WASTE PACKAGE PERFORMANCE ASSESSMENT FOR THE YUCCA MOUNTAIN PROJECT*

W. J. O'Connell, D. A. Lappa, and R. M. Thatcher
Lawrence Livermore National Laboratory
Livermore, CA 94550

ABSTRACT

We completed a first cycle of model development from a specification to a computer program, PANDORA-1, for long-term performance assessment of waste packages. The model for one waste package at a time incorporates processes specific to the unsaturated environment at the proposed Yucca Mountain, NV, site. PANDORA-1 models the most likely processes and several modes of waste alteration and release. The development identified information needs for future models; many processes, local details, and combinations will have to be examined. Integration of ensemble performance and quantification of uncertainties are modeling steps at higher aggregation. Methodologies for these steps include sampling, which is well studied; we have focused on several open questions. We can now calculate the amount of variance reduction available from Latin hypercube sampling; it is a limited reduction. A new method, controlled sampling, provides substantial variance reduction for a broad range of model functions. An uncertainty analysis test-bed program compares the new with old sampling methods.

INTRODUCTION

Since 1982 the Lawrence Livermore National Laboratory (LLNL) has been assigned responsibility by the US Department of Energy (DOE) Yucca Mountain Project for development of the waste package for emplacement in tuff, which includes the definition of the package environment, material development and testing, package design, performance assessment, and testing. The concepts, data, and plans for the waste package are presented in the Site Characterization Plan (SCP) (1).

Waste package systems performance assessment is oriented toward assessing the post-closure performance of the set of waste packages in the proposed repository in terms of performance goals set by the US Nuclear Regulatory Commission (NRC). The NRC regulations set long-term performance requirements on the engineered barrier system: substantially complete containment for a time period, and limited release rate for the post-containment period. The DOE conceptual design puts reliance on the components of the waste package in meeting these goals (see paper by Cloninger et al., this session). To assess performance with respect to the requirements, three levels of aggregation must be modeled: individual waste packages, the ensemble of waste packages within the repository, and uncertainty or probabilistic distribution of performance outcomes for the ensemble.

The performance assessment task within the project at LLNL assembles conceptual models and data from the tasks specialized in design, barrier materials, waste form materials, and near-field environment (see Fig. 1). These models are coupled within systems models at the three levels of aggregation, examining interactions among processes and evaluating the net long-term performance. The core model is PANDORA, a deterministic model evaluating the performance of one waste package at a time for a given set of initial and time-varying local conditions. An ensemble model will assess the performance of the set of waste packages, representing the range of conditions affecting the waste packages and integrating over the waste packages to

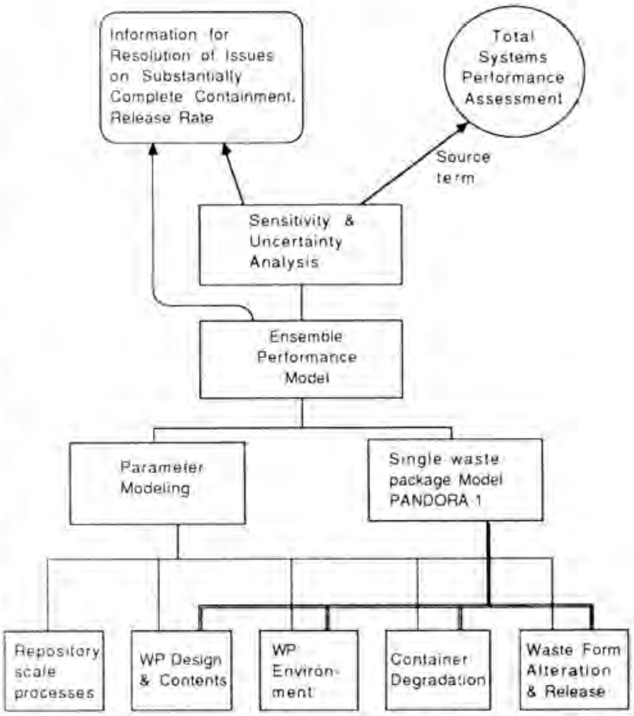

Fig. 1. Hierarchy of Models and Modeling Areas. The Detailed Models in the Specialized Areas Feed Concepts and Parametric Values to the System Models.

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find the net ensemble performance in terms of regulatory goals.

