Groundwater pathway sensitivity analysis and hydrogeologic parameters identification for waste disposal in porous media

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1 INTRODUCTION

The migration of radionuclides in a geologic medium is controlled by the hydrogeologic parameters of the medium such as dispersion coefficient, pore water velocity, retardation factor, degradation rate, mass transfer coefficient, water content, and fraction of dead-end pores. These hydrogeclogic parameters are often used to predict the migration of buried wastes in nuclide transport models such as the conventional advection-dispersion model (Freeze and Cherry 1979), the mobile-immobile pores model (Coats and Smith 1964), the nonequilibrium adsorption-desorption model (Ogata 1964), and the general group transfer concentration model (Yu et al. 1985b). One of the most important factors determining the accuracy of predicting waste migration is the accuracy of the parameter values used in the model. More sensitive parameters have a greater influence on the results and hence should be determined (measured or estimated) more accurately than less sensitive parameters. A formal parameter sensitivity analysis is carried out in this paper. Parameter identification techniques to determine the hydrogeologic parameters of the flow system are discussed. The dependence of the accuracy of the estimated parameters upon the parameter sensitivity is also discussed.

2 NUCLIDE TRANSPORT EQUATION

The one-dimensional nuclide transport equation in porous media can be expressed in the following partial differential equation (PDE):

$$\frac{\partial C}{\partial t} = \frac{D}{R_d}\frac{\partial^2 C}{\partial Z^2} - \frac{V}{R_d}\frac{\partial C}{\partial Z} - \lambda C - \frac{K}{R_d} C + \frac{\dot{M}}{R_d} \qquad (1)$$

where: C = dissolved concentration of radionuclide (kg m^{-3}); D = dispersion coefficient (m^2 s^{-1}); R_d = retardation factor = $1 + \rho_b K_d/\theta$;

ρ_b = bulk density of the porous medium (kg m^{-3}); K_d = distribution coefficient (m^3 kg^{-1}); θ = volumetric water content (m^3 m^{-3}); V = average pore water velocity (m s^{-1}); λ = radioactive decay constant (s^{-1}); K = degradation rate (s^{-1}); M = source releasing rate (kg m^{-3} s^{-1}); Z = distance along flow path (m); and t = time (s).

Numerous analytical solutions for various boundary and initial conditions have been solved for Equation 1. For the purpose of parameter sensitivity analysis, the simplest form of solution will be employed. The analysis procedures presented herein can be employed in more complicated solution forms and can be expanded to two- and three-dimensional cases. The simplest solution to Equation 1 is an infinite medium solution with planar source input, which can be obtained by the Fourier integral transformation method. Because the radioactive decay constant, λ, is a physical parameter that can be determined (measured) much more accurately than all the other parameters, λ can be deleted in sensitivity analysis. After correcting for radioactive decay, the infinite medium solution of the concentration at any point of interest, Z_1, can be written as:

$$C(t) = \frac{C_o}{R_d} \frac{1}{\sqrt{4\pi Dt/R_d}} \exp\left[- \frac{(Z_1 - Vt/R_d)^2}{4Dt/Rd} - \frac{K}{R_d} t \right] \quad (2)$$

where C_o = planar source concentration (kg m^{-2}).

In sensitivity analysis terminology, the concentration, C, in Equation 2 is the response function (output); the parameters (input) are D, R_d, V, K, and Z.

3 PARAMETER SENSITIVITY AND SENSITIVITY COEFFICIENTS

3.1 Definition

The sensitivity analysis of the nuclide concentration response function is developed as follows. This sensitivity analysis will show the fractional change of the concentration due to the fractional change of a parameter (Yu 1984).

Let dC denote the change in the concentration distribution that results from the perturbation dP of parameter P. Further, let dC/C denote the fractional (or percentage) change that results from the fractional (or percentage) change dP/P. Then the sensitivity coefficients, S_P, are given by the ratio of $\frac{dC}{C}$ to $\frac{dP}{P}$. That is,

$$S_P \equiv \frac{dC/C}{dP/P} = \frac{d(\ln C)}{d(\ln P)} \quad (3)$$

Note that S_P is a dimensionless number and represents the percentage change in output to the percentage change in input. Since

$$dC = \frac{\partial C}{\partial P} dP \quad (4)$$

with all other parameters fixed, therefore

$$S_P = \frac{\partial C}{\partial P} \cdot \frac{P}{C} \tag{5}$$

In other words, the sensitivity coefficient of a parameter P is the product of the partial derivative $\partial C/\partial P$ times the ratio of P/C. The partial derivative, $\partial C/\partial P$, is called the sensitivity of the response function C to a perturbation in the parameter P at a given point (Thomas 1982). The sensitivity can change from point to point and, for a given perturbation dP, the resulting change in C can be much larger than dP (if $\partial C/\partial P$ is large) or much smaller than dP (if $\partial C/\partial P$ is small).

