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METHODOLOGY USED FOR TOTAL SYSTEM PERFORMANCE ASSESSMENT OF THE POTENTIAL NUCLEAR WASTE REPOSITORY AT YUCCA MOUNTAIN (USA)

E. DEVONEC (1), S. D. SEVOUGIAN (1), P. D. MATTIE (1), J. A. MCNEISH (1), S. MISHRA (2)

(1) Duke Engineering and Services, 1180 Town Center Drive, Las Vegas, NV 89144, USA
(2) Duke Engineering and Services, 9111 Research Blvd, Austin, TX 78758, USA
E-mail: eve_devonec@ymc.gov

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ABSTRACT

The U.S. Department of Energy and its contractors are currently evaluating a site in Nevada (Yucca Mountain) for disposal of high-level radioactive waste from U.S. commercial nuclear plants and U.S. government-owned facilities. The suitability of the potential geologic repository is assessed, based on its performance in isolating the nuclear waste from the environment. Experimental data and models representing the natural and engineered barriers are combined into a Total System Performance Assessment (TSPA) model [1]. Process models included in the TSPA model are unsaturated zone flow and transport, thermal hydrology, in-drift geochemistry, waste package degradation, waste form degradation, engineered barrier system transport, saturated zone flow and transport, and biosphere transport. Because of the uncertainty in the current data and in the future evolution of the total system, simulations follow a probabilistic approach. Multiple realization simulations using Monte Carlo analysis are conducted over time periods of up to one million years, which estimates a range of possible behaviors of the repository. The environmental impact is measured primarily by the annual dose received by an average member of a critical population group residing 20 km down-gradient of the potential repository.

In addition to the nominal scenario, other exposure scenarios include the possibility of disruptive events such as volcanic eruption or intrusion, or accidental human intrusion. Sensitivity to key uncertain processes is analyzed. The influence of stochastic variables on the TSPA model output is assessed by "uncertainty importance analysis", e.g., regression analysis and classification tree analysis. Further investigation of the impact of parameters and assumptions is conducted through "one-off analysis", which consists in fixing a parameter at a particular value, using an alternative conceptual model, or in making a different assumption. Finally, robustness analysis evaluates the performance of the repository when various natural or engineered barriers are assumed to be
degraded. The objective of these analyses is to evaluate the performance of the potential repository system under conditions ranging from expected to highly unlikely, though physically possible conditions.

DEFINITION OF TOTAL SYSTEM PERFORMANCE ASSESSMENT

Performance assessment and total system performance assessment (TSPA) are terms with very specific meanings in the high-level radioactive waste management community. Performance assessment is a method of forecasting how a system or parts of a system, designed to contain radioactive waste, will behave over time. Its goal is to aid in determining whether the system can meet established performance requirements. A TSPA is the subset of performance assessment analyses in which all of the components of a system are linked into a single analysis (as defined in proposed 10 Code of Federal Regulations Part 63 [2] and in proposed 10 Code of Federal Regulations Part 963 [3]). A performance assessment treats both the engineered and natural system components. The engineered system is, to some extent, controllable, but the natural system is not. The responses of the total system extend over periods beyond those for which data have been, or can be, obtained.

![Figure 1 - Total System Performance Assessment Pyramid (adapted from Figure 1.1-1 in CRWMS M&O 2000)](image)

The process of constructing and implementing a TSPA is often described as a pyramid, where detailed information representing the various processes and components of a total system are distilled and linked into progressively more abstracted models used to analyze system performance (Figure 1). The base of the pyramid is built using all of the data and information collected by scientists and engineers involved in site characterization and engineering design. The base is large because it represents the composite of all the information gathered by a repository program. All of this information feeds the conceptualization of how various processes work. A conceptual model is a set of qualitative descriptions used to describe a system or subsystem for a given purpose. These models will need to be evaluated more or less stringently.
depending on how probable each is considered to be. The specific aspects for
describing a process on a larger scale are then extracted and incorporated into
computer models to deal with each of the relevant processes. Only information
determined to be a primary driver for the process makes it up the next level of the
pyramid. The upper level shows the final level of distillation of information into the most
critical aspects necessary to represent the total system. At this point, all of the models
are linked together in the TSPA model. These are the models used to forecast total
system behavior and estimate the likelihood that the behavior will comply with
regulations and ensure long-term safety.

