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AN EXAMPLE OF MONTE CARLO ANALYSIS APPLIED TO REPOSITORY SITING

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ABSTRACT

This report contains a detailed description of a Monte Carlo analysis of a hypothetical nuclear waste repository performed for the Lawrence Livermore Laboratory as part of their mock siting exercise. Field measurements had been used to construct a hydrology model of the geologic medium surrounding a nuclear waste repository, complete with specified uncertainties. The Monte Carlo analysis has been used to ascertain the uncertainty in the radioactive release from the repository given the uncertainty in the geohydrologic parameters, and correlation analysis has identified some input parameters that have a potentially large influence on the output (radioactivity release) uncertainty.

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1.

INTRODUCTION

1.1 PURPOSE OF THE MOCK SITING EXERCISE

The U.S. Nuclear Regulatory Commission (NRC) is charged with assuring that nuclear activities are conducted in a manner consistent with the public health and safety. Among its responsibilities is the licensing of proposed nuclear waste repositories. NRC has engaged the Lawrence Livermore Laboratory (LLL) of the University of California to develop various analytical tools to assist making decisions on repository license applications. In order to gain insight into the process of deciding whether a particular location is suitable for the disposal of nuclear waste, LLL is conducting a "mock siting" exercise.

In the mock siting exercise a location for a hypothetical repository was chosen. This location, referred to as Site A, had been extensively explored for the purpose of determining water production capability of the region. A large amount of measured data was assembled by Golder Associates at Site A, and even though the purpose of the exploration was other than repository siting, a large portion of the data would have been needed for a repository license application. Golder prepared an assessment of the Site A regional hydrology. They focused on the repository siting problem and compiled the measured data (Ref. 1).

LLL also engaged The Analytic Sciences Corporation (TASC) to evaluate nuclide transport potential at Site A and to use appropriate probabilistic techniques in order to assess

the range of uncertainty in performance of a hypothetical repository situated in the region.

1.2 RISK ASSESSMENT TOOLS

The NUTRAN nuclide transport program was developed by TASC to simulate the flow of radioactive contaminants in groundwater from a nuclear waste repository to the biosphere. The NUTRAN transport model is based on the assumption that the nuclear waste flow in groundwater is essentially one-dimensional except at points that form the junction of one-dimensional flow paths. The program solves the mass transport equations analytically in each one-dimensional segment and uses the output of the previous segment as the input to the next flow path. Thus, the accuracy of the method depends on the degree to which the actual flow path conforms to the assumed piecewise one-dimensionality.

Models of a wide variety of phenomena which directly affect the flow of the contaminant have been included in NUTRAN (Refs. 2 through 4). The time necessary for the repository to refill, the leaching behavior of the waste matrix, and the effect of solubility on the release rate of specific nuclides may each be computed by or be inputs to the model.

A great deal of uncertainty exists as to the regional hydrology at Site A despite the large number of measurements available to this study. Individual measured parameters are uncertain due to measurement error and spatial variability. Also, since the purpose of the measurements was estimation of water production capability, certain parameters of interest to repository siting had not been evaluated. Furthermore, there exist several possible hydrologic regimes (scenarios) which could fit the measured data.

Monte Carlo techniques can be used to assess the effect of the uncertainties such as those in a described scenario. In a Monte Carlo analysis, the solution of the problem (the amount of radioactivity released in this case) is viewed as a parameter of a hypothetical population (possible outcomes if a repository were to be built at Site A). A random number generator is used to construct a sample of the population of possible repositories from which statistical estimates of the parameter can be obtained. In practice this means the probability density functions (pdf's) of the hydrologic inputs are formed. Each uncertain input is sampled by randomly selecting a value based on its pdf. When all inputs have been assigned values, NUTRAN can be used to calculate some measure of the performance of this repository, such as release of waste to the biosphere. The process described above may be repeated several times. The result is a sample of the possible repositories and the computed performance of each repository in the sample. An estimate of the contribution of measurement uncertainty to the overall performance can be obtained from statistical analysis of the performance measures computed by NUTRAN for the repositories in the sample. Correlation analysis can be used to identify those inputs that most probably contribute to the overall uncertainty in repository performance. References 3 and 5 contain descriptions of repository risk analyses performed by TASC using the Monte Carlo techniques in conjunction with NUTRAN.

1.3 OUTLINE OF THE REPORT

In Chapter 2, the main components of the Monte Carlo analysis are presented in detail. The NUTRAN computer program is described. The repository model selected by Golder for

analysis and their probabilistic parameter values for this model are reviewed and the specific probabilistic inputs describing this model for the Monte Carlo analysis are presented in this Chapter. The method used to generate the random repository descriptions is discussed, the performance measures for the repository are defined, and the uses of correlation analysis are introduced. The results of the Monte Carlo and correlation analyses are presented and discussed in Chapter 3. Finally, in Chapter 4, the process of analysis, and the results obtained are reviewed with emphasis on what was learned, both procedurally and analytically.

2. COMPONENTS OF THE MONTE CARLO ANALYSIS

In this chapter the basic component used in the Monte Carlo analysis are discussed:

- The NUTRAN computer program
- The basic hydrology
- The probability density function (pdf's) of the geohydrologic parameters
- The method of selecting repository descriptions using the pdf's
- The statistics to be generated from the Monte Carlo trials and their meaning as performance measures
- The method of identifying those input parameters with potentially large influence on the uncertainty in repository performance (correlation analysis).

2.1 THE NUTRAN COMPUTER PROGRAM

The NUTRAN computer program (Refs. 2 through 4) calculates the release of radioactivity from a waste repository and the resulting doses to man due to transport in groundwater and the biosphere. The program is composed of four parts:

- The ORIGIN code, which calculates radio-nuclide buildup and decay
- The WASTE code, which calculates radio-nuclide transport in groundwater

- The BIDOSE code (Ref. 6) which takes account of transport in surface waters, biological transformations, and human living patterns to calculate doses to man from releases to the biosphere
- The WPLOT code, which combines the results of the other programs to calculate releases of radioactivity and doses to man.

