STATUS OF INTEGRATED PERFORMANCE ASSESSMENT OF THE WASTE PACKAGES AND ENGINEERED BARRIER SYSTEM

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ABSTRACT

Performance assessment of the engineered barrier system for a nuclear waste repository combines information from relevant disciplines and predicts the net long-term performance of the EBS in units of regulatory goals for performance. The performance assessment models are specific to the proposed Yucca Mountain, Nevada site. Early assessments are used for project planning and feedback. The EBS scenarios activity develops the scenarios and the consequent event sequences. Initial model development for single waste packages indicates that the radionuclide release rate performance is sensitive to the water flux, element solubilities, and/or the mode of water contact with the waste. The latter in turn depends on local scale hydrology and the modes of corrosion for the container material. For the release rate summed over waste packages, variations among waste packages and their near-field environments are anticipated. These variations place demands on data acquisition and modeling, as well as modulate the impact of localized changes of conditions. Sampling in uncertainty assessment is a subsequent step in examining the reliability of predictions made in the performance assessments. Advances made in sampling methods are referenced.

INTRODUCTION

The Yucca Mountain Project (YMP) of the U.S. Department of Energy (DOE) is currently evaluating the suitability of Yucca Mountain in southern Nevada as a nuclear waste repository site. Lawrence Livermore National Laboratory (LLNL) has been assigned by the YMP, since 1982, to plan, develop, and qualify the waste package subsystem, including study of package-environment interactions.

Perhaps the greatest challenge for the nuclear waste disposal system is to provide sufficient demonstration of waste isolation performance over a very long time period. The U.S. Environmental Protection Agency (EPA) has set a performance criterion for the total system for a 10,000-year time frame (40 CFR 191)[a]. The U.S. Nuclear Regulatory Commission (NRC) has additionally set performance criteria for subsystems, including the engineered barrier system (EBS), to be met under anticipated processes and events (10 CFR 60.113). Briefly, these criteria state that the EBS shall be designed to provide substantially complete containment of the waste within the waste packages for a period of 300 to 1,000 years after repository closure, and to limit release rates of radionuclides from the EBS for the subsequent time period.

BACKGROUND AND APPROACH

Performance assessment of the EBS is the predictive tool that combines the necessary information from all fields and assesses the net performance of the EBS. The waste packages are the principal elements of the EBS with respect to holding waste and delaying its release. Other elements such as the air gap in the borehole, a possible borehole liner, and configuration of the emplacement drifts, serve to shelter the waste packages from harmful impacts of the environment such as dripping water.

The performance assessment of the EBS is oriented toward the regulatory performance measures. The EBS performance assessments provide the radionuclide source term, i.e., release rates from the EBS into the total geologic repository system, for total system performance assessment oriented toward the EPA requirements. EBS performance assessments also evaluate whether the EBS subsystem will remain in compliance with the NRC performance requirements on substantially complete containment and limited release rates from the EBS. In examining these core assessments, system reliability and uncertainty assessments will identify and quantify uncertainties, determine the degree of reliability produced by reducing uncertainties and by building a defense-in-depth approach, and aid in determining whether there is reasonable assurance in the predictions of compliance with the NRC performance requirements.

The EBS performance assessments must be based on a fundamental understanding of the protective features of the

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[a] CFR indicates the U.S. Code of Federal Regulations

unsaturated tuff environment, the mechanisms controlling release of radionuclides from the waste packages, and radionuclide transport in the unsaturated, thermally varying near-field zone. The EBS system performance models integrate models of the fundamental mechanisms and provide for interfaces and interactions. The system modeling activity aims to assure that all relevant processes and interactions are identified and included. The system performance assessments must be capable of addressing both anticipated processes and events for the NRC's subsystem performance requirements, and unanticipated, potentially disruptive conditions that might exist during the required isolation periods, for the EPA's total system performance requirements (40 CFR 191) and for the NRC's required investigation of potentially adverse site conditions (10 CFR 60.122).

Early performance assessments are used for project planning and feedback. The early models are of necessity based on today's information, but they play a part in the iterative process of development. The early assessments highlight some of the information needed and show how it may be used, aid performance allocation and design requirements, and help synchronize the specialized modeling and measurement activities by assuring consistent assumptions and interfaces. Continuing performance assessments will provide feedback during the progress of site characterization and design activities.

