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GEOLOGIC WASTE DISPOSAL AND A MODEL FOR THE SURFACE MOVEMENT OF RADIONUCLIDES

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INTRODUCTION

In the following, a model for the surface movement of radionuclides is presented. This model, which is referred to as the Pathways Model, was constructed at Sandia Laboratories in a project funded by the Nuclear Regulatory Commission to develop a methodology to assess the risk associated with the geologic disposal of high-level radioactive waste. The methodology development involves work in two major areas: (a) models for physical processes, and (b) statistical techniques for the use and assessment of these models. The following presentation of the Pathways Model will involve topics from both areas. Additional information on the entire project can be obtained from its interim report (Campbell et al., 1978)

A model for the surface movement of radionuclides in the context of geologic waste disposal should permit consideration and assessment of the many factors that may affect both radionuclide distribution in the environment and our ability to predict such distribution. Desirable features include the following. First, due to (a) the possible diversity of specific waste disposal sites, (b) the changes which may occur at a particular site during the long time periods involved in radioactive waste disposal, and (c) the potential assessment and comparison of different sites, the model should be able to represent radionuclide movement in different physical settings. Second, the model should be able to represent radionuclide accumulation and possible reconcentration as well as dispersion and dilution. Third, as distribution coefficients and other factors influencing radionuclide movement are inexact known, the model should be

amenable to sensitivity analysis to determine (a) the relative importance of individual variables, and (b) the effects of uncertainty in knowledge of these variables. Fourth, as potential release periods in radioactive waste management are lengthy, it should be possible to determine the asymptotic behavior of the model. Fifth, as rainfall and other factors influencing radionuclide movement are functions of time (actually, stochastic processes), it should be possible to determine what effects the use of average values and other simplifying assumptions has on model predictions.

There are many models for the environmental movement of radionuclides. Recent surveys are provided by Hoffman et al. (1977) and Strenge et al. (1976). However, after considering existing models, it was decided that it would be more productive to construct a model tailored to the specific needs of the waste disposal project than to adapt an already existing model to those needs. Of the existing models, the Pathways Model has the greatest conceptual similarity with the HERMES model (Fletcher and Dotson, 1971).

THE PATHWAYS MODEL

For the environmental movement of radionuclides in the context of geologic waste disposal, there are two processes involved with distinctly different time scales. The first process is the long term distribution and accumulation of radionuclides in the surface environment. Radionuclide release to, movement through and removal from the environment will generally be very slow. The second process is the movement of radionuclides from the surface environment to man. Here, the time scale is much shorter. Therefore, the Pathways Model is divided into two submodels. One of these, the Environmental Transport Model, represents the long term distribution and accumulation of radionuclides in the environment. The other, the Transport to Man Model, represents the movement of radionuclides from the environment to man.

In the Environmental Transport Model, radionuclide movement is represented with a compartment model. With this approach, radionuclides in an area under consideration are divided into a number of "compartments" and then radionuclide movement between these compartments is represented by a system of linear differential equations. The basic idea is to place radionuclides which are in physical regions with different characteristics in different compartments and then to determine the distribution which results from radionuclide decay and from radionuclide movement between regions.

The Environmental Transport Model uses an algorithm to construct the radionuclide transport equations described in the preceding paragraph. The basis of this algorithm is a building block called a zone. A zone corresponds to a physical region in an area to be modeled. Further, each zone has four subzones (groundwater, soil, surface water and sediment) and various movements of water and solid material associated with these subzones are possible. It is the movements of water and solid material which are assumed to be responsible for radionuclide transport. In such movements, it is assumed that radionuclides are partitioned between the liquid and solid phases on the basis of distribution coefficients. A system of transport equations incorporating decay chain characteristics and regional diversity is constructed by linking a suitable number of these zones together. In this construction, each subzone has one uniformly mixed compartment associated with it for each radionuclide in the decay chain under consideration. A single zone is represented in Figure 1 and the linkage of a number of zones to represent the movement of a decay chain is represented in Figure 2.

In the Transport to Man Model, radionuclide movement is represented by a model based on simple food chains and concentration ratios. With this approach, food chains which originate in an affected area and lead to man are determined. Then, the radionuclide concentration in an affected food type is determined by the use of concentration ratios, and the amount of radionuclide consumed follows from the amount of food consumed and the radionuclide concentration in that food. This approach is the same as currently employed by the Nuclear Regulatory Commission (NRC, 1977).

A more detailed description of the Pathways Model is provided in Chapter 4 of the project's interim report (Campbell et al., 1978). Further, a user's manual which describes the

Fig. 1. Division of a Zone into Subzones. Arrows represent possible movements of water and solid material.

Fig. 2. Flows Associated with the Movement of a Chain of N Radionuclides through a System of M Zones. Figure 1 represents the flows associated with a single zone in greater detail.

model and the computer program which implements it is also available (Helton and Kaestner, 1979).