ORIGEN, which is fully described in Ref. 7, was used to calculate radionuclide inventories. The inventories were calculated using the standard reactor parameters for a light water reactor given in Ref. 6. A fuel of uranium enriched to 3.3% ^{235}U was assumed to be burned for 1100 days at an average power of 30 MW/MT. The neutron flux ϕ and the reactor spectrum parameters THERM, RES, and FAST were 2.92×10^{13} n/cm²-sec, 0.632, 0.333, and 2.0 respectively. Reprocessing was assumed to occur 150 days after the fuel is removed from the reactor.

The WASTE program was used to calculate the transport of radioactivity from the repository to the biosphere. This program begins by calculating the length of time required for the mined cavity to refill with water after decommissioning. For Site A, this time was negligible (two years if all parameters take their nominal values).

The WASTE program assumes that after the repository has resaturated and the canister corrodes, the waste matrix begins to leach. If the leaching is sufficiently rapid, some nuclides may be released faster than the water surrounding the canisters can dissolve them. The release rate of each element is checked against its solubility in the surrounding water and reduced when appropriate. Solubility limits were not considered for Site A analysis. This is a conservative assumption since solubility limits reduce the radioactive releases. If the

water contained in a storage room changes more slowly than the waste dissolves, the turnover rate limits how rapidly radioactivity leaves the storage room. This factor also was not included in this analysis.

WASTE calculates the flow of water within the repository corridors, storage rooms, and shafts by a method which takes account of the details of the repository's structure (Ref. 8). Because the relatively high natural permeability of the rock around the repository at Site A reduces the importance of details of flow within the repository, the repository at Site A was treated as a homogeneous plane source.

In the mathematical method used to calculate the transport of radionuclides in ground water (Ref. 9), the steady-state ground water flow pattern is approximated by a network of one-dimensional flow paths, which need not be straight. These flow paths or stream tubes are then analyzed using a simple one-dimensional model for the transport in each path. In this way, more complex situations can be analyzed approximately.

The model incorporates the effects of advection, chemical interactions, hydrodynamic dispersion, and radioactive decay. Provided that the stream tubes are sufficiently long compared to the characteristic dispersion length, the one-dimensional equation can be solved using a simple Green's function technique (Ref. 10). Each stream tube is considered in sequence and appropriate calculations are made at the junction of different streams.

The transport of the various components of waste is calculated under the assumption that all nuclides in a decay chain have the same retardation factor (Ref. 3). When nuclides in a decay chain have differing retardation factors, the results

are modified to take account of this by use of formulas derived in Ref. 11. In this study it was assumed that the waste from the generation of 10^6 MWe-yr of power was stored in the repository, and that all nuclides in a decay chain have the same retardation factor.

Radionuclides can reach man either by flow to surface water bodies or through withdrawal in wells. Doses to man are calculated from the outputs of the BIDOSE model. Doses to both individuals and the population, as well as releases to radioactivity, are calculated as functions of time; total releases and population doses integrated over all time are also computed. In addition, radionuclide concentrations in the ground water are calculated.

2.2 THE HYDROLOGY AT SITE A

The appendices of Ref. 1 contain a detailed discussion of Site A and the techniques used to determine the possible hydrology regimes in the region. Several hydrologic scenarios are discussed, however only one scenario is considered to be sufficiently likely to require detailed analysis with NUTRAN. In the next subsection the basic flow path model for this scenario is discussed and the uncertainties in the geohydrologic parameters which are used to define this scenario are provided in subsection 2.2.2.

2.2.1 The Basic Hydrology Model

Golder Associates devised the basic flow path model of the preferred hydrology at Site A. This model, containing five nodes and four flow paths, is shown in Fig. 2.2-1. The repository is located at node 1 in a layer of marlstone.

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(Not to scale - vertical scale exaggerated)

Figure 2.2-1 Basic Flow Path Model

Ground water leaving the repository flows downward to a lower aquifer (node 2) which is at a lower hydraulic head than the upper aquifer at that point. At the "hinge line" the aquifer heads are equal. To the right of the hinge line in the figure, the lower aquifer is at a higher hydraulic head than the upper aquifer. Consequently at node 3 the ground water flows upward to the upper aquifer (node 4). The ground water then flows in the aquifer to a discharge at node 5. Note that the lower aquifer ends at a large saline zone. The other most reasonable hydrology scenarios have the lower aquifer divert and flow perpendicular to the plane of the drawing. These scenarios are not considered in this report.

2.2.2 The Model Parameters and Their Uncertainties

The five node model described above was selected for Monte Carlo analysis using NUTRAN to simulate the flow of waste

from the repository to the biosphere. The inputs used in NUTRAN are briefly described below, and are presented in tables for easy reference. The basic values and quantitative uncertainties for the model parameters were developed by Golder Associates (see Ref. 1).

Intrinsic Properties of Flow Paths - The length, cross-sectional area, permeability, porosity and dispersion of each flow path are presented in Table 2.2-1. For purposes of this analysis, all of these variables are assumed to be independent. All variables are bounded below by 0, and porosity is also bounded above by 1. The value used for the permeability of the pathway from the depository to the local aquifer was ten times larger than actually found (Ref. 1). This discrepancy causes only a very small change in results.

Flow Path Head Drop - The hydraulic pressure head of each of the five nodes are inputs to NUTRAN for the Site A analysis. The heads are determined by arbitrarily setting the head of node 5 to zero and randomly generating the head drop between nodes 4 and 5. The head of node 4 is set equal to

TABLE 2.2-1
ASSUMED STATISTICS FOR PATHWAY INPUTS

Y-360R

PATHWAY	PATHWAY INPUTS					
	PARAMETER	LENGTH (m)	CROSS-SECTION (m ²)	PERMEABILITY (cm/sec)	POROSITY	DISPERSION (m)
Depository to Lower Aquifer	Distribution Median Uncertainty	lognormal 59.59 0.14	deterministic 2.82x10 ⁶	lognormal 8.56x10 ⁻⁷ 0.65	lognormal 0.09 0.5	lognormal 63 0.25
Lower Aquifer	Distribution Median Uncertainty	normal 4835 500	normal 1.25x10 ⁵ 2.09x10 ⁴	lognormal 2.39x10 ⁻³ 0.18	lognormal 0.015 0.5	lognormal 63 0.25
Lower to Upper Aquifer	Distribution Median Uncertainty	lognormal 119 0.14	deterministic 3.3x10 ⁶	lognormal 3.87x10 ⁻⁷ 0.5	lognormal 0.08 0.5	lognormal 63 0.25
Lower Aquifer	Distribution Median Uncertainty	lognormal 1.5x10 ⁵ 0.05	normal 2.89x10 ⁵ 4.10x10 ⁴	lognormal 9.16x10 ⁻⁴ 0.46	lognormal 0.012 0.5	lognormal 63 0.25

