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INVERSE PROBLEM IN RADIONUCLIDE TRANSPORT*

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INTRODUCTION

The disposal of radioactive waste must comply with the performance objectives set forth in 10 CFR 61 for low-level waste (LLW) and 10 CFR 60 for high-level waste (HLW). To determine probable compliance, the proposed disposal system can be modeled to predict its performance. One of the difficulties encountered in such a study is modeling the migration of radionuclides through a complex geologic medium for the long term. Although many radionuclide transport models exist in the literature, the accuracy of the model prediction is highly dependent on the model parameters used. The problem of using known parameters in a radionuclide transport model to predict radionuclide concentrations is a direct problem (DP); whereas the reverse of DP, i.e., the parameter identification problem of determining model parameters from known radionuclide concentrations, is called the inverse problem (IP).[1-6] In this study, a procedure to solve IP is tested, using the regression technique. Several nonlinear regression programs are examined, and the best one is recommended.

METHODOLOGY AND RESULTS

A general, one-dimensional nuclide transport model can be written as:[7]

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

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where C is the radionuclide concentration, D is the dispersion coefficient, R_d is the retardation factor, V is the water velocity, λ is the decay constant, K is the degradation rate, and $\dot{M}$ is the source input. This model has been solved both analytically and numerically for an infinite and semi-infinite medium.[7] With known radionuclide concentrations, the parameters can be estimated from the analytical or numerical solution by standard regression techniques such as least squares. Both linear and nonlinear least squares techniques have been used.[7] The advantage of using the least squares technique is that the calculated parameters are best linear unbiased estimators (b.l.u.e.).[8-9] The disadvantage of using this technique is that any outliers are very influential when there are only a few data points.

Solving IP using linear regression is a straightforward technique (science). Both simple linear regression and multiple regression, using the MINITAB statistical package,[10] have been successfully applied to determine radionuclide transport parameters such as dispersion coefficients and retardation factors.[11] Solving IP of the radionuclide transport equation using nonlinear regression is more of an art than a science. Two statistical packages have the capability to do nonlinear regression, i.e., SAS[12] and BMDP.[13] In the SAS package, the NLIN procedure solves the nonlinear regression problems. The user can choose from among the steepest-descent method, the modified Gauss-Newton method, the MARQUARDT method, and the secant (DUD) method. In the BMDP package, two programs -- 3R and AR -- solve nonlinear regression problems. The BMDP3R uses the modified Gauss-Newton method and the BMDPAR uses the secant method. These methods are discussed in detail in Ref. 7.

Extensive tests were done to compare the BMDP and SAS procedures. Table 1, which is a partial list of the test results, shows a comparison of two SAS and two BMDP programs using different initial conditions, with various parameters fixed to the true values. The concentration data were computer generated, using the parameters listed in Table 1 as the true values. Case 1 shows that if the parameter values are unbounded,

