SENSITIVITY STUDIES OF THE SWIFT RADIONUCLIDE TRANSPORT MODEL

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I. INTRODUCTION

Risk analysis is a vital part of any safety assessment of a proposed nuclear waste depository. Risk analysis results are expressed in terms of radiation-induced health effects and are calculated using mathematical models. These models describe the following processes: (1) radionuclide migration in groundwater from the depository to a discharge point in the surface environment, (2) radionuclide migration and accumulation in the surface environment, (3) human uptake, and (4) radiation dosimetry and health effects. There are large uncertainties associated with many of the input variables to these models so that ranges, rather than point values, are often specified. Consequently, the risk estimates themselves have large uncertainties. Therefore, point estimates of risk, without an indication of the possible distribution of results, are probably meaningless and may be misleading.

Given the importance of quantifying uncertainties in risk estimates, it is clearly important to identify those input variables which are major contributors to uncertainty in model output. It is also important to establish techniques to generate model output distributions with a limited number of computer runs for assumed ranges and distributions on model input variables. Such is the purpose of a sensitivity analysis.

The work reported here is part of a larger program funded by the Nuclear Regulatory Commission to develop a risk assessment methodology for geologic disposal of radioactive waste.

Two important parts of this methodology were used in this study, namely a numerical geosphere transport simulator and statistical techniques for analyzing transport calculations. The transport simulator is the Sandia Waste Isolation Flow and Transport (SWIFT) code [Dillon, Lantz, and Pahwa, 1978]. It is a three-dimensional, finite-difference model which solves conservation equations for fluid flow, heat transport, (possibly non-trace) solute mass, and radionuclides in trace quantities. The statistical techniques package [Iman, Helton, and Campbell, 1978] were designed to reduce the number of transport calculations and still make possible a reliable identification of important input variables. These methods are discussed further in Section III. To demonstrate the application of the transport and statistical methods, we have chosen a reference site and a particular depository-breachment scenario. The physical problem is described in the next section, and results from the sensitivity analysis are presented in Section IV.

11. PHYSICAL PROBLEM

The sensitivity analysis described in this paper was applied to a strictly hypothetical system. This system consists of both a reference site containing a nuclear waste depository [Campbell, et al., 1978] and a disruptive-event scenario for the possible release of radioactive materials from the depository to the biosphere. The reference site is located in a symmetrical upland valley and is shown in cross-section in Figure 1.

The crest of the ridge surrounding the valley is at an elevation of 6000 feet, and the crest is a surface- and ground-water divide so that the only water moving in the valley falls in the valley itself. The valley is drained by a major river, River L, which is at elevation 2500 feet. Tributaries to River L exist, such as River U, but they are normally dry. The valley receives 40 inches of rainfall per year, of which 16 inches are lost by evapotranspiration and the remaining 24 inches recharge the groundwater system. The geology of the site is also shown in Figure 1. The valley is underlain by crystalline bedrock which crops out only over a narrow width at the ridge crest surrounding the valley. This bedrock is assumed to be impermeable to groundwater flow. Over the bedrock is a sequence of sedimentary rock as shown in Figure 1. Nominal values of all hydraulic and thermal properties are given in Campbell, et al. [1978].

One disruptive event which conceivably could release radioactive waste from a depository such as that of the reference site is the formation of a U-tube. Here we assume seal failures of a shaft (30 feet in diameter) on the up-dip side and of a borehole (3 feet in diameter) on the down-dip

Figure 1. Geologic Cross-Section Through Reference Site

side. The shaft, for example, could be a man-materials connection to the surface, and the borehole could be a ventilation pipe. The U-tube, as shown in Figure 1, provides a flow path between the depository and the upper aquifer. The shaft and borehole are not extended through the upper shale and upper sand and gravel as there is no significant vertical hydraulic gradient.

Numerical simulations have been carried out for the full two-dimensional system of Figure 1 and for some selected three-dimensional systems in the near field of the depository using the SWIFT computer code. For the sensitivity analysis, however, a simplified one-dimensional representation of the full system and the U-tube was used. This representation is shown as a dashed line in Figure 1. Fluid flow in the simplified system was established using pressure boundary conditions taken from a full-system simulation, and radionuclides were introduced into the system from an assumed inventory and leach rate.