The third level model permits sensitivity and uncertainty analyses. Necessary inputs are some characterization of the uncertainties or distributions of input parameters of the ensemble model, including some characterization of correlations among inputs. Outputs from this level of analysis include a quantitative description of the uncertainty in the predicted ensemble performance, and the distribution of performance results in terms of a cumulative distribution function (CDF). The latter is transferred as the source term for the total system performance assessment. (The total system includes repository and site as well as engineered barrier system.)

In early activities, we developed and implemented the first cycle of the deterministic waste package performance model, PANDORA-1, and evaluated and developed ensemble/uncertainty methodologies. We also developed quality assurance procedures and planned (1,2) for the 1988-95 time period to develop data, models, interfaces among activities, and assessments on the topics needed for a license application.

The next section discusses the PANDORA-1 model and some of the information developed, as well as our approach to developing quality software. We then discuss ensemble and uncertainty analysis methodologies. Numerous techniques and reviews, e.g., (3), are available. We have focused on several outstanding questions: exactly how good is the widely used Latin hypercube sampling (LHS) (4), and might other methods better address our needs. Finally, we discuss a new sampling method, controlled sampling.

DETERMINISTIC MODEL PANDORA-1

PANDORA-1 (Lappa and Hardenbrook, in preparation) examines the performance of a single waste package within a range of conditions. The outputs are performance measures -- duration until first breach of the container and release rates of radionuclides -- that will be summed over packages by an ensemble model to compare with regulatory performance requirements. Our primary goals during the first cycle of model development were to identify concepts important to site-specific performance and to determine how well the performance of the waste packages could be predicted or bounded, given current knowledge about the conditions specific to the proposed Yucca Mountain site. Some secondary goals were to identify data needs and interfaces to plan the following cycles leading to license application; and to exercise quality control practices linked to software engineering practice, as a support to quality assurance.

Conceptual and specification development proceeded on two tracks. On one track, local scenarios, conceptual description of processes, and performance allocation to system elements were developed and reported in LLNL project reports and in the SCP (1). On a related track, an initial specification (5) for PANDORA-1 was completed and updated. For most submodels, the specification input was closed September 1987; for some submodels, updates based on recent experimental results were made as late as May 1988.

The local scenarios modeled in PANDORA-1 include the scenario expected for most waste packages, no contact with any significant amount of liquid water; and two less likely or unlikely scenarios involving dripping or flowing water contact. The latter scenarios require some assumptions, since conditions for fracture flow and mechanisms for dripping water and for water entry into a breached container remain to be investigated.

A model of diffusive contact and transport is deferred to the second cycle, PANDORA-2, because information is not yet available on the possible extent of continuous diffusive pathways. The likely situation under the unsaturated conditions is that water is preferentially absorbed in the porous matrix of the tuff; there is not enough water to fill fractures in the tuff and gaps between the tuff and package components. Then fractures and gaps are predominantly air-filled and serve as interruptions rather than conduits for connectivity of the water volume.

PANDORA-1 includes the most expected scenario for the bulk of the waste packages, i.e., no liquid water contact. Following closure, the near-field temperature will rise above the boiling point of the vadose groundwater. For several hundred years, the waste packages will exist within an air-steam atmosphere; the general uniform corrosion rate will be very low. During this period, some portion of the containers may be breached due to undetected fabrication defects or due to rare local variations in the environmental conditions. Even after the temperature of the near field drops below the boiling point, an entrant convective flux of groundwater is not expected because of the partially saturated condition together with the substantial capillary suction of the tuff. The expected environment will be humid air and possible small-area contact with moist tuff. Once containment is lost by any means, a fraction of the gaseous radionuclides, particularly carbon-14, but also in early failure cases krypton-85 and hydrogen-3 (tritium), will escape the waste package.

For a water-contact scenario in PANDORA-1, we assume that once the temperature of the near field drops below the boiling point, some water contacts and, after breach of the container, enters the waste package by unspecified means. The host rock water flux puts a limit on the package water flux. PANDORA-1 models general corrosion in steam-air and water environments; this corrosion proceeds very slowly for the container alloys under consideration, and hence is not a container breach mode. Localized corrosion modes are a central concern. They are not sure to occur (and indeed a goal of design and material selection is to avoid or minimize the occurrence of such modes), but they are conceivable. Predictive alloy-specific models for localized corrosion modes, and for local variations in container environment affecting corrosion, have not yet been developed.