TABLE 2.2-2
 ASSUMED STATISTICS FOR HEAD DROP INPUTS

T-3409

PATHWAY	METHOD OF CALCULATION	PARAMETER	HEAD DROP	GRADIENT	LENGTH
Depository to Lower Aquifer	generate head drop	Distribution Median Uncertainty	lognormal 42.90 0.10	-	lognormal 59.50 0.14
Lower Aquifer	generate gradient Head Drop = Gradient $\times$ Length	Distribution Median Uncertainty	-	lognormal 0.0015 0.2200	normal 4830 500
Lower to Upper Aquifer	generate head drop	Distribution Median Uncertainty	normal 16.0 1.6	-	lognormal 119.00 0.14
Upper Aquifer	generate gradient Head Drop = Gradient $\times$ Length	Distribution Median Uncertainty	-	lognormal 0.015 0.058	lognormal 1.5×10^4 0.05

this head drop. This process is repeated recursively with the head of each node set equal to the head of the succeeding node plus the head drop between the two nodes.

As is discussed in Ref. 1, the head drops between the two ends of the flow path were measured for the flow paths between the repository and the lower aquifer and between the lower and upper aquifers. However only gradients were measured for the two paths within the aquifers. For these two paths the head drop is generated as the product of the flow path length and gradient. These procedures are summarized in Table 2.2-2.

Waste Dissolution Properties - The resaturation time of the repository and dissolution time of the waste control the time and rate of waste release to the geosphere. They were generated randomly using the parameters summarized in Table 2.2-3. Resaturation Time is composed of a constant plus a random variable. The constant (32 years) is the sum of the average age of the waste in the repository and the time required for the repository to refill with water. The random

TABLE 2.2-3
 ASSUMED STATISTICS FOR VARIABLES CONTROLLING
 TIME AND AMOUNT OF WASTE RELEASE

T-3410

VARIABLE	METHOD OF CALCULATION	PARAMETER	
Resaturation Time (RT)	$RT = 32 + y$	Distribution of y	lognormal
		Median	60.0
		Uncertainty	0.23
Dissolution Time (DT)	$DT = 2000 \times (y/60)^{1.3}$	Distribution	lognormal
		Median	2000
		Uncertainty	0.30

variable is the time required for the ground water to dissolve the canister, thereby making the waste available for dissolution. This variable is assumed to have a lognormal distribution with a median of 60 years. The dissolution time for the waste is assumed to be directly correlated with the dissolution time of the canister, i.e., if the chemical composition of the ground water is such that the canister corrodes in a short period of time, the waste is also likely to dissolve in a correspondingly short time span. The dissolution time of the waste is assumed to have a lognormal distribution with a median of 2000 years and is calculated by scaling the randomly generated canister dissolution time.

Retardation Factors - The retardation factors for the nuclides in the waste were established by dividing the isotopes into three groups (^{129}I and ^{99}Tc in group I, the other fission products in group II, and actinides in group III), and assigning a common retardation factor to all nuclides in the same group. The minimum, preferred, and maximum retardation factors, B, for each group were estimated by LLL for water containing 10^3 and 10^4 parts per million (ppm) of dissolved solids (Table 2.2-4). Golder provided estimates of the dissolved solids (in

ppm) in the water, C, in each flow path of the repository model (Table 2.2-5).

TABLE 2.2-4
RETARDATION FACTORS FOR SELECTED
PARTICULATE CONCENTRATIONS

T-3411

CONCENTRATION OF DISSOLVED SOLIDS (ppm)	NUCLIDE GROUP I			NUCLIDE GROUP II			NUCLIDE GROUP III		
	MINIMUM	PREFERRED	MAXIMUM	MINIMUM	PREFERRED	MAXIMUM	MINIMUM	PREFERRED	MAXIMUM
1000	1	1	1	1	100	1000	1	100	10000
10000	1	1	1	1	5	10	1	10	100

TABLE 2.2-5
CONCENTRATION OF DISSOLVED SOLIDS BY PATHWAY

PATHWAY	CONCENTRATION OF DISSOLVED SOLIDS (ppm)
Depository to Lower Aquifer	1000
Lower Aquifer	7000
Lower to Upper Aquifer	10000
Upper Aquifer	1500

In order to produce pdf's for the retardation factors several assumptions must be made. The terms "minimum", "preferred", and "maximum" are understood as follows. "Preferred" is synonymous with "median". "Maximum" denotes a value of the quantity which is rarely exceeded. It is assumed that the "maximum" value lies two standard deviations above the mean, i.e. -- 97.73% of all observations will be below the maximum. "Minimum" refers to an absolute minimum since its value is

always given as 1 which is the smallest possible retardation. In the following, the minimum value is interpreted to lie two standard deviations below the median, i.e. -- the distribution function will be constrained so that 2.27% of the observations are exactly 1.

The method used to develop probability density functions for the retardation factors in pathways is outlined in Appendix A. In that appendix, the "log-linear" distribution for the fission product retardation factors is also defined.

Table 2.2-6 summarizes the probability distributions used for the retardation factors of each nuclide group in each flow path. The distribution of each B is either "deterministic" in which case only the constant value is given, "lognormal" in which case the median value of B and the uncertainty (the standard deviation of the logarithm of B) are given, or "log-linear" in which case the preferred and maximum values of B are given.