As an example, an early performance assessment will examine EBS-site interaction for a hypothesized site scenario, involving the cumulative movement of a waste-package-intersecting fault plane in excess of the movement allowed for in the design basis. This will aid in understanding the mechanisms and the impact of this potentially unfavorable site event, and thus what sizes and types of fault traces need to be searched for.

The EBS performance assessment (PA) models assemble conceptual models and data from the LLNL tasks specializing in modeling the near-field environment, container materials, waste forms, and engineering design concepts (see Figure 1). These areas in turn have overlapping needs for geochemical models as well as hydrological, mechanical, and materials process models. The scenario activity identifies site scenarios impacting EBS performance as well as EBS-scale scenarios. The scenario activity also identifies the EBS processes and event histories consequent to a scenario initiator.

Three types of assessment information are provided by the performance assessment models (see Figure 1). The first type is assessment of single waste package performance under different anticipated near-field environments. This information is useful to design activities. The second type relates to the performance of the set of all waste packages in the repository with respect to the NRC performance requirements on the EBS. This assessment also provides the source term for total system PA. The third type of assessment characterizes the reliability of the predictions made by the first two types of assessments.

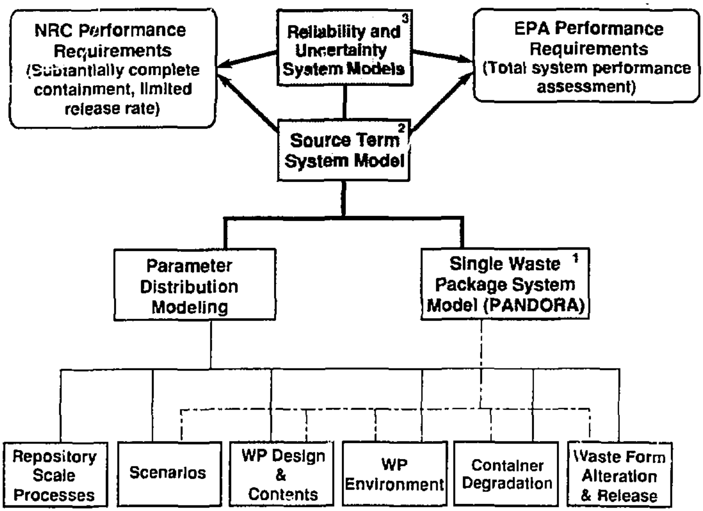

Figure 1. Hierarchy of models and their functional applications. Shading identifies PA models; numbers refer to types of information discussed in text.

PA ACTIVITIES AND PROGRESS

This section discusses developments to date and future plans. The physical processes and hence the conceptual models developed are site-specific for the unsaturated tuff medium at the proposed Yucca Mountain site.

Quality Assurance

The DOE has committed to conducting the Yucca Mountain Project under the controls of a quality assurance (QA) program acceptable to the NRC. In engineering management terms, QA provides management oversight for planning, controlling, documenting, and reviewing the technical work, for tracking safety-related uses of the technical work products, and for tracking the resolution and impacts of any open questions.

The transition from LLNL's previous QA program to an NRC-accepted QA program progressed during the past year. LLNL's revised QA program, quality procedures, and QA infrastructure implementation were successfully audited by DOE, with NRC and State of Nevada observers, in June 1989. LLNL's QA Program has been accepted by the NRC[1]. The LLNL Software QA Plan was accepted by the DOE Yucca Mountain Project Office (YMPO) in December 1989.

Planning prerequisites satisfied specifically for PA technical activity include the revision and approval by LLNL of the Scientific Investigation Plan for performance assessment, the writing and approval by LLNL of activity plans, and the identification and writing of activity-specific procedures. A Quality Procedure for internal interface control has been developed and released, since scenario and model development will involve extensive interaction with other technical areas in the LLNL Yucca Mountain Project. Individual software plans for computer-based model development activities are being written to particularize the application of the LLNL Software QA Plan.