PANDORA-1, given by assumption a container breach, also models waste alteration and release. Depending on how many cracks and breaches the container has, water may fill the container and overflow, or may trickle through. In the latter scenario, the water contact time and area are significant. The PANDORA-1 model accounts for the different release behaviors of various radionuclides in the glass waste and the components of spent fuel: fuel gap-grain inventory fraction, fuel matrix fraction, C-14 fraction available on the surface of fuel cladding, and gaseous as well as water-mediated releases. Release rates are, for some radionuclides, limited by their elemental solubility at the established conditions; and for other radionuclides, by the gap-grain fraction, the holdup in a partially failed container, and the alteration rate of the spent fuel matrix. The present model does not treat the presence of the spent fuel cladding or glass pour canister as barriers to release.

Figure 2 provides a general description of the grouping and relationships of the physical process submodels described above or identified as information needs for PANDORA development. The primary physical processes with which the model is concerned are: radionuclide inventories and decay, and the associated radiation field and heat generation rates; heat transport and resulting temperatures; geometric configuration, material properties, and mechanical stresses; the amount, chemistry, and contact mode of

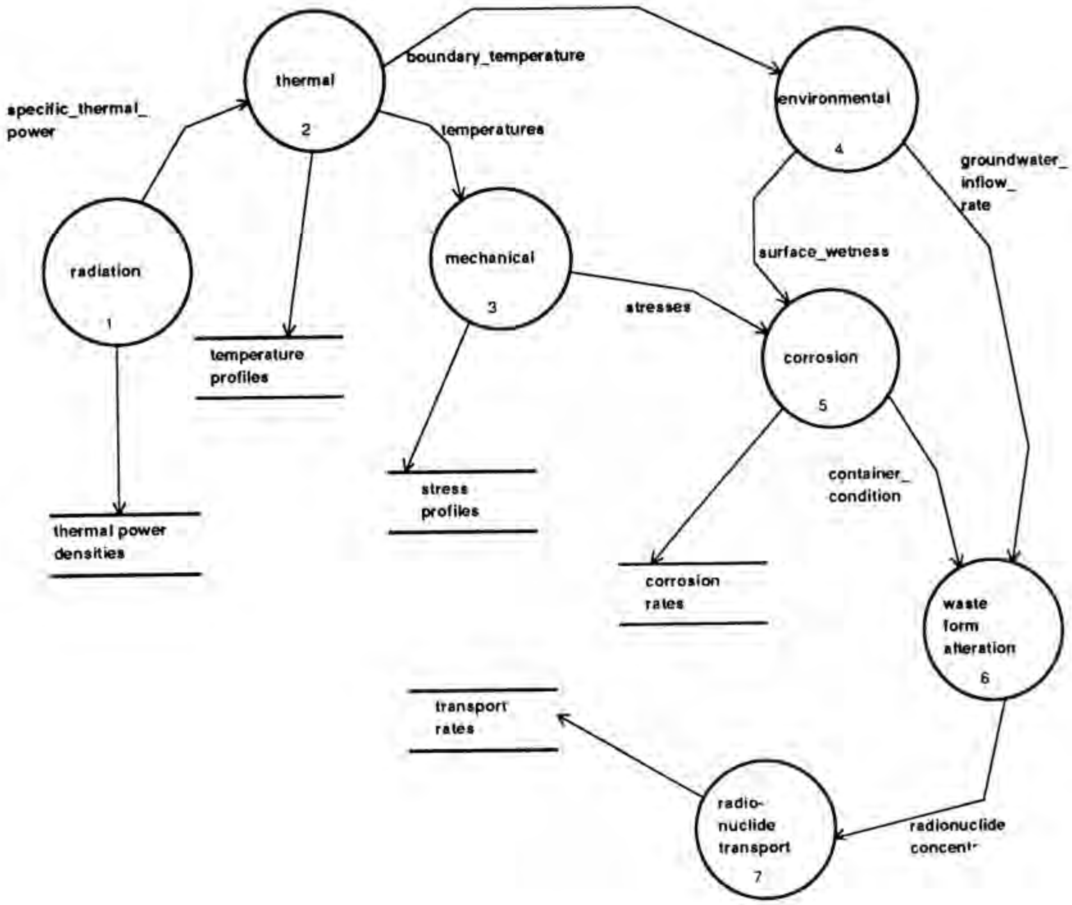

Fig. 2. Functional Data Flow Diagram for PANDORA.

groundwater/steam/vapors affecting the waste package; the alteration of container, waste form, and near-field native materials; the transport of radionuclides into and through the near-field; and synergistic effects.