It is felt that the division of the Pathways Model into the submodels Environmental Transport and Transport to Man and the construction of the Environmental Transport Model on the basis of compartments provides the capability to represent different types of radionuclide movement and also to assess both radionuclide dilution and possible reconcentration. By suitably defining the zones and subzones associated with the Environmental Transport Model and organizing the operation of this model in conjunction with the Transport to Man Model, it is possible to represent a variety of different and possibly diverse sites and also to represent different sets of conditions which could exist through time at a specific site. The computer program which implements the Pathways Model is written to permit, and indeed require, significant user involvement in its operation.

SENSITIVITY ANALYSIS

For the Pathways Model, an approach to sensitivity analysis based on regression analysis has been found to be productive. The overall approach is described in Iman et al. (1979) and applications of the approach to the Environmental Transport Model are described by Helton and Iman (1979) and Helton et al.

(1979). Basically, the idea is (a) to start with a set of input variables with selected ranges and distributions, (b) to select model inputs from these variables according to their ranges and distributions, (c) to generate model output with the selected inputs, and (d) to assess the relationship between model input and output by stepwise regression. Special techniques found to be useful include (a) Latin hypercube sampling to select values of input variables, (b) the rank transform to reduce the effects of nonlinearity in the relationships between model input and output, and (c) the FRESS (predicted error sum of squares) criterion to indicate overfit during regression analysis.

An example of a sensitivity analysis calculation is contained in Table 1. This example is taken from Table 6.10 of Helton and Iman (1979) and indicates variables affecting the buildup of U234 in a flood plain. It is assumed that U234 is entering a river and that various processes are acting to move it into the flood plain. The site and the assumptions underlying its derivation are described in Helton and Iman (1979). Approximately 30 independent variables were involved in the regression analysis which generated Table 1. The following variables actually appear in the table: B4- average soil subzone thickness, B7- a conversion factor such that the product of B7 and the pore volume of the soil subzone is equal to the annual water exchange between the soil subzone and the surface water subzone, B10- a conversion factor such that the product of B10 and the mass of solids contained in the soil subzone is equal to the annual solid exchange between the soil subzone and the surface water subzone, B12- the regional erosion rate, B42- the distribution coefficient for U234 in the soil subzone, and B43- the distribution coefficient for U234 in the surface water subzone.

The stepwise regression analysis which generated Table 1 was based on rank transformed data. The first two columns indicate the variables and cross products in order as selected by the regression analysis. The third and fourth columns contain R^2 values based on rank transformed data and interpolations

Table 1. Stepwise Regression Results for Variables Affecting U234 Concentration in a Flood Plain.

Step	Variable	Rank R^2	Raw R^2	St. Reg. C.
1	B43	0.614	0.368	0.745
2	B42	0.796	0.665	1.283
3	B42*B42	0.849	0.669	-0.866
4	B10*B43	0.878	0.702	0.254
5	B12*B43	0.901	0.812	-0.189
6	B4*B7	0.914	0.835	0.118

from rank transformed data to raw (i.e., untransformed) data, respectively. The Rank R^2 indicates how successful the regression model is in predicting the relative importance of variables in influencing the Environmental Transport Model while the Raw R^2 indicates how successful the regression model is in duplicating the Environmental Transport Model. The fifth column contains standardized regression coefficients for the individual variables in the regression model at the last step of the regression analysis. The absolute value of these coefficients provides a ranking of the relative importance of the individual variables in influencing the model. Many regression analyses of the form indicated here are presented in Helton and Iman (1979) and Helton et al. (1979).

ASYMPTOTIC BEHAVIOR

It is possible to show that, for a fixed rate of radionuclide input, the radionuclide concentrations as predicted by the Environmental Transport Model will increase monotonically to asymptotic limits. As the time required in many situations to reach steady state in the surface environment may be short relative to other processes involved in the release of radionuclides to the surface environment (i.e., groundwater transport), it may be desirable to use asymptotic values for radionuclide concentrations in the surface environment rather than calculating and using their values as functions of time. For the same zone and variables used in the generation of Table 1, the variation in time to 90 percent steady state and concentration at steady state for an assumed input rate of 1 atom/yr of Cm245 to the surface water subzone is represented in Table 2. This table is adapted from Tables 4.4 through 4.7 of Helton et al. (1979); this report contains numerous such compilations as well as sensitivity analyses similar to the one presented in Table 1 for the variables influencing time to 90 percent steady state and concentration at steady state. As the Environmental Transport Model is linear with respect to radionuclide input, such calculations can be scaled to represent other input rates.