EBS Scenarios

Earlier scenario development was done by Sandia National Laboratories as part of the site scenarios development, summarized in the Yucca Mountain Site Characterization Plan (SCP)[2] Section 8.3.5.13. Early conceptual developments identifying EBS processes and time evolution for the expected conditions scenario appeared in several reports, e.g., the reference environment for the waste packages,[3] thermal analysis,[4] and a "bathtub" water contact mode for waste form alteration and radionuclide release.[5]

The EBS scenarios activity has been expanded (SCP[2] Section 8.3.5.10.3.1) to address an NRC concern to assure attention to scenarios impacting the EBS subsystem, and to systematize the scenarios at the EBS scale and the EBS processes and event histories consequent to a scenario initiator.

The expanded activity for EBS scenarios has four subactivities. The first, scenarios identification, provides a listing of potential scenarios for the EBS. This subactivity has begun at Quality Assurance level 1 and is described in more detail below. The second subactivity, scenario delineation, requires the development and application of decision criteria. This subactivity's objective is to separate the scenarios into anticipated and unanticipated processes and events. The EBS subsystem performance under anticipated conditions is to meet the NRC requirements in 10 CFR 60.113. The third subactivity, scenarios quantification, develops and assembles the parameters of the near-field environment and of the waste packages and EBS. The fourth subactivity verifies the envelope of environmental conditions used as a basis in waste package design.

The EBS scenarios activity is needed to:

1. Provide a defensible basis for the selection of the set of EBS scenarios, processes, and boundary conditions, which are to be modeled and for which the performance of the EBS is to be assessed.

2. Provide a defensible basis for the set of near-field environmental conditions for which container and waste form testing and modeling capabilities must be established.

3. Provide for consistency and completeness in the assumptions and conclusions about the physical interfaces among the detailed processes and system elements being investigated.

The EBS scenarios identification subactivity identifies scenarios at the waste package scale, including local impacts of site-scale scenarios which may affect EBS performance, and scenarios initiated by local processes and events. For a specified site-scale scenario, the waste package-scale impacts and subsequent event history will differ for the various waste packages across the repository. The subactivity structures the scenario identification process and extends the scenarios to sequences of events leading to degradation of the waste package and eventual release processes for radionuclides. The subactivity will use applicable systems analysis tools such as structured expert opinion methods, failure modes and effects analysis, and event trees.

The current phase of the scenarios identification subactivity uses technical publications of Sandia National Laboratories on site-scale scenarios. Future phases of scenario work will involve interaction with Sandia. Procedures for external interface control, implementing the DOE Office of Civilian Radioactive Waste management (OCRWM) Systems Engineering Management Plan, will be developed.

Single Waste Package Assessment

The modeling goal of this activity is to take the environment and properties of each individual waste package, and model the time evolution of container degradation and subsequent radionuclide mobilization and release. The intended uses of the single waste package model are to be the kernel for the source term model (see below), to provide analyses for design options and for guidance on performance allocation and waste package design requirements, and to represent the interface and coupling among the processes studied in the specialized technical areas.

Early conceptual development,[6] extensions, and modeling have led to the first cycle of the Yucca Mountain-specific performance model, PANDORA-1 (see acknowledgments below).

Container degradation processes in the first PANDORA model are general corrosion in water vapor and liquid water. The model and data show that these processes are too slow to form a failure mode. To exercise the later process of waste form alteration, PANDORA-1 assumes a container breach when the uncorroded thickness decreases to a user-specified value.

Container failure will probably depend on localized corrosion, and will probably have the form of one or multiple small breaches, because of the corrosion-resistant properties of the alloys being considered for the Yucca Mountain site. Progress has been made in specialized studies aimed at developing alloy-specific and local-environment-specific predictive models of initiation and/or rates of localized corrosion modes.[7,8] Further progress will also require modeling or bounding of changes to the environment/container interface, e.g., rock movements to create a crevice needed for crevice corrosion.