This long list of processes includes many complex elements. In eliciting first-cycle models from the experts, we found that the uncertainties exceeded the knowns; indeed that is why the Project has an extensive Site Characterization Plan. Present assertions about the processes are limited. Notable problem areas are the long-term hydrology within a highly fractured, partially saturated, porous medium subjected to temporally varying thermal gradients and temperatures exceeding the boiling point of water; localized metal corrosion modes in an unsaturated environment; and the long-term chemical behavior of waste form/container/groundwater/tuff systems within a temporally varying radiation/thermal/hydrologic environment.

Other variabilities include conditions that vary with location in the repository; temperature varying with time; spent fuel type, burnup, and time out-of-reactor when emplaced; and vitrified high-level waste radionuclide inventory range and glass composition range allowed within the waste acceptance criteria.

Our work in assembling concepts and data, and in building a systems model, identified information needs. The identified needs are exemplified in the data flow diagram, Fig. 2; in the information needs, interfaces, and interconnected schedules published in the SCP (1); and in a more detailed long-range planning network being developed by the Project.

The qualitative conclusions of the first cycle of modeling are threefold. First, in the most common scenario, the containers will be in a steam or water vapor environment, and the corrosion rate is so low that the container will not breach during the first 10,000 years.

Second, to characterize the rare breaches requires advances beyond present predictive capabilities. That is, to demonstrate the first-order conclusion and to search for any container failure and waste release events, many processes, local details, and combinations must be modeled. For example, in the absence of substantial general corrosion, localized corrosion modes will probably control container failure. Among these modes, crevice corrosion requires a crevice and an electrolyte contact. Stress corrosion cracking requires electrolyte contact at a point where there is stress, such as weld residual stress. Thus the local modes of water contact become important--contact with moist porous rock, with a surface having fracture flow, or dripping. In turn, the water contact modes depend on interrelationships between rock hydrologic parameters and future changes in average water flow, and on local geometric or parameter variations. The rock mechanical responses, although not expected to be significant for stress on the container, may become significant for local variations in the water contact mode.

Third, radionuclide releases from a single wet package are complex; the performance of the ensemble of all waste packages will involve adding up many diverse single-package behaviors.The present model PANDORA-1, while limited, is a careful attempt to identify what can be asserted about long-term waste package behavior in the unsaturated environment. Due to present limitations in the knowledge base, any applications for performance predictions or for ranking the importance of processes and parameters should be reviewed and supplemented by qualitative or analytical arguments and expert judgment.

Quality assurance is an important concern throughout model development. There are, appropriately, considerable quality assurance constraints placed on the license application development process. Of these, perhaps the most critical for performance assessment are those surrounding software verification and model validation. Without a convincing demonstration of quality in our models and our means for exercising them on computers, we cannot expect to receive a license to construct from the NRC.

Consequently, we have spent considerable time and resources on developing and employing methods for assuring the quality in both our models and in our software. These methods include, specifically, the development of software requirements specifications, design specifications, test procedures, and accompanying documentation. All source code is highly commented internally and externally. Only highly structured, readily comprehensible source code is acceptable. The interface with the user is straightforward and involves considerable use of data range checking and error-flagging.

Currently, PANDORA is written in FORTRAN-77 running under BSD UNIX 4.2 SunOS release 3.5 on a SUN 3/110 workstation. Strict limitations have been placed on the use of FORTRAN-77 to assure the most structured source we could reasonably achieve. For example, the use of ENTRY points, COMMON storage, and the GOTO command are severely restricted or forbidden. The source code is extremely modular, facilitating maintenance and extension. All input and output is channelled through I/O-specific modules. For the next version of PANDORA we expect to use ADA as the programming language to support structured design and structured source code. We will continue to use CADRE Teamwork as the SA/SD tool. We also expect to develop a highly sophisticated window-based input preprocessor and a DISSPLA-based graphicpost-processor to enhance the User interface.

ENSEMBLE AND UNCERTAINTY ANALYSIS METHODOLOGIES

A second activity in performance assessment at LLNL is to evaluate performance of the ensemble of waste packages. This involves, first, determining the extent of similarity or variation in waste package and environmental parameters in the repository, and second, integrating the performance results over the *significant parameters*. A third activity, uncertainty analysis, determines the effect of input uncertainties in the model on the uncertainty of the output; this involves integrating over the ranges of probability distributions. Sampling is an effective approach in both applications for integration over a large number of variables.