The sensitivity of C with respect to a parameter P is denoted as C_P. That is,

$$C_P \equiv \frac{\partial C}{\partial P} \tag{6}$$

Substituting Equation 6 into Equation 5 results in

$$S_P = C_P \cdot \frac{P}{C} \tag{7}$$

3.2 Mathematical derivations

Applying Equations 3-7 to the concentration equation (Equation 2), the parameter sensitivities of the response function C(t) can be derived by elementary calculus. The results (Yu 1984) are:

$$C_D = \frac{\partial C}{\partial D} = \frac{C(t)}{D} \cdot \left[\frac{(Z_1 - Vt/R_d)^2}{4Dt/R_d} - \frac{1}{2} \right] \tag{8}$$

$$C_{R_d} = \frac{\partial C}{\partial R_d} = \frac{C(t)}{R_d} \cdot \left[\frac{Kt}{R_d} - \frac{(Z_1 - Vt/R_d)(Z_1 + Vt/R_d)}{4Dt/R_d} - \frac{1}{2} \right] \tag{9}$$

$$C_V = \frac{\partial C}{\partial V} = \frac{C(t)}{V} \cdot \left[\frac{V(Z_1 - Vt/R_d)}{2D} \right] \tag{10}$$

$$C_K = \frac{\partial C}{\partial K} = \frac{C(t)}{K} \cdot \left(- \frac{Kt}{R_d} \right) \tag{11}$$

$$C_{Z_1} = \frac{\partial C}{\partial Z_1} = \frac{C(t)}{Z_1} \cdot \left[- \frac{Z_1(Z_1 - Vt/R_d)}{2Dt/R_d} \right] \tag{12}$$

The sensitivity coefficients of the parameters can be obtained from Equations 8-12 and Equation 5. The results are:

$$S_D = \frac{(Z_1 - Vt/R_d)^2}{4Dt/R_d} - \frac{1}{2} \tag{13}$$

$$S_{R_d} = \frac{Kt}{R_d} - \frac{(Z_1 - Vt/R_d)(Z_1 + Vt/R_d)}{4Dt/R_d} - \frac{1}{2} \quad (14)$$

$$S_V = \frac{V(Z_1 - Vt/R_d)}{2D} \quad (15)$$

$$S_K = -\frac{Kt}{R_d} \quad (16)$$

$$S_{Z_1} = -\frac{Z_1(Z_1 - Vt/R_d)}{2Dt/R_d} \quad (17)$$

In order to get a more accurate indication of these sensitivity coefficients, a typical set of parameters is used to calculate sensitivity coefficients. This set of parameters is: $D = 0.001\ m^2\ h^{-1}$, $R_d = 2.0$, $V = 0.1\ m\ h^{-1}$, $Z_1 = 1.0\ m$, $K = 0.0625\ h^{-1}$, and $C_o = 1.0\ \mu Ci\ m^{-2}$.

The sensitivity coefficients of the parameters D, R_d, V, Z_1, and K at different times are presented in Table 1. The sensitivity coefficients change as time passes and there is a certain trend in how they change. Also, S_K has rather small absolute values compared to the others, which means that the concentration is rather insensitive to the degradation rate. The sensitivity coefficients have the same sign as the sensitivities of the concentration distribution. Thus, for negative sensitivity coefficients, the response function will change in the opposite direction of the perturbation--i.e., if the parameter is increased, then the concentration will decrease. Therefore, when an iterative method is used to estimate parameter values from nuclide concentration data, the sensitivity coefficients offer good information that can be used to (1) qualitatively determine in which direction to go to the next step, and (2) quantitatively predict how much a

Table 1. Parameter sensitivity coefficients

Time (h)	S_D	S_{R_d}	S_V	S_{Z_1}	S_K
3	119.92	-162.82	42.50	-283.33	-0.09
6	40.33	-75.65	35.00	-116.67	-0.19
9	16.31	-44.02	27.50	-61.11	-0.28
12	6.17	-26.29	20.00	-33.33	-0.38
15	1.58	-14.12	12.50	-16.67	-0.47
18	-0.22	-4.72	5.00	-5.56	-0.56
21	-0.44	3.10	-2.50	2.38	-0.66
24	0.33	9.92	-10.00	8.33	-0.75
27	1.77	16.08	-17.50	12.96	-0.84
30	3.67	21.77	-25.00	16.67	-0.94
33	5.90	27.13	-32.50	19.70	-1.03
36	8.39	32.24	-40.00	22.22	-1.13

parameter value should be changed. However, this application is hindered when there is more than one parameter as in the case of the nuclide transport equation.