Water contact with the waste package will occur only if there is some variation of the local environment away from its nominal condition, e.g., development of dripping or contact with moist rock. Detailed hydrothermal studies[9] predict the times when the temperature near a waste package drops below the boiling point and when a rewetting front starts to reach the rock near the waste package. Even then the rock is only partially saturated, and most or all water moves through the pore spaces of the rock, rather than by fracture trickling or dripping. The first PANDORA model takes the detailed calculation[9] as a boundary condition for temperature history and water presence, and simply assumes that a user-specified fraction of the gross water percolating near the waste package borehole drips into the waste package after it is assumed breached.

Waste form alteration and waste release are modeled using two assumed contact modes for water, the "bathtub" and trickle-through modes, and a mode with no liquid water. The following focuses on the modeling concepts used for the spent fuel waste form.

The "bathtub" model[5] assumes container breaches only above the fuel level, and dripping water, so the fuel can become immersed. The current model includes the observation in recent experiments by Wilson (summarized in Wilson and Bruton[10]) that, even after uranium in solution reaches a saturation level, concentrations of soluble elements such as Tc, Cs and I continue to increase in solution. This continuous rate is notionally associated with the matrix alteration rate. The "bathtub" model includes a filling period for the container as the fuel gradually becomes immersed, and assumes thorough mixing of solutes in the water within the container, and release as new water influx forces old water over the top.

The "trickle-through" model assumes multiple breaches of the container at top and bottom so that water can enter and then drain out. A fraction of the spent fuel surface is wetted by the trickle and thus participates in the alteration and release. A film of water is assumed to be maintained; the water mass moves down as a moving film, picking up solutes and exiting at the bottom.

In both modes of contact, diverse components of the spent fuel waste are accounted for. The C-14 component on the surface of cladding, the fraction of soluble and gaseous elements positioned in the spent fuel's cladding gap, and gaseous elements in the fuel matrix are considered. Matrix embedded elements include highly soluble elements whose release is limited by the rate of matrix alteration, and elements whose release rate from the waste package is limited by their solubility. Short-lived product radionuclides are coordinated with their parent radionuclides. Cladding and hardware radionuclides are presently treated as being lumped with the spent fuel matrix component.

In the no liquid water ("dry") mode, only release of gaseous radionuclides on the surface and in the cladding gap occurs.

Examples of release rates of matrix-limited and solubility-limited radioactive elements for a "bathtub" case are shown in Figures 2 and 3, for a waste package with 2.75 metric tons of initial heavy metal of PWR spent fuel with a burnup of 33,000 MWe-days. The example release rates shown are for a single waste package. The release rates to compare with regulatory limits are those for the sum over all waste packages. The latter is addressed under "Source Term Assessment" below.

In the matrix-limited case for technetium-99 (Tc-99) in Figure 2, a matrix alteration rate of 8.7×10^{-4} fraction/year is assumed, based on an interpretation of Tc-99 release rates at 85°C summarized in[10]. After the filling time, the initial concentration of Tc-99 in the water and the initial release rate are less than the maximum rate because the fuel was only

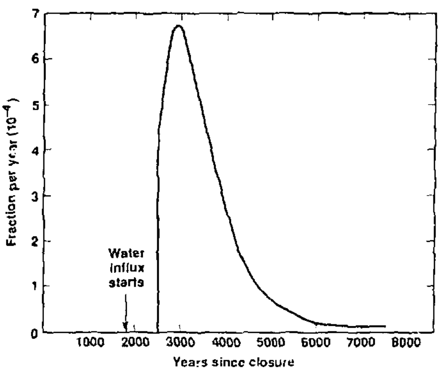

Figure 2. Illustrative release rate time history for Tc-99, for a "bathtub" contact mode. The gradual filling of the container with water, the eventual dissolution of the container's inventory of Tc-99, and the gradual refreshing of the water in the container influence the time history; see text. Given the assumed filling time and matrix alteration rate, the cladding gap inventory of Tc-99 makes a relatively small contribution to the initial release rate.

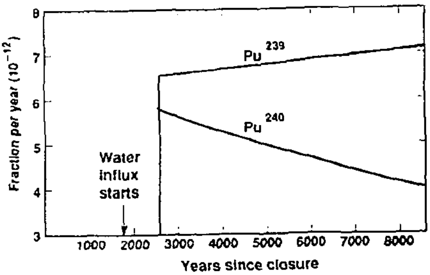

Figure 3. Illustrative release rate time histories for Pu-239 and Pu-240, for a "bathtub" contact mode. The plutonium in the exiting water is at a solubility limit. The proportion of isotopes changes with time.

gradually immersed during the filling period. The release rate peaks when all the Tc-99 in the package has been released into solution, and then declines as new water enters and mixes with the contained water.