The sampling approach takes a sample from the input domain, and evaluates the model at each input to get a

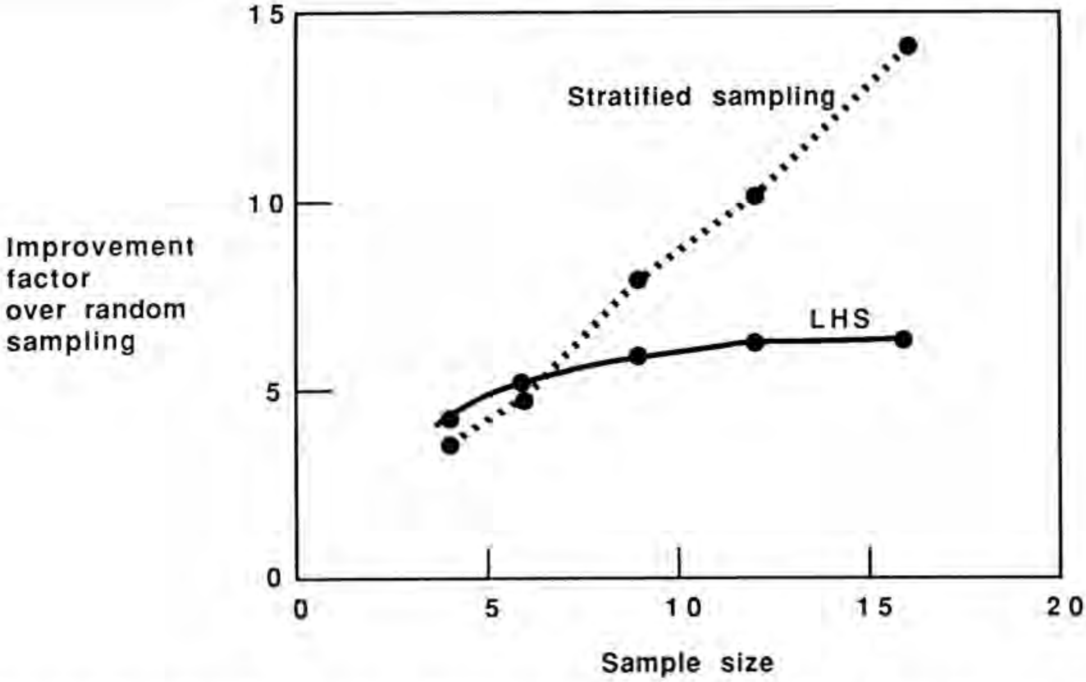

Fig. 3. Effect of LHS and Stratified Sampling as Variance Reduction Techniques, For a Selected Monotonic Function, Eq. 2. The Vertical Axis, Improvement Factor, is the Ratio of Variances of the Estimators of the Mean.

sample of the outputs. The mean of the output sample is an estimate of the integral or of the mean of the output variable. The output sample can also be used to obtain estimates of the variance and fractiles in the cumulative distribution function (CDF) of the output. Each estimate is itself a single value drawn from a random variable, whose variance depends on the sample size and on the sampling method.

Numerous sampling methods have been used; low variance of estimators is desired. Stratified sampling (6, Chapter 4) reduces the variance of estimators as compared to that attainable with simple random sampling. Latin hypercube sampling (LHS) (4) also often reduces variance. The variance of estimators from LHS has been, however, difficult to evaluate for most specific cases, with formulas and inequalities available in Ref. (4). Andres (3) expressed a widely held consensus: "The variance of a Latin hypercube estimator cannot easily be determined."

We have developed a simple formula for calculating the variance of the estimator of the mean using LHS, for a model of the form, for example:

$$Y = A + \sum_i f_i(X_i) + \sum_{ij} s_i(X_i)s_j(X_j) \qquad \text{(Eq. 1)}$$

plus higher order terms; where X_i's are the inputs, Y is the output of the model, and f_i, s_i are functions of one variable X_i with zero means; and A is a constant. Higher terms of the expansion are considered using products of the same s_i's. The different f_i's in the linear terms indicate that higher order terms in one variable may be combined into the one-variable term. The formula (O'Connell, in preparation) for the variance of the estimator of the mean is a long series of one-line equations, simple in that it involves at most two-dimensional sums and analytical one-dimensional integrals for cell means, when applied to a model of the double-sum form of Eq. 1.