As information flows up the pyramid, it becomes more abstracted, as depicted by the
decreasing width of the pyramid. However, abstraction is not synonymous with
simplification. If a particular component model cannot be simplified without losing
essential aspects of the model, it ceases to move up the pyramid and becomes part of
the TSPA calculation tool. The level of complexity used to represent a process is also
dictated by the sensitivity of the results of the TSPA to that particular process. The
more sensitive the process or parameter, the more detailed the model representation
tends to be. However, the degree of complexity is also limited by the state of
knowledge concerning the model.

MAJOR STEPS IN THE YUCCA MOUNTAIN PERFORMANCE ASSESSMENT

In general, the goal of performance assessment is to provide decision makers with a
reasonable estimate of the realistic future performance of the disposal system and a
clear display of the extent to which uncertainty in the present understanding of the
system affects that estimate (proposed 10 Code of Federal Regulations Part 63 [2]). In
order to capture the full detail of the uncertainty and variability in the behavior of the
repository system, the Yucca Mountain TSPA uses a probabilistic approach. This
approach was adopted by the U.S. Environmental Protection Agency (EPA) in 1985 in
the original radiation protection standards [4], and it is similar to that adopted by many
other repository programs internationally. The major steps of the TSPA approach are:

1. A series of TSPA scoping analyses were performed between 1991 and 1998,
sponsored by the U.S. Department of Energy (DOE). During the iterative process of
performing these analyses, knowledge was gained regarding the TSPA methods
and approach, and regarding the key features, events and processes (FEPs) that
most significantly impact postclosure performance of the potential Yucca Mountain
repository system. Additional information about the relevant FEPs was collected
from non-DOE-sponsored TSPAs, process model workshops and analyses, NRC
Issue Resolution Status Reports, expert elicitations, and external oversight groups.

2. Once identified, the FEPs are combined to avoid redundancy, then classified, and
finally screened using defined criteria to identify those that should be included in the
TSPA analysis and those that can be excluded.
3. Scenarios (i.e., representations of possible future states of the potential repository) are constructed using the retained FEPs. Scenarios are subsequently screened, by retaining only those that represent the conditions of greatest relevance to regulatory requirements and the long-term safety of the site. An estimate of the probability that the chosen scenarios will occur must be provided. The following major scenarios were retained:

- **Nominal Scenario** – Considers FEPs expected to occur during the time period of evaluation.

- **Disruptive Event Scenario** – Considers igneous disruption (i.e., volcanism) as an additional event that has a low probability of occurrence during the time period of evaluation. This scenario class includes two scenarios, igneous intrusion (indirect releases via groundwater) and volcanic eruption (direct releases).

- **Human Intrusion Scenario** – Considers a stylized event of human intrusion into the potential repository as defined in the governing regulations.

4. Models are developed to represent components of the system that are potentially important in the chosen scenarios.

5. Parameter uncertainty is accounted for by developing distributions of values for parameters that have natural variability or are imprecisely known. Each distribution describes a range of values within which the true value is believed to fall. However, single values are used to describe properties that are well known or for which uncertainty has been shown to have little or no effect on overall performance.

6. Calculations are performed using the TSPA model. Uncertainty associated with the selection of scenarios is included in the TSPA by conducting separate analyses for each scenario. Uncertainty associated with the model parameters is included in the TSPA by conducting multiple calculations for each scenario using values sampled from the ranges of possible values (Monte Carlo analysis). Each individual calculation uses a different set of sampled input values. In a statistical sense, the result of each individual TSPA calculation represents a different possible realization of the future performance of the system, consistent with the uncertainty in the input parameters.

