

US EPA ARCHIVE DOCUMENT

Uncertainty in Model Predictions—Plausible Outcomes from Estimates of Input Ranges

Presented at Brownfields 2002, Charlotte, North Carolina, Nov 13-15, 2002

James W. Weaver, Caroline L. Tebes-Stevens, Kurt Wolfe
Ecosystems Research Division
National Exposure Research Laboratory
Office of Research and Development
United States Environmental Protection Agency
Athens, Georgia 30605

Models are commonly used to predict the future extent of contamination given estimates of hydraulic conductivity, porosity, hydraulic gradient, biodegradation rate, and other parameters. Often best estimates or averages of these are used as inputs to models, which then transform them into output concentrations. Despite this evident certainty, all properties of the subsurface are both uncertain, because of imperfect measurement methods, and subject to point-to-point variability, because of geologic heterogeneity. Where used as purely predictive tools (i.e., in the absence of model calibration to field data), uncertainty and variability lead to the need for assessment of the plausible range of model outcomes. For Brownfields sites, the need to provide rapid assessment of contamination may not allow extensive field and modeling studies, where calibration data sets would be obtained. In those and other cases there is a need for evaluation of model uncertainty given input variation. Our approach is to use all combinations of input parameters to determine the earliest and latest first arrivals, the lowest and highest peak concentration, the shortest and longest duration of contamination, and the lowest and highest risk scenarios. Results of simulations show that even moderate ranges of input variation generate significant differences in model predictions. These differences are greater than obtained from simple one parameter at a time uncertainty analyses, because of combined influences of multiple parameters. For example, hydraulic conductivity, porosity and gradient together determine the seepage velocity, and variation of each of parameter needs to be considered in order to determine the extremes of velocity. The extreme parameter sets were found to be different for some of the four predicted model outputs (first arrival, maximum concentration, duration, risk). This result shows that selection of worst case parameter set depends on the desired output of the model. The simulations showed that the best and worst case parameter sets for first arrival time, maximum concentration and duration were consistent across all simulations and could thus be selected *a priori*. Those for risk, however, could be determined only by performing an uncertainty analysis for each input parameter set.

Introduction

Models are commonly viewed as useful tools for understanding contaminant transport (Oreskes et al., 1994) and determining future risk (ASTM, 1995). The degree of predictive capability of subsurface transport models has, in fact, not been established (e.g., Miller and Gray, 2002, Eggleston and Rojstaczer, 2000). Thus models are more likely to provide a framework for understanding transport than for predicting future exposure and risk. Commonly, models are calibrated to field data to demonstrate their ability to reproduce contaminant behavior at a site. This process implies a degree of correctness in understanding and provides the first step toward demonstration of predictive ability. For screening sites, however, sufficient data may not be collected for calibrating a model. How then should models be used in situations where they cannot or will not be calibrated? What are the ranges of output, given uncertainty in inputs? Can worst case parameter sets be selected that always provide a bound on plausible outcomes? This paper addresses these questions through an approach to uncertainty analysis.

Approach

A simple analytical solution of the transport equation was used to determine uncertainty in model outputs. This model is a solution of the mass balance equation for transport of solutes in ground water, given by

$$R \frac{\partial c}{\partial t} = -v_x \frac{\partial c}{\partial x} + D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} + D_z \frac{\partial^2 c}{\partial z^2} - \lambda c \quad (1)$$

where R is the retardation factor [dimensionless], c is the concentration [M/L³]; t represents time [T]; x, y, and z are the three cartesian coordinate directions [L]; v_x is the x-direction seepage velocity [L/T], D_x, D_y and D_z are the three components of dispersion [L²/T], and λ is a first order loss coefficient [T⁻¹]. This form of the transport equation is based on the assumption that the dispersion constants are independent of time and space that ground water flow is one-dimensional, steady and uniform, that biodegradation is adequately represented by a first order process. With boundary conditions specified as

$$\begin{aligned} c(0) &= \begin{cases} c_0 & ; t < t_p \\ 0 & ; t > t_p \end{cases} \\ \frac{dc}{dx}(\infty) &= 0 \end{aligned} \quad (2)$$

a solution can be obtained for a one-dimensional case where the transverse and vertical components of dispersion are assumed negligible (van Genuchten and Alves, 1982) or a similar three dimensional case (Leij and Bradford, 1994). The one-dimensional case is useful because of rapid computation of its results and is used in the following.

