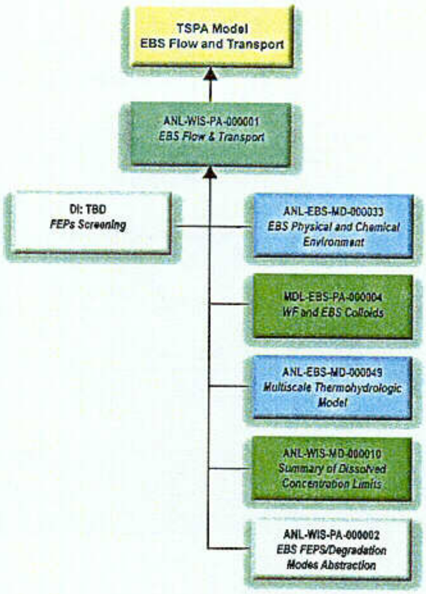

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Figure G-5. Engineered Barrier System Flow and Transport Document Hierarchy

C18

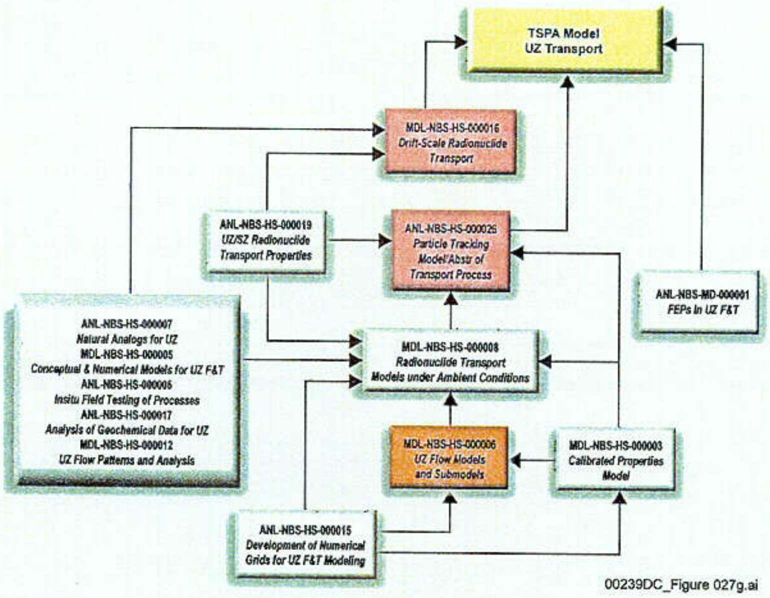

Figure G-6. Unsaturated Zone Transport Document Hierarchy

C19

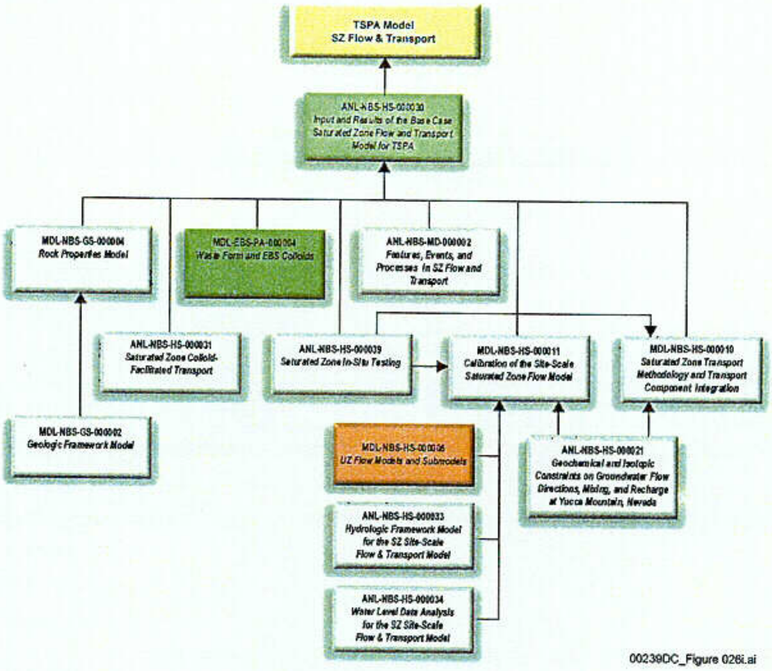

Figure G-7. Saturated Zone Flow and Transport Document Hierarchy

C20

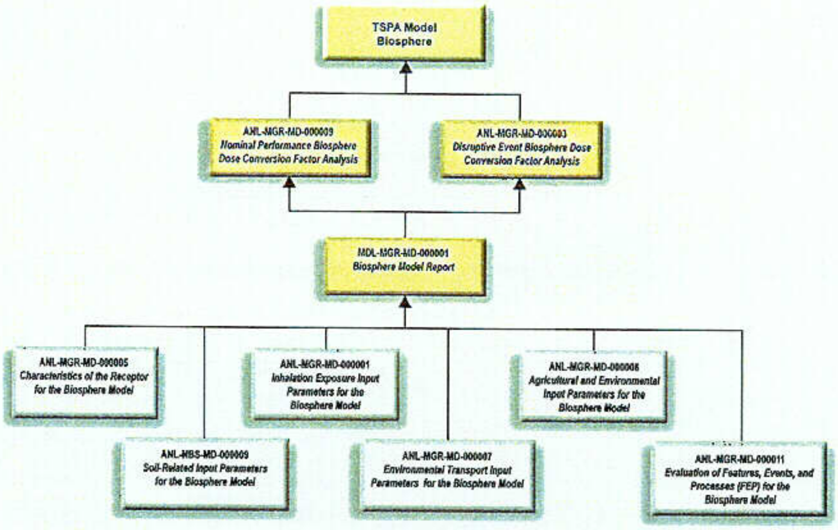

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Figure G-8. Biosphere Document Hierarchy