TABLE 2.2-6
PROBABILITY DISTRIBUTION OF RETARDATION FACTORS

T-3412

	NUCLIDE GROUP I	NUCLIDE GROUP II	NUCLIDE GROUP III
Repository Distribution to Lower Aquifer	Deterministic	Log-linear	Lognormal
Median/(Preferred)	1.0	(100.0)	100.0
Uncertainty/(Maximum)	-	(1000.0)	1.0
Lower Aquifer	Deterministic	Log-linear	Lognormal
Median/(Preferred)	1.0	(7.83)	15.85
Uncertainty/(Maximum)	-	(19.31)	0.60
Lower to Upper Aquifer	Deterministic	Log-linear	Lognormal
Median/(Preferred)	1.0	(5.0)	10.0
Uncertainty/(Maximum)	-	(10.0)	0.5
Upper Aquifer	Deterministic	Log-linear	Lognormal
Median/(Preferred)	1.0	(65.0)	78.48
Uncertainty/(Maximum)	-	(501.2)	0.95

Conceptually, a repository has been built corresponding to one of the random descriptions (except for retardation factors) and isotopes of only one of the nuclide groups have been placed in this repository. The retardation factors for that group in each flow path are independent of the repository and hence can be randomly generated according to the cdf's of B in the flow paths. Such an experiment will produce radioactivity release rates for that nuclide group. This experiment may also be repeated with each of the other two nuclide groups and will produce results for each group separately. However if all three groups are buried in a single repository there should be some correlation between their respective retardation factors. No such correlation was included in producing the retardation factor for this study because of the very sparse data on retardation at Site A. Hence, one should view each Monte Carlo run not as one experiment summed for all three groups but rather as three separate experiments, one for each nuclide group.

2.3 THE MONTE CARLO AND CORRELATION ANALYSIS METHODS

In the Monte Carlo analysis repository descriptions are randomly generated based on the input parameter pdf's described in Section 2.2. The NUTRAN computer code is then used to compute the radioactive release from each randomly-generated description. Three descriptors of the radioactive release are singled out as measures of repository performance. The distributions of these three descriptors and some simple statistics for the results are used as measures of repository performance and the uncertainty in that performance due to the uncertainties in the hydrogeologic parameters. Correlation analysis between the inputs and the performance measures for the fifty models helps to identify some parameters with potentially large influences on the uncertainty in the performance measures.

In this section the method used to validate the random descriptions is discussed and the performance measures are defined, and the correlation technique is explained.

2.3.1 Validation of the Random Repository Descriptions

Three variables were selected from the generated inputs and subjected to goodness-of-fit tests to ascertain whether or not they were properly generated. The variables are the permeability, cross-section and retardation factor for the fission products in the upper aquifer and are generated from a lognormal, normal and log-linear distribution respectively. For all three variables there is no significant difference between the observed and theoretical populations using the Kolmogorov-Smirnov goodness-of-fit test (Ref. 12). Furthermore, since all random variables used in this study are normal, lognormal or log-linear, these goodness-of-fit tests indicate that the random variables used in the Monte Carlo analysis are correctly generated from their specified probability distributions.

2.3.2 Performance Measures for the Repository

The performance measures were chosen to assess the effectiveness of Site A as a barrier to waste release. The site serves as a barrier by delaying the transport of waste from the repository to the biosphere. During this delay, radioactive decay can significantly reduce the quantity of waste reaching the biosphere. Decay is a nonlinear process in time, so relatively small delays may cause significant decreases in the radioactive release from the repository.

The ability of the site to function as a barrier is measured in this study by the peak flow rate of radioactivity to the biosphere (Ci/yr), the time when the peak flow rate occurs (yr), and the total outflow of radioactivity from the

repository for all time (Ci). Each of these three measures is computed for each of the three nuclide groups. The initial inventory of the repository is assumed to be 10^6 MWe-yr of waste.

2.3.3 Correlation Analysis

The uncertainty in repository performance caused by the uncertainties in the input parameters is calculated using Monte Carlo techniques. In this way the gross effect of all uncertainties was ascertained. The next step in the analysis is an attempt to point out some input parameters that significantly contribute to the uncertainties in the radioactive releases. Correlation analysis is the statistical method by which significant relationships may be identified.

Since the true distribution of the outputs is not known, it is not valid to utilize a correlation coefficient which requires a known distribution. A correlation coefficient which is independent of distribution (i.e., "non-parametric") is the Spearman rank correlation coefficient (Ref. 12) which was originally developed as a tool for finding dependence relationships between variables which need not be quantifiable but which can be ranked in order e.g., the artistic ability of a person. Spearman called these rankable variables "qualitiles".

In its original conception the Spearman coefficient was used to check for dependence between two qualitiles as follows. The two qualitiles being studied were paired for each observation. The qualitiles were ranked separately and the ranks were correlated based on the difference in rank of the pair formed from each observation. The correlation coefficient obtained in this manner is 1 if the ranks in each pair agree. In this case, the rank relationship between the members

of one set of qualittiles determines the rank relationship between the members of the second set of qualittiles for all observations; they are the same relationship. A correlation coefficient of -1 is obtained for a complete reversal of ranks. In this case knowledge of the rank relationships between members of one set of qualittiles completely determines the rank relationships in other set; the relationship is reversed. Spearman argued that it was unlikely that the correlation coefficients would be near ± 1 if the two qualittiles were independent random variables. In order to quantify this argument the probability that two independent qualittiles would have a given rank correlation coefficient was computed. This probability, "the probability of independence", can be used to determine those pairs of qualittiles that are likely to be related.

The Spearman coefficient, then, is a tool with which monotonic relationships between pairs of variables can be identified. It should be noted that the relationship identified is qualitative and not quantitative. It is possible to have high correlation between an input and output variable and have very little spread in the output distribution (c.f., the discussion of Nuclide Group I in Section 3.1). The high correlation means only that the ranks of the variables are closely matched, regardless of the range of values of each variable. If both variables have reasonably large spreads in distribution and are highly correlated, then it is possible that a great deal of information may be gained by studying the relationship between them. Another point to note is that the Spearman coefficient cannot identify non-monotonic relationships, e.g., if two variables are related by a quadratic relationship, the coefficient may be near zero. However, there is no correlation coefficient at present which can identify unspecified non-monotonic relationships between variables.

The probability of independence is a measure of chance occurrences, and should be used with the same caveats applicable to any statistical study. If one is interested in identifying input-output pairs which are almost certainly dependent then restricting attention to those pairs with a probability of independence less than 0.01 or 0.05 may be appropriate. However, if one is attempting to determine possible dependencies in order to clarify the crucial issues in a repository licensing exercise it may be reasonable to consider a more liberal cutoff value.

An example of spurious correlation is appropriate here. For convenience the correlation coefficients were calculated for all possible pairs of inputs and outputs. A correlation coefficient of 0.28 was found between the time of peak flow for Nuclide Group II and the retardation factor in the upper aquifer of Group III. The probability of independence for such a correlation with 50 samples is 0.047, yet the variables are independent, for the latter does not enter into the calculation of the former. The presence of the spurious correlation does not negate the validity and potential importance of the other variables which have also passed through the filter. However, it is a reminder of the effect of a chosen significance level on a study of this type.