The above derivations (Equations 4-17) assume that only one parameter is uncertain whereas all others are fixed. A more general case is that in which all parameters are uncertain; in this case, the total differential of the concentration may be expressed as:

$$dC = \frac{\partial C}{\partial D} dD + \frac{\partial C}{\partial R_d} dR_d + \frac{\partial C}{\partial V} dV + \frac{\partial C}{\partial K} dK + \frac{\partial C}{\partial Z_1} dZ_1 \qquad (18)$$

Dividing Equation 18 by C yields:

$$\frac{dC}{C} = S_D \frac{dD}{D} + S_{R_d} \frac{dR_d}{R_d} + S_V \frac{dV}{V} + S_K \frac{dk}{K} + S_{Z_1} \frac{dZ_1}{Z_1} \qquad (19)$$

That is, the total percentage change is the sum of all the changes caused by individual parameters, which is the parameter percentage change times its own sensitivity coefficient. There are infinite combinations of the individual parameter percentage change that will result in the same total concentration percentage change. Thus, it is difficult to estimate parameter values from concentration data by an iterative method (see further discussion below).

3.3 Graphic illustration

Listing of calculated values in a table, such as Table 1, is one way to show sensitivity coefficients. A large number of long tables may be needed to show the S_p values at different conditions (different parameter values and times). Another way of showing parameter sensitivities is by using figures. Figures 1-5 illustrate how the concentration breakthrough curve (BTC) changes with a single parameter whereas all others are fixed to the values defined in Section 3.2.

Familiarity with these figures and the parameter sensitivities will be useful in interpreting computer model results and in predicting the results before actually running the model (Yu et al. 1984b, 1985a). Hence, a significant amount of computer costs may be saved if it is known that changing an insensitive parameter in a rather expensive code will not affect the results.

4 PARAMETER IDENTIFICATION

The parameter identification problem is called the Inverse Problem (IP) in the literature (Neuman 1973; Sagar et al. 1975). The IP is the reverse of a Direct Problem (DP). In the DP, concentrations are determined from known parameters and boundary conditions; whereas, in

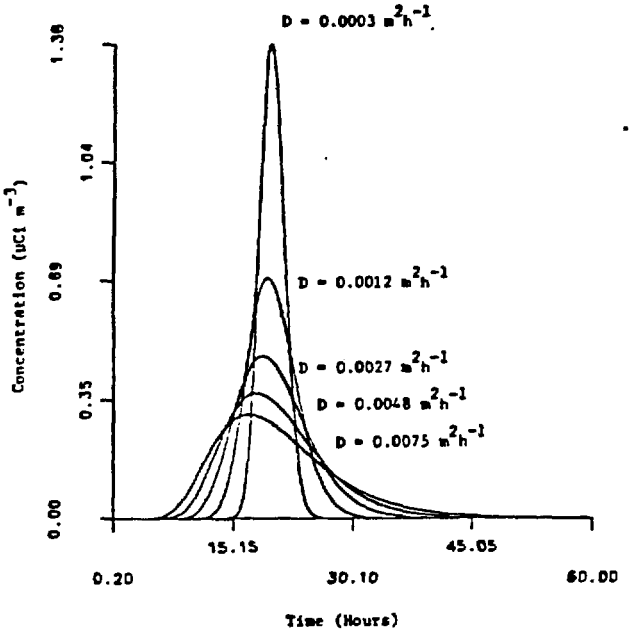

Figure 1. Breakthrough curves with different dispersion coefficients.