7. Results of preliminary performance assessments are analyzed at the system and subsystem levels to identify the models and parameters that have the greatest effect on the behavior of the system [1]. Examples of system performance measures are dose to humans, concentration of radionuclides in groundwater, and cumulative radionuclide releases from the system. Interpretation of these results helps guide testing for site characterization, model development, repository design, and compliance with applicable long-term requirements.
CONCEPTUAL MODELS AND INFORMATION FLOW FOR THE NOMINAL SCENARIO

A schematic representation of the repository system (the repository drift is located approximately 300m below the surface, and 300m above the water table) and the major processes relevant to its performance is shown in Figure 2. It illustrates the individual component models that together must be analyzed in evaluating the behavior of the Yucca Mountain repository system. These components comprise the individual building blocks of the TSPA analysis. For the nominal scenario presented in this paper, the repository system is represented by eight major process models: Unsaturated Zone Flow, Engineered Barrier System Environments, Waste Package and Drip Shield Degradation, Waste Form Degradation, Engineered Barrier System Transport, Unsaturated Zone Transport, Saturated Zone Transport, and Biosphere.

Figure 2 – Representation of the Repository and the Major Components of the TSPA (adapted from Figure 1.8-1 in CRWMS M&O 2000 [1])
These major process models are represented in Figure 3, along with the sub-models they are built on. This figure shows a stylized conceptualization of the TSPA model hierarchy and information flow between the process models. Radionuclide transport is the primary consideration for information flow among the TSPA models. The TSPA model architecture and information flow is a sequential calculation in which each spatially based transport model may be run in succession, with output as “mass versus time” from an upstream spatial domain serving as the input of mass versus time for the spatial domain immediately downstream. Two key factors in accurately representing the information flow for the overall system are: (i) information and assumptions passed up the model pyramid must be consistent, and (ii) the parameters that most affect performance in the detailed process models must be appropriately represented in the subsequent subsystem and total system models, including the appropriate uncertainty range of the parameters.

**Nominal Scenario TSPA Model**

![Diagram of TSPA Model](image)

Figure 3 - Process Model Factors included in Total System Performance Assessment for the Nominal Scenario (adapted from Figure 3.1-3 in CRWMS M&O 2000 [1])

**CODE ARCHITECTURE AND NUMERICAL MODELS**

The overall information flow discussed above forms the basis for the architecture of the TSPA computer code. The executive driver program, or integrating shell, that links all the various component codes is GoldSim [5]. It is a probabilistic sampling program that
ties all the component models, codes, and response surfaces together in a coherent structure that allows for consistent parameter sampling among the component models. The GoldSim program is used to conduct multiple realization runs of the system. These yield a probability distribution of dose rate in the biosphere that shows uncertainty in dose rate based on uncertainty in all the component models.

Figure 4 provides a better understanding of the TSPA model code architecture (i.e., the actual computer codes used and the information transfer between codes). It includes both the codes run prior to the GoldSim program and those run in real time that are coupled to or within the GoldSim program. An important method of information transfer amongst the various codes is the use of response surfaces, which are multidimensional tables of output from one model to be used as input in another model. Based on the schematic information transfer shown in Figure 4, some response surfaces generated by codes external to GoldSim only provide data to other codes external to GoldSim. Other response surfaces, such as liquid saturation, temperature, and seepage flux, are directly incorporated into GoldSim as data tables that influence such things as waste form degradation rates. Not all couplings or all models are shown in Figure 4, (e.g., in-drift geochemical modeling is too complex to show all of its aspects in this figure).

![Figure 4 - TSPA Code Configuration: Information Flow Among Component Computer Codes (adapted from Figure 2.2-3 in CRWMS M&O 2000 [1])]
RESULTS AND SENSITIVITY ANALYSES

For any given scenario (nominal or disruptive), the Monte Carlo methodology requires the TSPA computer model to be evaluated for each of the equiprobable parameter sets sampled from their prescribed distributions. Thus, each realization results in a total dose history (i.e., table of dose rate as a function of time). The aggregation of all dose histories produces a picture of the overall uncertainty in predicted performance. Results of the TSPA model simulation for the nominal scenario, using 300 realizations, over 100,000 years is presented in Figure 5. The dose rate histories for all realizations (gray lines) provide an indication of the overall spread in model results given the uncertainties in the inputs. The mean dose rate history was calculated at each point in time and superimposed on the figure, as well as the median (50th), 5th, and 95th percentiles. The broad range in projected dose rates at any given time is due to the uncertainty and variability of TSPA model parameters, and their interaction with one another, which can be complex and highly nonlinear.