3. RESULTS OF THE STATISTICAL ANALYSIS

In this section the results of the Monte Carlo and correlation analyses are presented (Section 3.1) and discussed (Section 3.2). In order to provide a frame of reference for the following material, Appendix B contains the results of the NUTRAN analysis of a repository model in which all parameters have their "preferred" values. (See Section 2.2.)

3.1 NUMERICAL RESULTS

Fifty randomly generated repository descriptions were analyzed with the NUTRAN computer code and the values of the three performance measures for each of the three nuclide groups were calculated for each description. The choice of a sample size of fifty was based on the limited time and resources available to the project. A larger sample of randomly generated repositories would have produced better estimates of the performance measures, however, the purpose of the mock siting exercise was to gain insight into the regulatory process rather than to very accurately study site A. The choice of the sample size was made with this purpose in mind.

The results are summarized in Fig. 3.1-1 through 3.1-9 which show histograms of the results. Table 3.1-1 contains summary statistics of the 50 outputs. The "interquartile spread" is one-half of the difference between the 75th and 25th percentile values.

Figure 3.1-1 Histogram of Peak Flow Rate for Nuclide Group I

Figure 3.1-2 Histogram of Peak Flow Rate for Nuclide Group II

Figure 3.1-3 Histogram of Peak Flow Rate for Nuclide Group III

Figure 3.1-4 Histogram of Time of Peak Flow for Nuclide Group I

Figure 3.1-5 Histogram of Time of Peak Flow for Nuclide Group II

Figure 3.1-6 Histogram of Time of Peak Flow for Nuclide Group III

Figure 3.1-7 Histogram of Total Flow for Nuclide Group I

Figure 3.1-8 Histogram of Total Flow for Nuclide Group II

Figure 3.1-9 Histogram of Total Flow for Nuclide Group III

TABLE 3.1-1
SUMMARY STATISTICS OF MONTE CARLO ANALYSIS

T-3413

VARIABLE	STATISTICS			
	MEAN	STANDARD DEVIATION	MEDIAN	INTERQUARTILE SPREAD
<u>Peak Flow Rate (Ci/yr)</u>				
Nuclide Group I	3.6×10^2	2.8×10^2	2.7×10^2	1.3×10^2
Nuclide Group II	1.0×10^3	6.3×10^3	8.8×10^1	5.2×10^1
Nuclide Group III	3.5×10^2	7.2×10^2	1.0×10^2	1.5×10^2
<u>Time of Peak Flow Rate (yr)</u>				
Nuclide Group I	1.2×10^3	1.0×10^3	8.7×10^2	6.0×10^2
Nuclide Group II	1.6×10^4	2.7×10^4	6.3×10^3	6.6×10^3
Nuclide Group III	4.8×10^4	1.9×10^5	9.3×10^3	1.2×10^4
<u>Integrated Flow (Ci)</u>				
Nuclide Group I	4.4×10^5	1.3×10^3	4.4×10^5	7.1×10^2
Nuclide Group II	3.6×10^5	7.9×10^5	2.6×10^5	8.8×10^3
Nuclide Group III	5.7×10^5	5.3×10^5	4.5×10^5	2.8×10^5

The results of the correlation analyses are difficult to present in a concise format. A significance level of 0.05 for the probability of independence was used to determine which results would be reported in the following. This significance level does not represent a judgment of what is significant, but rather a judgment about how much information is both convenient to present and useful for discussion.

The Spearman rank correlation coefficient was calculated between each measure of the radioactive release at Mock Site A and each of the uncertain input variables used to calculate that measure. Tables 3.1-2 through 3.1-4 contain abbreviated results of the correlation study for Nuclide Groups I through III respectively. Each table contains information on those input variables that are sufficiently correlated to the output measure listed that the probability of independence between the input and output are less than 0.05. One of the input variables, dissolution time, was generated by scaling the randomly generated resaturation time. The correlation coefficients for these two variables and any other variable are identical. For this reason, they are jointly listed in

TABLE 3.1-2
INPUT VARIABLES CORRELATED WITH PEAK FLOW RATE,
TIME OF PEAK FLOW RATE AND INTEGRATED FLOW - NUCLIDE GROUP I

T-3414

VARIABLE	CORRELATE	SPEARMAN CORRELATION COEFFICIENT	PROBABILITY OF INDEPENDENCE
Peak Flow Rate (Ci/yr)	Waste Release	0.99	0.0001
Time of Peak Flow Rate (yr)	Waste Release	0.48	0.0004
	Permeability of Upper Aquifer	-0.28	0.048
Integrated Flow (Ci)	Waste Release	0.92	0.0001

the tables below as "Waste Release" since they control the time and rate of waste release. In addition, only the gradients in each pathway and not the head drops at each node were included in the correlations.

TABLE 3.1-3
INPUT VARIABLES CORRELATED WITH PEAK FLOW RATE,
TIME OF PEAK FLOW RATE AND INTEGRATED FLOW - NUCLIDE GROUP II

T-3415

VARIABLE	CORRELATE	SPEARMAN CORRELATION COEFFICIENT	PROBABILITY OF INDEPENDENCE
Peak Flow Rate (Ci/yr)	Retardation Factor in Upper Aquifer	-0.55	0.0001
	Waste Release	0.53	0.0001
	Porosity in Upper Aquifer	-0.48	0.001
	Permeability between Repository and Lower Aquifer	0.28	0.048
Time of Peak Flow Rate (yr)	Retardation Factor in Upper Aquifer	0.67	0.0001
	Porosity in Upper Aquifer	0.50	0.0002
	Waste Release	0.34	0.016
Integrated Flow (Ci)	Retardation Factor in Upper Aquifer	-0.71	0.0001
	Porosity in Upper Aquifer	-0.47	0.0005
	Waste Release	0.30	0.037
	Porosity in Lower Aquifer	-0.29	0.039

3.2 DISCUSSION

The purposes of the analyses reported above were to determine the performance of the hypothetical repository at Site A, to find the uncertainty in that performance, and to point out certain variables that may contribute significantly to radioactive release. Each purpose is designed to provide significant information concerning a possible repository at Site A. Whether significant information can be developed

with the small sample size -- fifty randomly generated repository descriptions -- used in this project is doubtful. The mock siting exercise was undertaken to gain a better understanding of the tools and procedures needed for the regulatory process. Hence, the results are treated as significant information below despite the fact that a larger sample would doubtlessly provide more accurate estimates of repository performance.