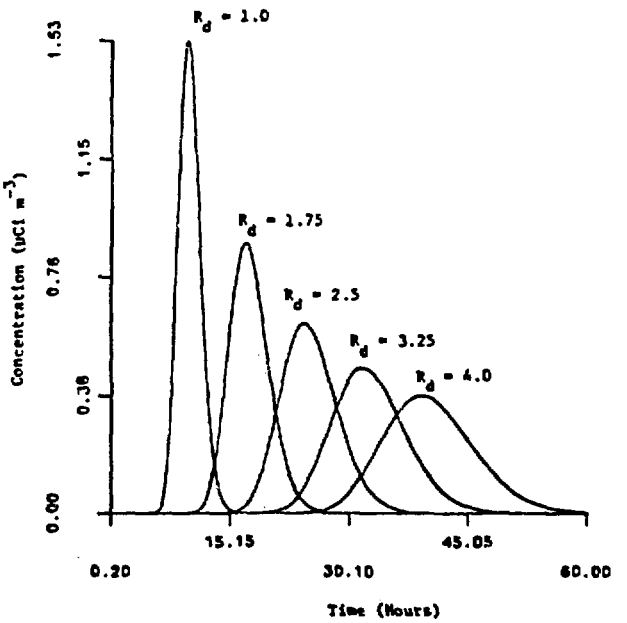

Figure 2. Breakthrough curves with different retardation factors.

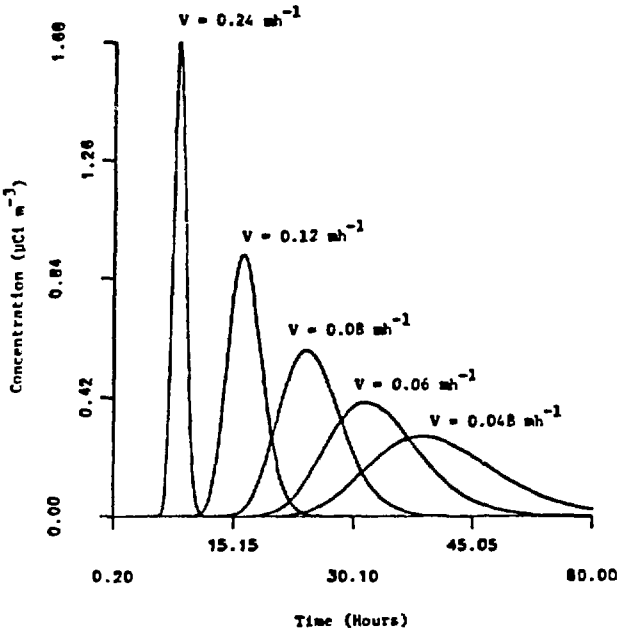

Figure 3. Breakthrough curves with different average pore water velocities.

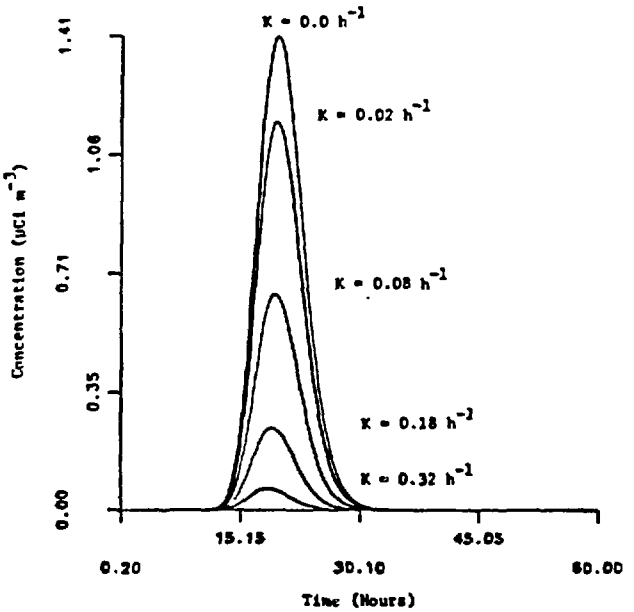

Figure 4. Breakthrough curves with different degradation rates.

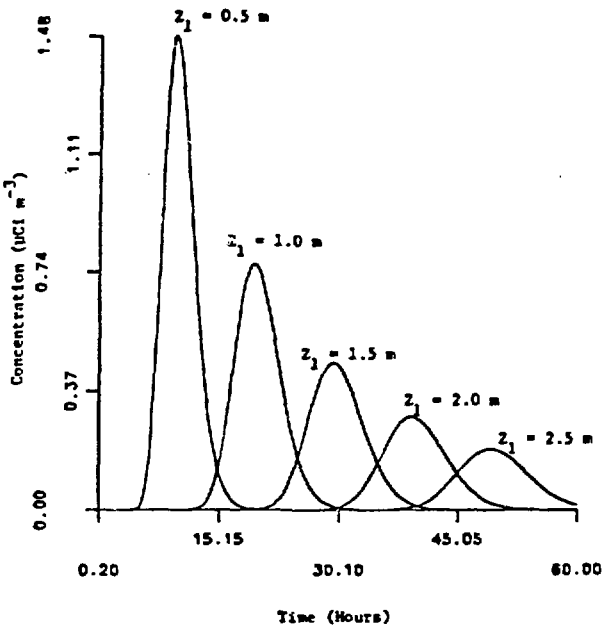

Figure 5. Breakthrough curves with different path lengths.