In the solubility-limited case for plutonium (Pu) in Figure 3, the element has reached its solubility limit. The assumed solubility value represents a maximum based on several potential chemical conditions. The changing proportions in isotope release follow the fractional composition of the isotopes in the total element inventory.

An example for a soluble radionuclide, Tc-99, in a trickle-through case is shown in Figure 4. It is assumed that a fraction of the fuel within the container is wetted and kept wet by the flowing water. The time for a drop of water to enter and exit is assumed to be determined by the movement of the surface film of water. The matrix alteration rate for the wetted fuel surface is assumed to be the same as in the saturated case. In the example the wetted surface fraction is assumed to be 1%. These assumptions indicate data needs. An order of magnitude calculation can provide some initial perspective. A groundwater percolation flux of 0.5 mm/year and a "catchment area" with a radius of 0.8 meters, slightly

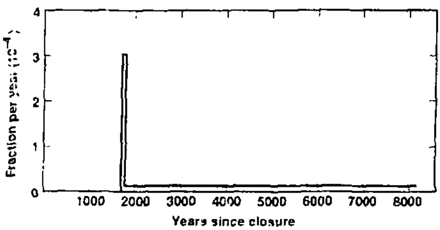

Figure 4. Illustrative release rate time history for Tc-99, for a trickle-through contact mode. A fraction of 0.01 of the spent fuel surface is assumed to be wetted; see text. The cladding gap component of that wetted fuel fraction exits as a short pulse. The matrix component is released gradually.

larger than a vertical emplacement borehole's cross section, give a water volume of 1 liter per year. At 20 drops per cm^3, this is one drop of water per half hour. This will probably drip from one point, and drain out. The amount of spent fuel that can be kept wet by a footprint of one trickling drop is rather small. On the other hand, the wetted surface area could increase in future millenia if the surface roughness of the spent fuel increases due to progressive alteration.

Some simple observations on sensitivity can be drawn from inspection of the models and the sample calculations. The release rate of Tc-99 is sensitive to the choice of "bathtub" or trickle-through case, because the rate is sensitive to the fraction of wetted fuel surface area. The release rate of Tc-99 is not sensitive to the water flux value in the trickle-through case, except possibly indirectly if the wetted surface area increases. The release rate of Tc-99 is only indirectly sensitive to the water flux value in the "bathtub" case, via container fill time and water refresh time. The release rate of Pu is not sensitive to the choice between "bathtub" or trickle-through case except for its starting time, but it is directly sensitive to the water flux value.

Concepts under consideration for future PANDORA models include evaporation of some of the entering water, the development of breaches at the bottom of the "bathtub" from the inside, and a possible diffusive mode of water contact, waste alteration, and release.[11] Nitao[12] has pointed out that under partially saturated hydrological conditions, water would be preferentially absorbed by tuff with its small-radius grain and pore sizes. To maintain a water film through container cracks and over spent fuel elements, development of small-radius surface texture, i.e., high surface roughness, would be necessary.

PANDORA-1 includes models for heat generation rate, temperature profile inside the waste package, and thermal stress. Future versions will add radiation profile and mechanical stresses which may influence corrosion modes and waste form processes. An extension currently being planned for PANDORA will incorporate new information in the near-field, container materials, and waste forms areas, and will extend the range of anticipated waste-package scenarios. PANDORA-1 was developed with use of software engineering and software lifecycle methods, which will aid in the transition to the revised QA program.

Source Term Assessment

1. Concepts. We are developing concepts for the first version of the Yucca Mountain-specific source term model, i.e., the containment and release rate performance summed over waste packages. The first model will be for anticipated processes and events. The task is non-trivial because different waste packages are subjected to different conditions, and the largest contributors to net release rate will probably come from a small number of packages with off-average conditions.