Overall repository performance was estimated by computing with the NUTRAN computer code the typical values of three performance measures for each of the three nuclide groups.

TABLE 3.1-4
INPUT VARIABLES CORRELATED WITH PEAK FLOW RATE,
TIME OF PEAK FLOW RATE AND INTEGRATED FLOW - NUCLIDE GROUP III

T-3416

VARIABLE	CORRELATE	SPEARMAN CORRELATION COEFFICIENT	PROBABILITY OF INDEPENDENCE
Peak Flow Rate (Ci/yr)	Retardation Factor in Upper Aquifer	-0.62	0.0001
	Porosity in Upper Aquifer	-0.50	0.0002
	Porosity in Lower Aquifer	-0.41	0.0035
	Waste Release	0.29	0.041
Time of Peak Flow Rate (yr)	Retardation Factor in Upper Aquifer	0.72	0.0001
	Porosity in Upper Aquifer	0.45	0.0009
	Porosity in Lower Aquifer	0.36	0.01
	Permeability in Upper Aquifer	-0.32	0.02
Integrated Flow (Ci)	Retardation Factor in Upper Aquifer	-0.70	0.0001
	Porosity in Upper Aquifer	-0.50	0.0002
	Porosity in Lower Aquifer	-0.38	0.0065
	Permeability in Upper Aquifer	-0.29	0.042

Fifty repository descriptions were randomly generated using probability distribution functions for the input variables. The performance measures for these repository models were calculated using NUTRAN. Both the mean and median of the performance measures (Table 3.1-1) are estimates of the typical repository performance.

The distributions of the output parameters for the models (Figs. 3.1-1 through 3.1-9) and the basic parameters describing these distributions (Table 3.1-1) are measures of the uncertainty in repository performance. Finally, correlation analysis was used to identify some input parameters that may significantly effect the output measures.

The tasks described above are relatively easy to perform. The amount of difficulty varies with the complexity of the model. However, the NUTRAN computer program has an interactive Monte Carlo input generator which greatly reduces the problem of producing randomly generated repository models. Moreover, the input generator may be readily "customized" to accommodate the "eccentricities" of a particular repository model, and thereby provides a flexible tool capable of generating analyses of very complicated flow models.

The use of the information obtained with the methodology will be illustrated by the following discussion of conclusions that may be drawn about the Site A repository from the analyses.

The typical repository performance was estimated by the median and mean of the 50 Monte Carlo trials (Table 3.1-1). The median and the values for the repository with preferred values reported in Appendix B are in fair agreement. The histograms of the outputs (Figs. 3.1-1 through 3.1-9) indicate a

"tail" on most of the output measures. This tail is caused by the skewed distributions used for most of the input variables. Because of this skewness it is unlikely that the median of the runs would completely agree with a run using all median values. The mean of the runs is often far different from the median. This is because a single run with an extremely large output value can dominate this statistic. Such is the case of mean value of the peak flow rate of Nuclide Group II. In this case the mean value is 12 times larger than the median due to a single large, but statistically possible, result (see Fig. 3.1-2).

The uncertainty of the results can be estimated using the standard deviation or the inter-quartile spread of the Monte Carlo runs. The large standard deviations indicate a number of very large results and suggest that Site A is not well characterized. The histograms of the outputs (Figs. 3.1-1 through 3.1-9) also indicate that peak flow rates many times higher than the median are definite possibilities.

The analyses performed in these studies were designed to assess the effectiveness of the site and region as a barrier to waste flow. Performance measures based on the number of curies of radiation reaching the biosphere were chosen to determine the quality of that barrier. The median values of the performance measures and their uncertainties provide important information on the influence of the geohydrologic parameters on the ability of that barrier to prevent the waste from reaching the biosphere.

Table 3.1-1 indicates that the integrated flow in curies is the performance measure with the smallest uncertainty. The behavior of the repository as a barrier to waste release may be inferred from this measure. Table 3.2-1 shows

the quantity of curies of each nuclide group originally placed in the repository, the median total number of curies of that nuclide group which reach the biosphere, and the fraction of the original inventory of each group which flows through the barrier to the biosphere.

TABLE 3.2-1
THE REPOSITORY AS A BARRIER

NUCLIDE GROUP	AMOUNT OF WASTE ORIGINALLY EMPLACED* (Ci)	AMOUNT OF WASTE REACHING BIOSPHERE (Ci)	FRACTION OF WASTE REACHING BIOSPHERE
I	4.48×10^5	4.46×10^5	0.996
II	4.06×10^9	2.57×10^5	6.33×10^{-5}
III	3.67×10^7	4.52×10^5	0.0123

*Assuming 10^6 MWe-yr of 30 year old high-level waste with plutonium stowaway.

The fraction released for each nuclide group is determined by whether the nuclides with the largest contribution to the group inventory are kept in the geosphere long enough to undergo significant decay. For example, the group I inventory is dominated by the inventory of ^{99}Tc with a half-life of over 200,000 years. Thus the inventory of group I nuclides undergoes almost no decay since the median time of peak flow is less than 1,000 years. However, the original group II inventory is dominated by ^{90}Sr and ^{137}Cs which are each in the geosphere for about 200 half-lives at the median time of peak flow and thus contribute almost nothing to the radioactive release to the biosphere.

Some parameters that may contribute to the large uncertainties are suggested by the correlation results summarized in Tables 3.1-2 through 3.1-4.

The values of all radioactive release measures for Nuclide Group I may be dependent on the waste release properties (Table 3.1-2). If the flow time through the repository model is short in comparison to the width of the waste input pulse then the input pulse width will dominate the peak flow rate (Ref. 3). The time when waste starts to flow will determine the peak flow time if the other parameters do not greatly change the total flow time through the system. However some parameters that can affect total flow time may weaken the dependence. This is indicated in Table 3.1-2 by the sharply smaller value of the correlation coefficient of waste release to time of peak flow than to the other output measures. Finally, though there is a high correlation between integrated flow and waste release, the integrated flow for Group I is practically constant. The integrated flow is determined by the amount of decay which occurs during the time required for all of the waste to leave the flow system which, in turn, is controlled for Group I nuclides by the time when flow begins. However the total amount of decay for Group I nuclides is small because of the short total flow time of the biosphere of these nuclides. Hence, the integrated output is essentially constant.