We find that LHS is effective in variance reduction only to the extent that the model Y has a large component of single-variable terms. For multi-variable terms, the variance remains about the same as from random sampling and is in some cases higher. For combinations such as Eq.1 the variance reduction is limited. Stein (7) has found the same association of variance reduction with the degree of separability into single-variable terms, for the asymptotic case of large sample size.

As a concrete example, consider

$$Y = (X1 + 1/2)*(X2 + 1/2) \qquad \text{(Eq. 2)}$$

where X1 and X2 are independent and uniformly distributed on [-1/2, 1/2]. This function is monotonic in X1 and X2, hence by an inequality in Ref. (4) it is known that LHS gives lower variance than does random sampling. But now we know it is not very much lower. Figure 3 shows that the variance reduction with LHS reaches a plateau. Stratified

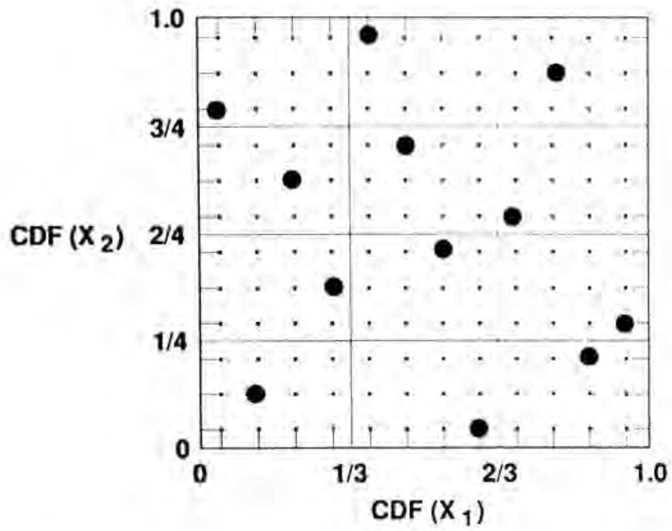

Fig. 4. Illustration of a Controlled Sample With Two Variables.

sampling, by contrast, provides a variance reduction that steadily improves with sample size.

Having demystified LHS, we now list our requirements and examine a new sampling scheme providing substantial variance reduction for a broad range of model functions.

We have examined existing methods of uncertainty analysis for feasibility and applicability to the system model, PANDORA. PANDORA output uncertainty due to input uncertainties is assessed from estimated CDF(Y) curves, where Y is a PANDORA model output random variable. Our particular needs for PANDORA reliability analyses are heavily influenced by several existing conditions. These are summarized as follows:

1. The sampling method used to estimate CDF(Y) curves must make efficient use of samples of limited size, because the computer cost of evaluating PANDORA for each output value Y in the sample is significant.

2. The estimated distribution of Y must be reasonably accurate over the full range of Y. Later, if necessary, we can use a biased sampling technique to improve the accuracy of an output variable at any specified part of its distribution curve.

3. PANDORA is a complex model. We cannot assume any "prior" knowledge of the behavior of any output random variables. Any information that is available before any evaluations have been made will be used to advantage, but our sampling methodology must perform effectively on a complex model whose behavior is unknown before any model evaluations have been studied.

The following sampling features together indicate our adopted strategy for accommodating these conditions:

1. Represent all portions of each input probability distribution in the sample. (The Latin hypercube sampling method contains this feature.)

2. Distribute the sample points so that all parts of the sample space are represented in the sample. (The stratified sampling method contains this feature.)

THE CONTROLLED SAMPLING METHOD

We have developed the controlled sampling method which combines these two sampling features (Thatcher, in preparation). The procedures for implementing them in the controlled sampling method are summarized as follows:

1. Separate the sample space into "cells" of equal probability. The number of cells, NC, becomes the sample size. One sample point (a vector) will lie in each cell.

2. Select NC values from each input distribution (scalar), so that they are separated by equal probabilities along the distribution curve. Use each input value in exactly one sample point.

3. Procedures (1) and (2) define many candidate controlled samples. The controlled sampling method selects one of these by a random assignment of the input values to become components of the sample points in the cells.