As indicated in the Introduction, fluid flow and radionuclide transport are controlled by hydrological and geochemical variables whose values are not generally well known for any given site. For the reference site, this uncertainty was defined by the Delphi method. Earth scientists from Sandia Laboratories, the U.S. Geological Survey and INTERA Environmental Consultants were assembled for the purpose of assigning a range and a distribution to each hydrological and geochemical parameter.

The results of this effort are shown in Table 1 for the simplified U238 chain, $U238 \rightarrow U234 \rightarrow Th230 \rightarrow Ra226$. The ranges chosen are global in nature and, as such, are somewhat broader than one might reasonably expect for a particular site.

Table 1. Parameter Ranges and Distributions

<u>Variable*</u>	<u>Range</u>	<u>Distribution</u>
ϕ_s	0.005 - 0.20	Log Normal
ϕ_a	0.05 - 0.30	Normal
K_s	0.01 - 50 ft/d	Log Normal
K_a	1.0 - 50 ft/d	Log Normal
α	45 - 500 ft	Uniform
$k_d(U)$	10^{-2} - 10^5 cm ³ /g	Log Uniform
$k_d(Th)$	10^{-2} - 10^5 cm ³ /g	Log Uniform
$k_d(Ra)$	10^{-2} - 10^3 cm ³ /g	Log Uniform
τ	10^3 - 10^7 y	Log Uniform

*Variable definitions:

ϕ = porosity, K = hydraulic conductivity, α = dispersivity,
 k_d = distribution coefficient, τ = leaching time of a constant-rate leach model, s = shaft and borehole, a = aquifer.

III. DESCRIPTION OF STATISTICAL METHODS

For the physical problem described above, we present results for the total (integrated) radionuclide discharge in the 10^5 -year time period following depository closure. The pertinent questions are:

1. Which variables, of those listed in Table 1, have a significant effect upon the total discharge and what is their relative importance?
2. What relationships exist between the distributions of model input and model output?

Conceptually, the manner in which the first question is answered is based on a simple geometrical picture such as the one shown in Figure 2. The dependent variable Y is given as a function of the two independent variables X_1 and X_2 over their respective ranges. Surface S is called the response surface. In general, the value of the dependent variable Y is known only at certain discrete points (i.e., for particular values of X_1 and X_2) as indicated by the crosses in Figure 2. In the physical problem addressed in this paper, the discrete points are known as a result of transport calculations with the SWIFT code. The

Fitting of the response surface by stepwise regression is of central importance to the sensitivity analysis as this process selects the important independent variables. In addition the standardized regression coefficients derived from the regression analysis provide a basis for determining the relative importance of the independent variables. Thus, the first question posed at the beginning of this section may be answered through response-surface construction.

Although simple in concept, response surface construction involves several statistical procedures. There is, for example, preliminary variable assessment using partial correlation coefficients, stepwise regression for construction of the response surface, protection against overfit, use of t-test to establish significance levels for the independent variables, and various tests to examine the effect of input variable distribution assumptions on the output variable distribution. Details of these procedures can be found in Iman, Helton and Campbell [1978] and in references cited therein. Here, however, we wish to highlight two relatively new statistical techniques which were used.

The first technique is Latin Hypercube Sampling (LHS) [McKay, Conover, and Beckman, 1970] which minimizes, relative to other commonly used schemes, the number of model calculations required for response surface construction. (For the numerical radionuclide transport simulator used here, the calculations can be quite expensive.) LHS yields a global selection of points and the fitted response surface yields an unbiased estimate of cumulative distributions functions and mean values for the model output. It is for these reasons that LHS is being used for sensitivity and risk analysis.

A brief description of LHS is provided in the following discussion. First the independent variable ranges X_i are divided into intervals I_{ji} based on equal probability. Values T_{ji} are

then randomly selected from each of these intervals. Secondly, the values T_{ji} are randomly mixed for each of the variables X_i to form the input vectors. For the simple four-point example of Figure 2 each variable range is divided as shown below,

and the four input vectors of independent variables are $T_1 = (T_{31}, T_{12})$, $T_2 = (T_{11}, T_{22})$ and $T_3 = (T_{41}, T_{32})$, $T_4 = (T_{21}, T_{42})$.