Uncertainty

Several approaches to sensitivity and uncertainty analysis have been developed. Generally these require knowledge of parameter values and their statistical distributions including correlations between individual parameters. In our approach we assume that site investigations are not sufficiently detailed to determine values for some of the parameters, let alone their statistical distributions and correlations. A brief accounting of the model inputs is given as follows: Porosity and dispersivity are essentially never determined on a site-specific basis, despite their importance in determining model outcomes. Biodegradation rate constants may be estimated from simple techniques (Buscheck and Alacantar, 1995), but these require adherence to a suite of restrictive assumptions that limits the results by the same considerations that we are attempting to address in this work. Parameters measured in the field are subject to uncertainty because of spatial variability (hydraulic conductivity and fraction organic carbon) or temporal fluctuations (gradients). The forcing parameters of the model, initial concentration and duration, are rarely known, because contamination is normally discovered years after a release occurs.

There is a similar lack of knowledge of statistical distributions of the inputs. A widely-used alternative is to assume knowledge of the statistical properties by using scientific literature values as substitutes. These approaches allow assignment of probabilities to the various outcomes. This approach suffers from obvious lack of site-specificity and where results depend strongly on these distributions it is not possible to determine how much error is introduced into results from these assumptions. Alternatively, if it is assumed only that plausible ranges of input parameters are known, similar outcomes can be determined, but probabilities cannot be assigned. Because of lack of knowledge of the underlying probability distributions, we implemented the latter approach to assess uncertainty in model outputs.

Nine parameters of the one-dimensional model are assumed to be variable. Tables 1a and 1b list parameters and their treatment in the model. All seven parameters of the model were allowed to be variable, as were the concentration and duration of the source. The chemical, distance to receptor, and minimum concentration of concern are taken as fixed for a given analysis. With this selection of inputs there are two values each for nine parameters. This leads to a

total of 2^9 or 512 unique combinations of parameters. This calculation highlights an assumption of this method: That each parameter value is equally likely and can occur in combination with each other parameter value. The large number of parameter combinations is the reason to seek models that execute rapidly. Hence the interest in the one-dimensional model.

Table 1a. Parameter inputs, their treatment in the model as fixed or variable and the values used in the example problems.

Quantity	Treatment	Example Problem Values		
		Low		High
<i>Model Parameters</i>				
Hydraulic Conductivity	variable	Low Scenario	15 ft/d	50 ft/d
		High Scenario	108 ft/d	328 ft/d
Porosity	variable	0.20		0.25
Gradient	variable	0.001		0.005
Fraction Organic Carbon	variable	0.0001		0.001
Organic Carbon Partition Coefficient	variable	31 L/kg		106 L/kg
Dispersivity	variable	0.1 * estimate from Xu and Eckstein (1995)		10 * estimate from Xu and Eckstein (1995)
Half Life	variable	Low Scenario	100 days	730 days
		High Scenario	4000 days	6000 days

Table 1b. The problem definition, its treatment in the model as fixed or variable and the values used in the example problems.