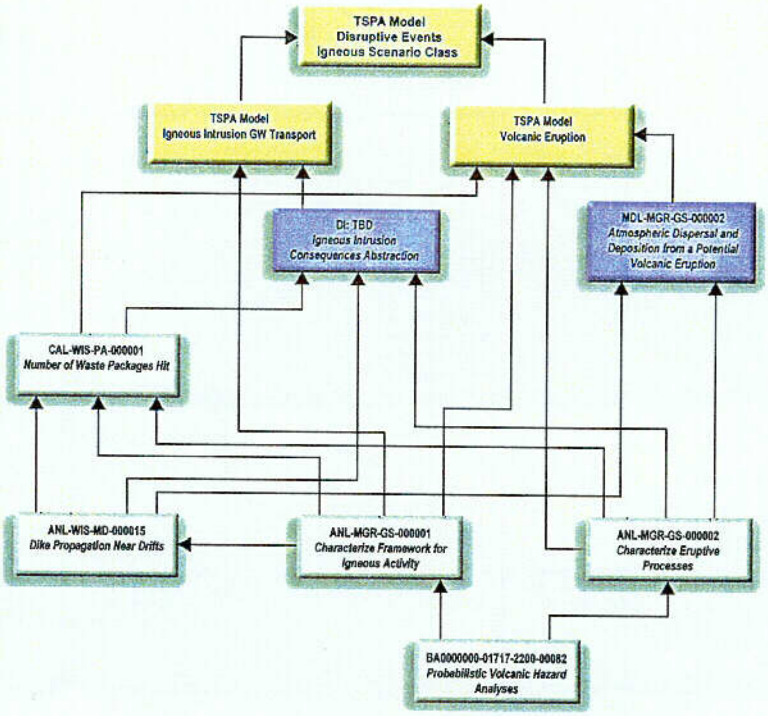

Figure G-9. Disruptive Events Igneous Scenario Class Document Hierarchy

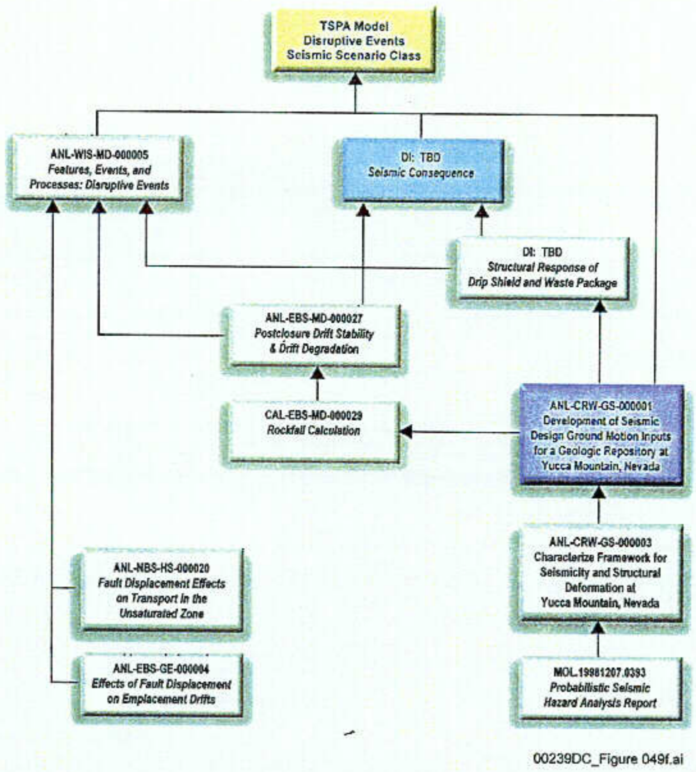

Figure G-10. Disruptive Events Seismic Scenario Class Document Hierarchy

C23

Table G-1. Key Documents that Directly Support TSPA-LA

Model	Document Title	Doc. ID	Document Control ID
Unsaturated Zone Flow			
Climate	Future Climate Analysis	U0005	ANL-NBS-GS-000008
Infiltration	Analysis of Infiltration Uncertainty	U0095	ANL-NBS-HS-000027
Mountain-Scale Flow Model	UZ Flow Models and Submodels	U0050	MDL-NBS-HS-000006
Drift Seepage	Abstraction of Drift Seepage	U0120	ANL-NBS-MD-000005
Drift Scale Coupled Processes	Abstraction of Drift Scale Coupled Processes	N0125	ANL-NBS-HS-000029
EBS Environment			
EBS Thermal-Hydrologic Environment	Multiscale Thermohydrologic Model	E0120	ANL-EBS-MD-000049
EBS Chemical Environment	EBS Physical & Chemical Environment Model	E0100	ANL-EBS-MD-000033
	In-Drift Precipitates/Salts Analysis	E0105	ANL-EBS-MD-000045
Waste Package and Drip Shield Degradation			
Waste Package and Drip Shield Degradation	WAPDEG Analysis of Waste Package and Drip Shield Degradation	W0050	ANL-EBS-PA-000001
Waste Package General and Localized Corrosion	General Corrosion and Localized Corrosion of Waste Package Outer Barrier	W0035	ANL-EBS-MD-000003
Drip Shield General and Localized Corrosion	Generalized Corrosion and Localized Corrosion on Drip Shield	W0085	ANL-EBS-MD-000004
Stress Corrosion Cracking of Waste Package and Drip Shield	SCC of Drip Shield and Waste Package Outer Barrier and the Stainless Steel Structural Material	W0095	ANL-EBS-MD-000005
Waste Form Degradation and Mobilization			
Radionuclide Inventory	Radionuclide Screening	F0015	ANL-WIS-MD-000006
	Initial Radionuclide Inventories	F0016	ANL-WIS-MD-000020