The correlation results in Table 3.1-3 indicate that the radioactive release of Nuclide Group II is more dependent on the retardation and porosity of the upper aquifer than on the waste release properties. The qualitative arguments in Ref. 3 indicate that the peak flow rate should be about equally affected by these three quantities. However the effect of each quantity increases with the uncertainty of that quantity.

This is qualitatively reasonable because the variation of the product of several variables with different uncertainties should be most dependent on the variable with the largest uncertainty.

Table 3.1-4 indicates that for Nuclide Group III the radioactive releases are most dependent on the retardation and porosity of the upper aquifer and the porosity of the lower aquifer. The waste release properties have only a small effect. Qualitatively, the large retardation factors of Group III cause the flow time to the biosphere to be much longer than the duration of waste release, so those parameters which contribute most to the velocity in the longer flow paths tend to dominate the release measures.

In summary, analysis of Site A has indicated that the large uncertainties in some input variables cause a large uncertainty in repository performance. The correlation analysis has helped to identify some variables which may contribute to the large uncertainty. If the values of these parameters could be more precisely determined the uncertainty in the performance measures may be greatly reduced. In a licensing review the measures of typical performance and the uncertainty in these measures may be prime considerations in deciding whether or not to grant the license. In the event that a positive decision on the license is not possible based on the measured data, further study of the significant variables found in the correlation analysis may help to reduce uncertainty and show whether the site is adequate.

One point should be made in closing. The correlation analysis was used to identify several variables that contribute to uncertainty. In each case these variables could have been predicted using simple qualitative arguments. The use of these qualitative arguments is possible for Site A because the

repository model is simple and the hydrologic regime in the region does not offer a great deal of resistance to waste flow. In an actual repository licensing evaluation it is likely that the hydrology will be better known so that the flow model will be more complex. Consequently, the important parameters contributing to uncertainty will not be identifiable by simple arguments. In this type of situation correlation analysis will be very useful to identify the important input parameters.

4. ADEQUACY OF THE SITE ASSESSMENT METHOD

In a repository licensing study a large amount of measured data is analyzed in order to describe the possible hydrologic regimes in the region. The problem of describing regimes has two parts: first, the data must be analyzed to produce a series of possible flow scenarios; second, the range of values of all parameters needed to compute waste transport in each scenario must be given. The description of the site is adequate for the purpose of licensing if the series of possible flow scenarios covers all likely situations and if the uncertainties of the parameters in each flow scenario is sufficiently small that the uncertainties of repository performance measures in that scenario are reasonably well defined. When the description and models are adequate the licensing body will be able to understand the ranges of repository behavior to be expected at the site and, from this understanding, be able to judge the merits of the site as a possible repository location.

The analyst's part in this process is to determine the repository performance measures and their uncertainties for each of the hydrologic scenarios, and to suggest ways to decrease these uncertainties if they are too large. The method used to determine the performance measures and to reduce their uncertainties is illustrated in Fig. 4-1. The geological data for each scenario and a computer model of a repository are used in a Monte Carlo analysis. The summary statistics from this analysis are examined and a determination is made on whether site acceptance is possible. If it is not, correlation analysis is employed to determine some of the variables that contribute significantly to the large uncertainty. These variables

Figure 4-1 A Method for Characterizing Site Performance

are more intensively studied in the field to reduce the uncertainties in their values and the entire process is iterated. As more and better data becomes available, the use of more detailed models may become justified.

The mock siting exercise was performed to gain insight into the process of repository regulation. The test consisted of a Monte Carlo analysis, and a subsequent correlation analysis performed because the site was not adequately characterized by the initial set of geologic data. However, no iteration of the measurement process was performed, since in this study it was not intended to perform further field measurements of the identified parameters. The study did illustrate the feasibility of

- Using Monte Carlo analysis to calculate repository performance measures and their uncertainties
- Using correlation analysis to determine input variables which may be significant contributors to the uncertainty.

The analyses performed in these studies were designed to assess the effectiveness of the site and region as a barrier to waste transport. Performance measures based on the number of curies of radiation reaching the biosphere were chosen to determine the quality of that barrier. The median values of the performance measures and their uncertainties provide important information on the influence of the geohydrologic parameters on the ability of that barrier to prevent the waste from reaching the biosphere.

Spatial variability and measurement error are the principal reasons why geoscientists must present uncertain repository descriptions. Thus, the analyst's assessment of the potential of a site to act as a barrier to waste flow must be stated in the language of uncertainty. The process described in this report is aimed at reducing the uncertainty in the repository assessment and may eventually provide regulators with enough information to accurately determine whether to grant a license for a repository at the site.

Assessing the repository as a barrier to the transport of radioactivity is only part of the system evaluation process. Since different nuclides can have different impacts on humans, biological transport and accumulation models (such as the BIDOSE portion of NUTRAN) must be used to evaluate the effects of the waste nuclides that penetrate the repository barrier and enter the biosphere. However, such models contain their own set of parameters with uncertainties. In order to focus on barrier uncertainties, radiation dose calculations using these models were not made within this study. Appendix B illustrates dose calculations based on the Site A repository and an assumed human usage pattern in the Site A region.

APPENDIX A
PROBABILITY FUNCTION OF
THE RETARDATION FACTORS

The problem of determining pdf's for the retardation factors of each nuclide group in each pathway is addressed in this Appendix. These pdf's are based on the information in Tables 2.2-4 and 2.2-5.

The paucity of the given data causes two problems for the estimation of the uncertainty of the retardation factor in a given flow path. The first problem is finding an appropriate interpolating function for the minimum, preferred, and maximum values of B as a function of C. The second problem is expressing in an analytic form the cdf of B in a flow path from its minimum, preferred and maximum values. The emphasis here is on the requirement of analyticity which is necessary for generating the random variable in a computer.