![Figure 5 - Simulated Annual Dose Histories for the Nominal Scenario](image)

Sensitivity analysis provides a useful and structured framework for unraveling the results of probabilistic performance assessments by examining the sensitivity of the TSPA model results (and their uncertainties) to the uncertainties and assumptions in model inputs. Three major methods are used.

First, uncertainty importance analysis is performed in order to identify which input parameters have the greatest influence on the spread (uncertainty) of the probabilistic model results. This is accomplished qualitatively using scatter plots, and quantitatively using statistical methods such as correlation-regression analysis and classification and regression tree analysis. The analyses are carried out using results from the probabilistic calculations at a fixed point in time, with the sampled inputs corresponding to each of the realizations being treated as independent variables and the computed outputs being treated as dependent variables.
Figure 6 is an example of regression analysis, which is a tool for quantifying the strength of input-output relationships in the TSPA model. To this end, a stepwise linear rank regression model is fitted between total dose at a given time (or some other performance measure) and all randomly sampled input variables. Parameters are ranked on the basis of how their exclusion would degrade the explanatory power of the regression model. The importance ranking metric used for this purpose is the uncertainty importance factor, which is defined as the loss in explanatory power ($R^2$-loss) divided by the coefficient of determination ($R^2$) of the regression model. Note that the uncertainty importance factor also quantifies what proportion of the total spread (variance) in total dose explained by the regression model can be attributed to the variable of interest. Figure 6 shows how uncertainty importance factors change with time for the key uncertain variables. Over the first 100,000 years, the stress corrosion cracking (SCC) outer lid stress profile is seen to be consistently the most important, followed by the median general corrosion rate of the Alloy-22 outer and middle lids. Note also the slow but steady increase in importance for saturated zone groundwater flux with time.

The second method is the probabilistic “one-off” analysis, which consists in modifying a parameter of interest from its original value while all other parameters are kept unchanged. In the TSPA implementation, the parameter of interest is given a single value (its 5th or 95th percentile value, whichever yields the more conservative model outcome), while all other parameters are characterized using their full probability distributions. This method analyzes the resiliency of the reference system when its parameters take extreme values. For instance, Figure 7 illustrates how the mean predicted dose rate is affected when the residual hoop stress state at the closure lid welds is fixed at the 95th and 5th percentile values of its uncertainty distribution.
The last type of analysis examines the robustness of the system by simulating potential repository performance when barriers (e.g., unsaturated zone, drip shield, waste package) are assumed to be degraded (or enhanced), one at a time or in combination. These analyses were conducted by fixing key parameters affecting the performance of each barrier near the extreme of their uncertainty distributions (5th or 95th percentile). In many of the analyses, several parameters are simultaneously set to unlikely values. The objective of such analyses is to examine the contribution of each of the barriers, and to determine the overall resiliency of the potential repository system to extreme conditions that are unlikely, but within the range of those believed physically possible. For instance, Figure 8 compares the mean nominal-scenario dose curves for the degraded and enhanced unsaturated zone flow and transport cases, along with the mean dose curve for the nominal-scenario base case.
SUMMARY REMARKS

The Total System Performance Assessment for the Yucca Mountain Site Recommendation Considerations Report is the culmination of a large body of scientific work. Scientific and engineering information has been integrated into a consistent picture of the overall repository system to project the future evolution of the potential repository system. Result uncertainty due to various assumptions and the current state of knowledge has been assessed by conducting a probabilistic analysis. Quantitative results of the TSPA are used to guide the future direction of the Yucca Mountain Project, as it proceeds towards the issuance of a Site Recommendation Report to the Secretary of Energy, the President, and the Congress of the USA.

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