the IP, parameters or boundary conditions are determined from known concentration data. Detailed discussion of the IP and DP may be found in Neuman (1973) and Yu (1984).

The current methods for solving the IP may be classified into two categories, i.e., indirect and direct methods. The indirect method is essentially an iterative one consisting of a repetitive solution of the DP. The DP is first solved with certain initial guesses of the parameters. The final values of the parameter vector are obtained iteratively by minimizing the error functional, which represents the difference between the model prediction and the actual observations of the dependent variable. A flow chart of the indirect method is shown in Figure 6. One important step in the flow chart is the performance analyzer. As explained in Section 3, when there is more than one parameter, it is hard to decide the correct direction of the next step. In other words, determining the parameter correction vector in Figure 6 is very difficult. Besides this difficulty, the indirect method needs nuclide concentration data at different positions to approximate the spatial derivatives in the numerical model.

The direct method of solving the IP treats the parameters as independent variables that are solved directly. If the solution to the PDE can be obtained, then the parameters can be estimated from the solution by standard regression techniques such as the least squares method. Both linear and nonlinear least squares methods have been used (Yu 1984; Yu et al. 1984a, 1984b, 1985a).

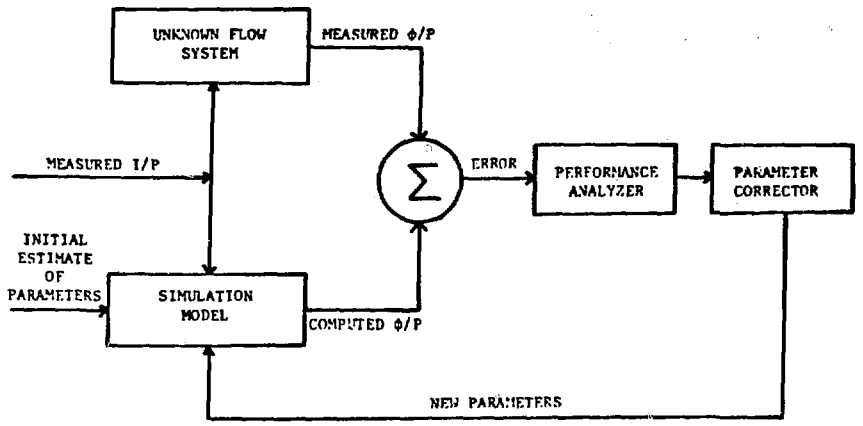

Figure 6. Flow chart of indirect calibration approach. Source: Adapted from Yu 1984.

The advantage of using the least squares method is that the parameters found are best linear unbiased estimators (b.l.u.e.) (Neter and Wasserman 1974). That is, the parameters are linear in C(t) with minimum mean square residuals and their expectation values are the true parameters. Also, even when the parameters are dependent, the least square method can still be used to estimate them. The disadvantage of using the least squares method is that when there are only a few data points, any outliers are very influential.

A linear regression technique has been developed (Yu et al. 1984a) that uses either the simple linear regression or the multiple regression to determine the effective dispersion coefficient and retardation factor simultaneously. The degradation rate and the water velocity can also be determined if the initial concentration is known (Yu 1984). More parameters can be determined if the nonlinear regression technique is applied (Yu 1984; Yu et al. 1985a). Constraints on the combination of parameters may be needed when using a nonlinear regression program such as BMDPAR (Dixon 1983). It must be emphasized that parameters determined by regression techniques (especially nonlinear regression) may not be the "true" parameters of a particular site, but they are the effective (representative) parameters that can be used in a solute transport model to predict the migration of wastes.

5 SUMMARY

The results of the groundwater pathway sensitivity analysis carried out in this study show that the degradation rate is a rather insensitive parameter. The parameter identification techniques currently being used include linear and nonlinear regression methods. More sensitive parameters should be determined more accurately because they have a greater influence on the prediction results.

6 ACKNOWLEDGMENT

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