In-Package Chemistry	In- Package Chemistry Abstraction	F0170	ANL-EBS-MD-000037
Cladding Degradation	Clad Degradation - Summary and Abstraction	F0155	ANL-WIS-MD-000007
Waste Form Degradation	CSNF Waste Form Degradation: Summary Abstraction	F0055	ANL-EBS-MD-000015
	Defense HLW Glass Degradation	F0060	ANL-EBS-MD-000016
	DSNF and Other Waste Form Degradation Abstraction	F0065	ANL-WIS-MD-000004
Dissolved Radionuclide Concentration Limits	Summary of Dissolved Concentration Limits	F0095	ANL-WIS-MD-000010
Waste Form and EBS Colloids	Waste Form and EBS Colloids	F0115	MDL-EBS-PA-000004
EBS Flow and Transport			
EBS Flow and Transport	EBS Flow and Transport	E0095	ANL-WIS-PA-000001
Unsaturated Zone Transport			
UZ Particle Tracking	Particle Tracking Model/Abstraction of Transport Process	U0065	ANL-NBS-HS-000026
Drift Scale Radionuclide Transport	Drift-Scale Radionuclide Transport	U0230	MDL-NBS-HS-000016
Saturated Zone Flow and Transport			
SZ Convolution	SZ Transport Abstractions	S0055	ANL-NBS-HS-000030
1D SZ Transport	SZ Transport Abstractions	S0055	ANL-NBS-HS-000030
SZ Flow and Transport	SZ Transport Abstractions	S0055	ANL-NBS-HS-000030

Table G-1. Key Documents that Directly Support TSPA-LA (Continued)

Model	Document Title	Doc. ID	Document Control ID
Biosphere			
Biosphere	Biosphere Model Report	B0090	MDL-MGR-MD-000001
	Nominal Performance Biosphere Dose Conversion Factor Analysis	B0065	ANL-MGR-MD-000009
	Disruptive Event Biosphere Dose Conversion Factor Analysis	B0055	ANL-MGR-MD-000003
Disruptive Events			
Seismic Activity	Seismic Consequence	TBD	TBD
Igneous Intrusion	Igneous Intrusion Consequences Abstraction	TBD	TBD
Volcanic Eruption	Atmospheric Dispersal and Deposition from a Potential Volcanic Eruption	T0125	MDL-MGR-GS-000002