Figure 4 illustrates the controlled sampling method as applied to a model with two input random variables, X_1 and X_2. CDF(X) is plotted instead of X along either distribution. The sample space has been separated into 12 cells of equal probability (assuming the input variables are independent). The 12 equally spaced marks along either margin identify the 12 input values from each input distribution that are used in the sample. The 12 large dots represent a controlled sample that was chosen by the random draw procedure. The 11 small dots in each cell suggest potential alternative controlled sample points that the random draw procedure might have selected.

We have constructed an uncertainty methodology testbed code, and compared the performances of controlled (C), Latin hypercube (L), and simple random (R) sampling methods on several models. We used test models with simple formulas, so that we could evaluate large samples and calculate nearly "true" CDF distribution curves for them. The performances of samples of limited size were measured as the average deviations between their estimated CDF(Y) curves and the "true" CDF(Y) curve. The results from tests on two models are presented below. The models are:

Model 1: $Y = U_1 + (U_1 - 0.5)^2 + 0.1U_2 + 0.2(U_2 - 0.5)^2$

Model 2: $Y = 1.0/[1.0 + 100.0 * (U_1 - U_2 - 0.1)^2)]^{1/2}$

where U_1 and U_2 are independent and uniformly distributed on [0,1].

Model 1 is separable. Analytically, we would predict better performance by Latin hypercube samples than by simple random samples from this type of model. Model 2 is more complex. On this basis, we would predict about the same performance by Latin hypercube and simple random samples for Model 2. Our test results are consistent with these analytical predictions.

Figure 5 illustrates our performance measure for single samples. The solid line is a graph of the true CDF(Y) curve for model 2. The estimated curves for single samples of size 49 from the three comparison methods are indicated. The average deviation for each sample is the average of the absolute values of the vertical distances between the true and the estimated curves.

To measure performances of the different sampling methods, the average performance of 50 samples from each method was computed. For either model, the sample sizes were the same for the three comparison methods. The test results for both models are presented in Table I.

TABLE I
AVERAGE ABSOLUTE DEVIATION OVER 50 SAMPLES

Model	Avg. Abs. Deviation By Sampling Method			Sample Size	Performance Ratios
	C	L	R		
1	0.016	0.019	0.052	40	L/C = 1.19
					R/C = 3.25
2	0.023	0.042	0.045	49	L/C = 1.83
					R/C = 1.96

The performance of (L) was much better than (R) for Model 1, but only slightly better than (R) for Model 2. The performance of (C) was much better than (R) for both models, and slightly to much better than (L). The slight improvement in the performance of (R) for Model 2 versus