The second technique from the response surface methodology which we wish to highlight is rank regression [Iman and Conover, 1979a]. The motivation here stems from the nonlinearity which is frequently present in the dependence $Y = f(X_1, X_2, \dots)$ of the basic response variable upon the independent variables. If, however, the dependence is monotone, as it frequently is for transport calculations, then it may be linearized with the rank transformation. The concept of a rank transform is simple in that each variable (independent and dependent) is replaced by its corresponding rank. For example, the smallest value of X_1 is replaced by the rank 1, the next smallest by the rank 2, and so on. Thus the original discrete valued function is replaced by the rank-transformed function $R(Y) = f[R(X_1), R(X_2), \dots]$. It is this transformed function which is fitted with a response-surface using stepwise regression and which is used to establish the significance and relative importance of the independent variables.

To answer the second question posed at the beginning of this section, i.e., the relationship of distributions of output variables to the assumed distributions of input variables, we can either propagate new distributions through the fitted response surface or reweight the base set of Latin hypercube input vectors as outlined in Iman and Conover [1979b] to reflect different distribution assumptions. This aspect of the analysis thus provides a means of assessing the sensitivity of model output to the distribution assumptions of the input variables. The utility of this procedure is demonstrated in the next section for the physical problem discussed in Section II.

IV. RESULTS AND CONCLUSIONS

To identify the important input variables for the system described in Section II and to establish relative importances of these quantities, stepwise regression analysis was performed on the total discharge to River L. The ranking of input variables for total discharge is shown in Table 2.

Table 2. Input Variable Ranking for Total Discharge.

<u>U238</u>	<u>U234</u>	<u>Th230</u>	<u>RA226</u>
$k_d(U)$	$K_d(U)$	$k_d(Th)$	$k_d(Ra)$
	τ	τ	K_s
	K_a	K_a	
	ϕ_a	ϕ_a	
N	30	28	47
R ²	0.657	0.850	0.909

The number N of nonzero values for each isotope which were used in the stepwise regression analysis are shown in the table. (Runs which produced no discharge during 10^6 years were omitted.) The R² values, if multiplied by 100, represent the percent of the output variation (expressed in ranks) which is assigned to the input variables selected by stepwise regression.

For each isotope, the distribution coefficient K_d ranked as the most important variable. The leach rate τ , hydraulic conductivity in the aquifer K_a and shaft K_s , and shaft porosity ϕ_a enter as less important variables.

Figure 3 shows cumulative distributions of total discharge for U238. The solid line represents results from the original SWIFT calculations. Even only 30 nonzero values were used to fit the response surface, the agreement is quite good. The agreement between SWIFT and the response surface curves for U234, Th230 and RA226 (not shown) is of similarly high quality.

Figure 4 shows cumulative distributions of total discharge for U238 where zero values have been included. These results are included to show the sensitivity of SWIFT output to the distribution assumption for the distribution coefficient (K_d). The curve labelled LU represents the original SWIFT results where a log-uniform distribution was used for the K_d values. To obtain the curve labelled LN, the original input vectors were reweighted to represent a log-normal distribution for the K_d values.

In conclusion we note four things: (1) Our simulation and statistical techniques appear to be applicable to a field-scale waste-isolation problem. (2) Transport variables have been constructed with less than 50 calculations by the geosphere-transport simulator. (3) The dispersivity is unimportant because total releases are used, and therefore, details of the shape of the breakthrough are unimportant. (4) The dominance of the distribution coefficient in each case is reasonable in view of the rather large values of the upper bound for this quantity (10^3 cm³/g for U and Th and 10^3 cm³/g for Ra).

Figure 3. Cumulative distributions of total discharge relative to source. The solid line represents results from SWIFT. The dotted line represents results from fitted response surface. Calculations which produced zero discharge are excluded.

Figure 4. Cumulative distributions of total discharge relative to source. The solid line represents results from SWIFT with log uniform distributions for K_d values. The dashed line was obtained by reweighting SWIFT results to represent log normal distributions on K_d values.

V. BIBLIOGRAPHY

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