TABLE 1 Comparison of SAS and BMDP Regression Programs

Case No.	Method	Dispersion Coefficient	Retardation Factor	Water Velocity	Path Length	Degradation Rate	Initial Concentration	Bounds Set	Iteration No.	RSS	IBM3033 CPU Time (s)
1	Initials	20	2	10	100	0.1	5	-	-	-	-
	MARQUARDT	13.40	2.449	8.006	137.0	0.2284	-4.924	No	5	0.002703	1.07
	BMDP3R	20.00	2.000	10.00	100.0	0.1000	5.000	No	5	0.003953	1.30
	DUD	779.0	90.63	-1185	27253	1114.	54143	No	8	0.002679	0.90
	BMDPAR	972762	9419	-154582	-2021192	3.019	-80030	No	6	0.003029	1.28
2	Initials	20	2	10	100	0.1	5	-	-	-	-
	MARQUARDT	30.00	10.00	20.00	120.00	0.1500	5.5	Yes	1	0.002679	0.98
	BMDP3R	20.00	2.000	10.00	100.00	0.1000	5.000	Yes	5	0.003953	1.35
	DUD	30.00	10.00	20.00	120.00	0.1500	5.500	Yes	0	0.002679	0.89
	BMDPAR	6.003	2.090	8.334	117.0	0.05687	4.288	Yes	50	0.0000	1.51
3	Initials	20	2	10	100	0.1	Fixed	-	-	-	-
	MARQUARDT	30.00	10.00	20.00	120.00	0.1500	-	Yes	1	0.002679	0.94
	BMDP3R	20.00	2.000	10.00	100.00	0.1000	-	Yes	5	0.003333	1.33
	DUD	30.00	10.00	20.00	120.00	0.1500	-	Yes	0	0.002679	0.86
	BMDPAR	30.00	1.931	8.000	90.00	0.1500	-	Yes	18	0.002391	1.34
4	Initials	20	2	10	Fixed	0.1	Fixed	-	-	-	-
	MARQUARDT	20.00	2.000	10.00	-	0.1000	-	Yes	0	0.002649	0.98
	BMDP3R	20.00	2.000	10.00	-	0.1000	-	Yes	5	0.002649	1.33
	DUD	30.00	10.00	10.00	-	0.1500	-	Yes	0	0.002679	0.82
	BMDPAR	7.890	3.159	11.81	-	0.04154	-	Yes	50	0.0000	1.47
5	Initials	20	2	Fixed	Fixed	0.1	Fixed	-	-	-	-
	MARQUARDT	30.00	10.00	-	-	0.1500	-	Yes	1	0.002679	0.96
	BMDP3R	20.00	2.000	-	-	0.1000	-	Yes	5	0.003144	1.33
	DUD	30.00	10.00	-	-	0.1500	-	Yes	0	0.002679	0.84
	BMDPAR	10.00	4.000	-	-	0.02000	-	Yes	50	0.000000	1.61
6	Initial	20	2	Fixed	Fixed	Fixed	Fixed	-	-	-	-
	MARQUARDT	30.00	10.00	-	-	-	-	Yes	1	0.002679	0.93
	BMDP3R	20.00	2.000	-	-	-	-	Yes	5	0.004445	1.34
	DUD	30.00	10.00	-	-	-	-	Yes	0	0.002679	0.83
	BMDPAR	10.00	4.00	-	-	-	-	Yes	25	0.000000	1.44
True Values		10.0	4.0	15.0	109.2	0.02	4.0	-	-	-	-
Upper Bound		30.0	10.0	20.0	120.0	0.15	5.5	-	-	-	-
Lower Bound		1.0	1.0	8.0	90.0	0.0	3.5	-	-	-	-

i.e., from $-\infty$ to $+\infty$, the programs either converged to unrealistic values or remained on the initial estimate. Cases 2-6 show that all programs except BMDPAR remained on either the boundary values or the initial values; only BMDPAR converged to parameters with acceptable residual sum of squares (RSS), although it took more iterations and, thus, was more expensive to run. The BMDPAR even converged to the true parameters when the other three were fixed to true (known) values (Case 5). The three fixed parameters are initial concentration, path length, and water velocity. The three determined parameters are dispersion coefficient, retardation factor, and degradation rate. Based on these results, the BMDPAR seems to be superior to other programs. Hence, BMDPAR can be used as the first trial program in solving the IP. If the RSS of using BMDPAR is not acceptable, then other programs may be used to seek improvement.

DISCUSSIONS AND CONCLUSION

An important factor determining the convergence of a nonlinear regression program used to solve the IP is the set of initial values used. A bad estimate of the initial value makes the program either converge to local minimum or not converge at all. There is no universal method to determine the initial values. It is the user's own judgment, based on experience and accessible information. This study demonstrates that it is desirable to set reasonable bounds for parameters to be estimated. It is also desirable to choose a different set of initial values and then use the least RSS parameters as the optimum parameters. The IP is an important tool for estimating parameters used in a radionuclide transport model for predicting the performance of a radioactive waste disposal system over the long term. Successful use of this tool will provide higher confidence in such predictions.

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