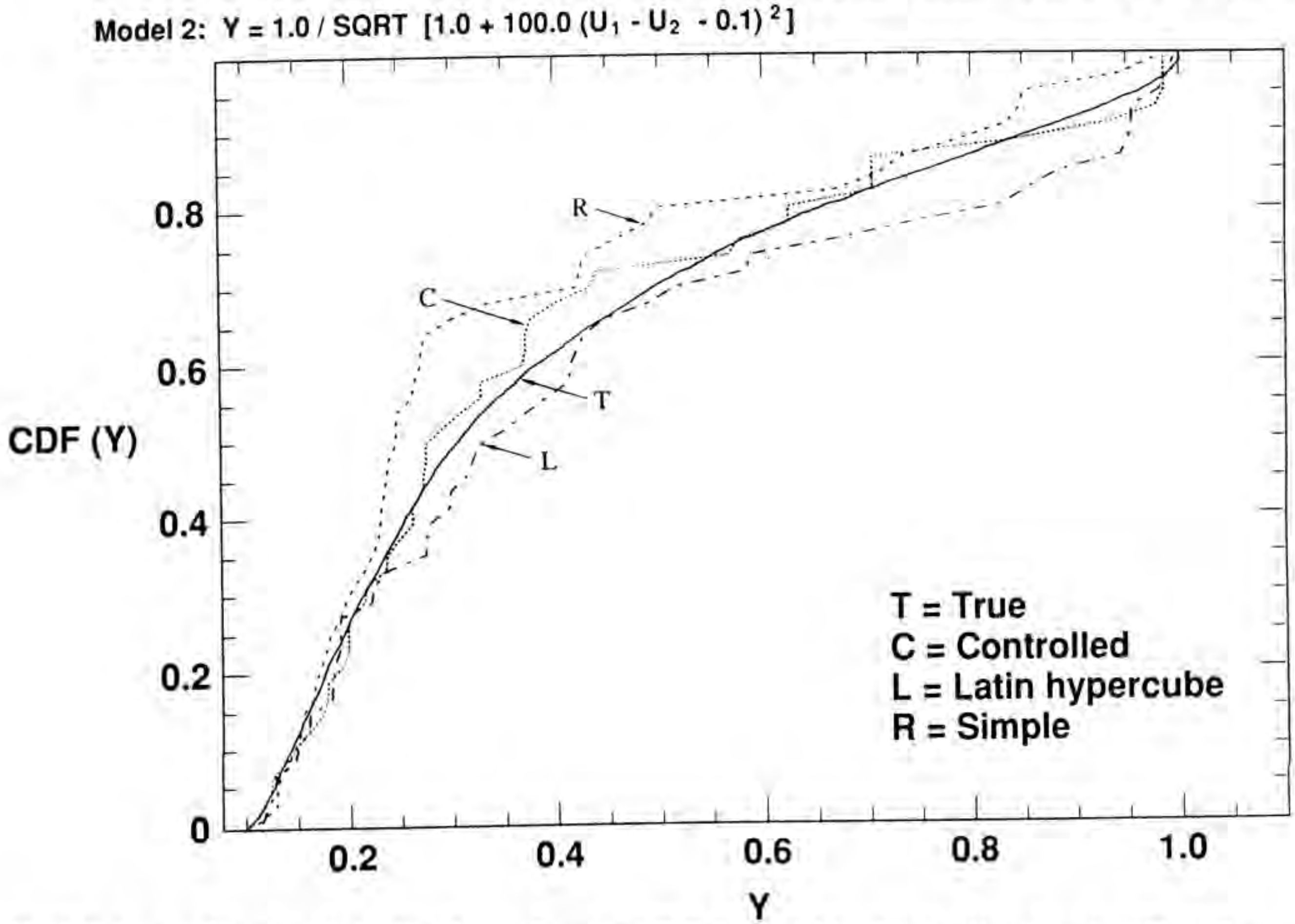

Fig. 5. Estimates of the Cumulative Distribution Function (CDF) for Model 2 as Obtained by a Sample of Fixed Size (49) Using Different Sampling Methods. The Average Deviation of the CDF From the True CDF is a Measure of Performance of the Sampling Method. Fifty Samples of This Type Provided the Data for Table I.

Model 1 can be attributed to the slightly larger sample size.

Additional tests are planned comparing controlled sampling with stratified sampling. A further variation on the controlled sampling approach is to consider the selected points as median indicators of selected subcells, and to select the evaluation points randomly within the indicated subcells. The selection of subcells then has the same structural features as controlled sampling. Tests are planned comparing this local-randomization approach with the point approach used by controlled sampling. Coupling of PANDORA-1 as the core model in the ensemble/uncertainty test-bed code will then be the next step.

REFERENCES

1. U.S. Department of Energy, Office of Civilian Radioactive Waste Management, *Site Characterization Plan, Yucca Mountain Site, Nevada Research and Development Area, Nevada*, Report DOE/RW-0199 (December 1988).
2. K. G. EGGERT, W. J. O'CONNELL, and D. A. LAPPA, "Scientific Investigation Plan for NNWSI WBS Element 1.2.2.5.L, NNWSI Waste Package Performance Assessment," UCID-20967, Lawrence Livermore National Laboratory (October, 1986).
3. T. H. ANDRES, "Statistical sampling strategies," in *Uncertainty Analysis for Performance Assessments of Radioactive Waste Disposal Systems, Proceedings of a Workshop, Seattle, Wash., 24-26. February, 1987* (OECD Nuclear Energy Agency, Paris, France; 1987).
4. M. D. MC KAY, R. J. BECKMAN, and W. J. CONOVER, "A comparison of three methods for selecting values of input variables in the analysis of output from a computer code," *Technometrics* 21, 239 (1979).
5. W. J. O'CONNELL and R.S. DRACH, "Waste Package Performance Assessment: Deterministic System Model Program Scope and Specification," UCRL-53761, Lawrence Livermore National Laboratory (October 1986).
6. R. Y. RUBINSTEIN, *Simulation and the Monte Carlo Method*, John Wiley and Sons, New York.
7. M. STEIN, "Large sample properties of simulations using Latin hypercube sampling," *Technometrics* 29, 143-151 (1987).