The interpolation function assumed was

$$\log B = \frac{1}{a_1 C + a_2} \quad (A-1)$$

with the values of the constants a_1 and a_2 to be determined from the two given points on each curve. Equation A-1 was chosen since it conforms to a priori judgments concerning the relationship between B and C, i.e. -- for large C, B goes to 1; for small C, B becomes large. This arbitrary procedure may be subject to considerable error; however, the data to which it is applied is extremely judgmental and the procedure is not expected to significantly affect the large uncertainties which are inherent in the data.

Equation 1 has the form

$$\log B = \frac{9000 \log B_1 \log B_2}{C(\log B_2 - \log B_1) + 10000 \log B_1 - 1000 \log B_2} \quad (A-2)$$

where a_1 and a_2 are evaluated from the given data and B_1 and B_2 are the values of the retardation factors at $C=10^4$ and $C=10^3$ respectively.

Note that $B=1$ at both C_1 and C_2 for the minimum retardations of each nuclide group and also for the preferred and maximum retardations of group I nuclides. Substituting $B_1=B_2=1$ into Eq. A-2 yields $B=1$ for each of these cases, and, hence, B does not depend on C . Equation A-2 was used to compute the preferred and maximum B 's for the fission products (group II) and the actinides (group III) using the data in Table 2.2-4. Table A-1 contains the results obtained for the preferred and maximum retardation factor of group II and III nuclides for the concentration of dissolved solids in each flow pipe.

For a given flow path, the probability distribution of B for each nuclide class is determined from the minimum, preferred, and maximum values of B given in Table A-1. For the nuclides in group I, B is set equal to 1 in all cases.

The actinides (group III) were assumed to have a log-normal distribution with the preferred values as median and the minimum and maximum values lying 2 standard deviations away in either side. This assumption is based on common practice and is reinforced by the fact that for each flow path the product of the minimum and maximum values of B equals the square of the preferred values -- a necessary condition for the lognor-

mal distribution. Note that if this condition is satisfied by the values of B given at the concentrations of 10^3 and 10^4 ppm of dissolved solids, it will automatically hold at every value of C if Eq. A-2 is used to compute the minimum, preferred, and maximum values of B at that concentration.

The probability distribution of B for the group II nuclides is not lognormal since the values of B given in table A-1 for these nuclides do not satisfy the necessary condition discussed in the previous paragraph. However, if the preferred value of B is assumed to be the median and the minimum and maximum values are assumed to be two standard deviations from the median then 3 points are determined on the cumulative distribution function (cdf) of the retardation. It is convenient to work with the base 10 logarithm of B ($\log B$), and the cdf of this variable will be interpolated from the three given points.

The problem of finding an analytic expression for the cumulative distribution of $\log B$, $F(x)$, is addressed by assuming that the function is a quadratic and that it fits the minimum, preferred, and maximum value of B calculated with Eq. A-2. This quadratic cdf can be used in a computer to randomly generate values of the retardation. Let P denote the preferred value of B and M denote the maximum value of B. Since the minimum value of B=1, there is no symbol assigned to this quantity. Thus, based on the assumed interpretation of the given values in terms of the cdf:

$$F(0) = \text{Prob}(\log B \leq 0) = \text{Prob}(B \leq 1) = 0.0227 \quad (\text{A-3a})$$

$$F(\log P) = \text{Prob}(\log B \leq \log P) = \text{Prob}(B \leq P) = 0.5 \quad (\text{A-3b})$$

$$F(\log M) = \text{Prob}(\log B \leq \log M) = \text{Prob}(B \leq M) = 0.9773 \quad (\text{A-3c})$$

In order to interpolate the values of $F(x)$ at other points x with $0 \leq x \leq 1$, assume

$$F(x) = ax^2 + bx + c$$

where a , b , and c are constants to be determined from Eqs. A-3a through A-3c.

The resulting expression for F is

$$F(x) = \frac{.4773}{\log P \log M (\log P - \log M)} [(\log M - 2 \log P) x^2 + \{2(\log P)^2 - (\log M)^2\} x] + 0.0227 \quad (A-4)$$

Figure A-1 shows the cdf computed for the logarithm of the retardation factor of group II nuclides in the upper aquifer. The random variable, B , corresponding to this cdf is determined by generating a random variable y from a uniform distribution with $0 \leq y \leq 1$, and solving

$$F(x) = y \quad (A-5)$$

for the corresponding x . Then $B=10^x$ is the random variable. This type of distribution will be referred to as "log-linear".

Table 2.2-6 summarizes the probability distributions used for the retardation factors of each nuclide group in each flow path. The distribution of each B is either "deterministic" in which case only the constant value is given, "lognormal" in which case the median value of B and the uncertainty (the standard deviation of the logarithm of B) are given, or "log-linear" in which case the preferred and maximum values of B are given.

Figure A-1 CDF for the Retardation Factor of Nuclide Group II in the Upper Aquifer

APPENDIX B
PERFORMANCE OF THE MEDIAN REPOSITORY

A repository based on the "preferred" (median) values of the input parameters (see Section 2.2) has been analyzed with NUTRAN.

The rate of release of radioactivity to the biosphere for this repository is illustrated in Fig. B-1, and numerical results are presented in Table B-1 for each nuclide group.

Figure B-1 is illustrative of the general behavior of the repository data used in this study. The flow of nuclide group I is seen as the "square wave" which begins at about 200 years and continues to about 3000 years. As the group I flow declines, the group II flow begins. Because retardation factors for groups II and III are not very different in the case considered, the group III outputs begin shortly thereafter. The "bump" in the output curve at about 6000 years, marked by the arrow, is the transition point where group III flow begins to dominate the release.

This repository was used with the reference river system described in Ref. 3 to compute the whole body equivalent dose to an individual whose life style involves maximum usage of those parts of the biosphere that are contaminated by the radioactivity. Calculated doses are shown in Fig. B-2.

These results are illustrative only since the reference river system does not exist at Site A.

Figure B-1 Release Rate of Radioactivity for the Selected Repository Data

TABLE B-1
RESULTS OF MEASURED VALUE RUN

	NUCLIDE GROUP I	NUCLIDE GROUP II	NUCLIDE GROUP III
Peak Flow Rate (Ci/yr)	2.4×10^2	1.3×10^2	3.2×10^2
Time of Peak Flow Rate (yr)	6.1×10^2	4.4×10^3	5.4×10^3
Integrated Flow (Ci)	4.5×10^5	2.6×10^5	6.4×10^5

Figure B-2 Whole Body Equivalent Case for Selected Repository Data

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