The existence of variation in conditions among the waste packages is an essential part of the performance allocation for meeting the EBS performance requirements. This is included in the performance allocation in the SCP[2] Sections 8.3.5.9 and 8.3.5.10. Different waste packages are expected to have different local environments (e.g., contact or no contact with liquid water), and the times of initial breaches and/or wettings of waste packages are expected to be spread out over time. Differences in container contents, other stochastic differences, and temperature field differences may also be expected. These will lead to differences in the results for the individual waste packages being summed over.

To produce the source term while taking the differences among waste packages into account, the source term model (see Figure 5):
(1) determines the ranges and distributions of the local environments, contents, and other parameters of the waste packages;
(2) determines the performances of the waste packages, for each waste package or for a sample, using PANDORA as a basis:
(3) sums results over the waste packages.

The determination of the distributions of local environments should address the site scenario, variations in geologic behavior and designed features over space for the given site scenario, and variations in relevant fine-scale local details of events or properties, or at least bounding characterizations of these local details. Container responses will likely be sensitive to local details of rock movement and water flow as well as to broadly varying properties such as temperature. Details of container alteration will be important to the subsequent processes of waste form alteration and release. Structuring the qualitative differences in the possible sequences of details may be done with tools such as failure modes and effects analysis and event trees.

2. Example. An example source term calculation can be used as an outline of the process, and as a sensitivity study to show the importance of data to be developed in the future. The calculation should not be considered definitive in terms of model outputs. Some processes listed in the SCP and expected to be relied on to help the EBS subsystem meet the performance goals, and for which characterization or design work is planned, are not yet included in our model of EBS performance.

Many elements of data are not yet available. To get the assessment process going, as a substitute for data we use parameter performance allocations from the SCP[2] Section 8.3.5.10 as assumptions.

For the distribution of local environments among the waste packages for the anticipated-conditions scenario, the SCP allocates that nine tenths of the waste packages shall remain dry, while one tenth may become "wet". The "wet" condition is specified only to the extent of limiting the amount of groundwater flux in or near the borehole to 20 liters/year. To be more specific, we proportion among the two wet contact modes modeled in PANDORA-1: we assume 0.1 of the wet packages have the "bathtub" mode and 0.9 of the wet packages have the trickle-through mode. Further, we assume the water influx in the wet cases is 1 liter/year as in the earlier examples in this paper rather than the upper bound of 20 liters/year allocat‹ ¹ in the SCP.

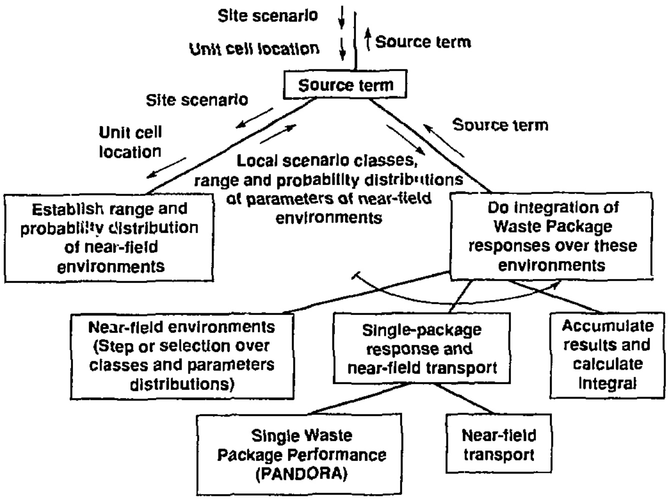

Figure 5. Structure chart for the source term model. The source term model calculation involves three major functions: the determination of the distribution of near-field environments and other parameters, the determination of single waste package responses, and a sum or integral. The figure uses the conventions for computer program structure charts. Activities or computer subroutines are in boxes. Data flows are arrows with nearby labels. Equal-level activities are done from left to right; the arc indicates repetition of activities.

The times of water contact and container breach are to be spread out in time, at least over 100 years according to the SCP performance allocation. Differences in the temperature field or stochastic differences in localized environmental changes or corrosion responses would contribute to this spread in time. We first do a sum over containers that fail at the same time, with container proportions as described above of 0.9 dry, 0.01 "bathtub" contact mode, and 0.09 trickle-through contact mode. The further sum of these sets over the range of failure times is a step we will only indicate qualitatively here.