TIME VARYING PARAMETERS

In the Environmental Transport Model, as will probably be the case for any model used to represent the surface movement of radionuclides, many parameters are based on "averaged" water and solid flow rates. Often, mean annual flow rates are used whereas the flow rates are (at best) periodic functions or (more realistically) periodic stochastic processes. It is desirable to assess the effect that the replacement of parameters with their average values has on model predictions. Such a study has been initiated for the Environmental Transport Model (Brown and Helton, 1979).

Table 2. Time to 90 Percent Steady State and Concentration at Steady State for an Assumed Input to the Surface Water Subzone of 1 atom/yr of Cm245. Time is in years; surface water concentration is in atoms/L; all other concentrations are in atoms/kg.

		<u>Ground Water</u>	<u>Soil</u>	<u>Surface Water</u>	<u>Sedi- ment</u>
Time to	Minimum	.10E+03	.10E+02	.10E+01	.10E+02
90%	Maximum	.28E+05	.51E+04	.27E+03	.44E+03
Steady	Average	.11E+05	.34E+03	.20E+02	.72E+02
State	St. Dev.	.10E+05	.43E+03	.33E+02	.65E+02
Conc. at	Minimum	.12E-16	.14E-13	.35E-13	.42E-12
Steady	Maximum	.13E-09	.38E-09	.94E-13	.45E-09
State	Average	.30E-11	.37E-10	.54E-13	.75E-10
	St. Dev.	.11E-10	.58E-10	.14E-13	.87E-10

That study investigates the effects of multiplying the coefficient matrix for the radionuclide transport equations by a periodic function and by a periodic stochastic process. The function and the stochastic process were picked to mimic observed hydrologic patterns. For the periodic hydrologic process, it was possible to calculate bounds on the difference between predictions made with the untransformed and transformed coefficient matrix; for the stochastic hydrologic process, there was less success at obtaining analytic assessments of the untransformed and transformed cases and computer simulations were used to obtain an indication of their differences. Overall, the variation was not large between concentrations calculated with averaged yearly values and with either periodic or periodic stochastic perturbations of these values. This is especially true as the uncertainty in some of the other parameters which are used as model input (particularly distribution coefficients) can produce much larger variation in model predictions.

REFERENCES

- Brown, J. B., and Helton, J. C., 1979, "Risk Methodology for Geologic Disposal of Radioactive Waste: Effects of Variable Hydrologic Patterns on the Environmental Transport Model," Report No. SAND79-1909, Sandia Laboratories, Albuquerque, NM.
- Campbell, J. E., Dillon, R. T., Tierney, M. S., Davis, H. T., McGrath, P. E., Pearson, F. J., Shaw, H. R., Helton, J. C., and Donath, F. A., 1978, "Risk Methodology For Geologic Disposal of Radioactive Waste: Interim Report," Report No. SAND78-0029, Sandia Laboratories, Albuquerque, NM.

- Fletcher, J. F., and Dotson, W. L. (Compilers), 1971, "HERMES - A Digital Computer Code for Estimating Regional Radiological Effects from the Nuclear Power Industry," Report No. HEDL-TME-71-168, Hanford Engineering Development Laboratory, Richland, WA.
- Helton, J. C., Brown, J. B., and Iman, R. L., 1979, "Risk Methodology for Geologic Disposal of Radioactive Waste: Asymptotic Properties of the Environmental Transport Model," Report No. SAND79-1908, Sandia Laboratories, Albuquerque, NM.
- Helton, J. C., and Iman, R. L., 1979, "Risk Methodology for Geologic Disposal of Radioactive Waste: Sensitivity Analysis of Pathways Model," Report No. SAND79-1393, Sandia Laboratories, Albuquerque, NM.
- Helton, J. C., and Kaestner, P. C., 1979, "Risk Methodology for Geologic Disposal of Radioactive Waste: User Manual for Pathways Model," Report No. SAND78-1711, Sandia Laboratories, Albuquerque, NM.
- Hoffman, F. O., Miller, C. W., Shaeffer, D. L., and Garten, C. T., 1977, "Computer Codes for the Assessment of Radionuclides Released to the Environment," Nuclear Safety 18, pp. 343-354.
- Iman, R. L., Helton, J. C., and Campbell, J. E., 1978, "Risk Methodology for Geologic Disposal of Radioactive Waste: Sensitivity Analysis Techniques," Report No. SAND78-0912, Sandia Laboratories, Albuquerque, NM.
- Strenge, D. L., Watson, E. A., and Droppo, J. G., 1976, "Review of Computational Models and Computer Codes for Environmental Dose Assessment of Radioactive Releases," Report No. BNWL-B-454, Battelle Pacific Northwest Laboratories, Richland, WA.
- U.S. Nuclear Regulatory Commission, 1977, "Calculation of Annual Doses to Man from Routine Releases of Reactor Effluents for the Purpose of Evaluating Compliance with 10 CFR Part 50, Appendix I," Regulatory Guide 1.109, Revision 1.