The example release rates for packages with the two water contact modes were shown in Figures 2 and 4 for a selected radionuclide, technetium-99 (Tc-99). For the dry contact mode there is zero release. Doing a weighted sum of these results, all starting in the same year, we get the result shown in Figure 6. Except for the one-year early peak, the result is slightly below the NRC's performance goal of 1×10^{-5} fraction/year. Introducing a spread of initiation times will reduce the pulsed peak value.

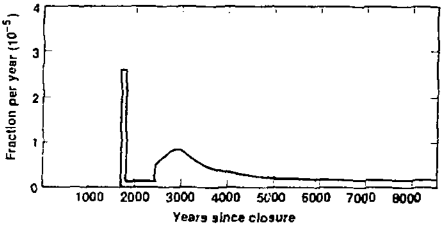

Figure 6. Illustrative release rate for Tc-99, a sum over waste packages experiencing dry, "bathtub", and trickle-through water contact modes; with equal times of initial water entry into a breach. Further summation over packages with different times of water contact will produce a *source term* for the Tc-99.

As a sensitivity consideration, it is apparent that if we were to assign the "bathtub" case for all the "wet" 10% allocated by the SCP, then the calculated release rate over all the waste packages would be as high as 6.7×10^{-5} fraction/year. This value is greater than the NRC's performance goal (remember that other elements from the SCP performance allocation are not in the model yet). This example sensitivity calculation shows that improvements in demonstration of EBS system performance can be obtained by studying hydrology (how much water gets into the borehole and into a breached container) and container corrosion (if a container is breached, can we expect multiple breaches to develop). Activities to address these questions are already in the SCP; here we wish to illustrate their importance.

Geochemical principles also influence the waste matrix alteration rate, which is a key parameter in the calculation. The trickle-through mode provides a perhaps significantly different geochemical environment for wetted fuel (low water to fuel ratio and more air), and a longer time period of alteration for which the chemical mechanisms and rates must be predicted. Activities to study these issues are also planned in the SCP.

Reliability and Uncertainty Assessment

One major element of the reliability of model predictions is the distribution of model output due to the distributions of inputs. Estimation of the mean and distribution of the output is often done using a sampling method: sampling on inputs, calculating the model, and doing statistics on the sample of outputs. We have looked theoretically and by numerical experiments at the variance reduction and robust performance for a range of model types when using Latin hypercube sampling and several other methods. We have developed a new method which combines features of several methods, and are extending tests of the method. Sampling is also under evaluation for doing an integration in the source term problem when the number of variables to be integrated over is large.

We looked at several existing sampling methods. Latin hypercube sampling (LHS) is a popular sampling method for variance reduction, but it has not been possible in practice to calculate how much variance reduction you get in any application.[13] Now we can calculate this and we find that the variance reduction from LHS is quite limited,[14] in many applications not much better than simple random sampling.

A new sampling method, controlled sampling, combines several features from LHS and stratified sampling methods, plus new features. It has robust performance over a variety of models like stratified sampling, and a variance lower than LHS as shown by numerical experiments,[14] and is expected to show a variance lower than simple stratified sampling.

SUMMARY

Performance assessment is oriented toward regulatory performance requirements, and is site specific. EBS scenario development and event sequence development lead into single-package PA, which provides the kernel for PA summed over all waste packages. Study of variations among waste packages and their near-field environments will be needed in the summed performance assessment for two reasons. First, a single assumed bounding case may provide too pessimistic an overestimate of radionuclide release rates. Second, in more realistic assessments the likely median condition will provide no radionuclide release, but variations may provide some release. Sampling in uncertainty assessment is a subsequent step in examining the reliability of predictions made in the performance assessments. Advances in sampling methods were referenced.

ACKNOWLEDGMENTS

This paper has used information from several studies not yet at the published report stage. D. [illegible] and C. Hardenbrook completed and implemented the single waste package performance model PANDORA-1. R. Thatcher developed and tested the controlled sampling method. W. O'Connell derived the amount of variance reduction attainable by the Latin hypercube method.

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