Quantity	Treatment	Example Problem Values		
		Low		High
<i>Problem Definition</i>				
Source Concentration	variable	10 mg/L		30 mg/L
Source Duration	variable	1500		3000
Chemical	fixed	benzene		benzene
Distance to receptor	fixed	Low Scenario	50 ft	50 ft
		High Scenario	500 ft	500 ft
Minimum Concentration of Concern	fixed	0.005 mg/L		0.005 mg/L

Simulation

The model gives concentrations at certain locations and times, so that breakthrough curves (concentrations histories at given points, see Figure 1) or concentration distributions (plumes at given times) could be determined

directly from the solution. In order to compare various scenarios, four outputs are generated from the modeled breakthrough curves: 1) first arrival time, 2) maximum concentration, 3) duration of contamination, and 4) risk factor. This first three of these are illustrated in Figure 1. Cancer risk is normally determined from an expression of the form (US EPA, 1989)

$$Risk = I SF = \frac{CW ED EF IR}{BW AT} SF$$

where I is the intake in mg/kg-day, SF is the cancer slope factor (kg-day/mg), CW is the concentration in water (mg/L), ED is the exposure duration (days), EF is the exposure frequency (days/year), IR is the injection rate (liters/day), BW is the body weight (kg), and AT is the averaging time (years). Since concentrations on the breakthrough curve change with time, the effect of the transient in concentration is included in the risk equation by using the substitution:

$$CW ED = \int_{t_0}^{t_a} CW(t) dt$$

where CW(t) are the modeled concentrations, t_0 is the contaminant first arrival time, t_a is the last time that the concentration is above the threshold. Thus the integral of concentration versus time gives a measure of relative risk. The model accumulates results and determines the best and worse cases for each of the four chosen breakthrough curve outputs.

In addition to variable parameters, four scenarios were created to simulate a variety of conditions and determine if the model behavior was similar despite variation in parameter values. Two ranges each of hydraulic conductivity and half life were selected (Table 1a). These variables were chosen to vary because they have a direct effect on model outputs: Hydraulic conductivity affects advective transport rates and thus the arrival times and duration of contamination, and the half life impacts maximum concentration. Risk is affected by both of concentration and duration. The scenarios are generally comparable with each other with the exception that the receptor is closer to the source in the low conductivity scenario. This selection was made so that there would be complete breakthrough curves for all combinations of parameters in each scenario.

Results

Table 2 shows the extreme cases for four problem scenarios (see Table 1): High and low conductivity aquifers, and high and low biodegradation rates. These results show the magnitude of possible outcomes given the range of inputs used. The high and low conductivity scenarios have a different distance to the receptor (500 ft versus 50 ft), so the first arrival time results are not directly comparable. In going 10 times further in the high conductivity scenario the arrival time is approximately 2.5 times greater than the low conductivity scenario (20 days/7.9 days), indicating proportionately earlier first arrival in the high conductivity scenario. The high

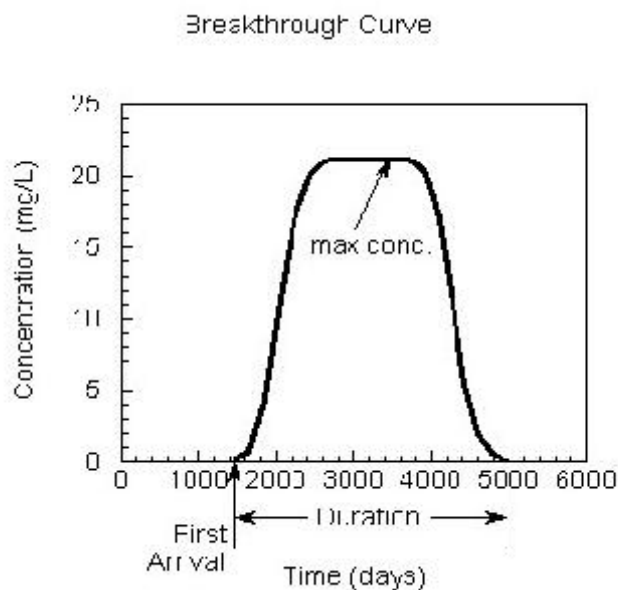


Figure 1 Illustration showing the relationship between the first arrival time, maximum concentration and duration of contamination. The first arrival time and duration are determined relative to a given threshold concentration, that is usually a maximum contaminant level or other concentration of concern.

conductivity scenarios can have the shortest maximum durations (column 6, rows a and b). The minimum durations are in part determined by the source duration (which at a minimum is 1500 days). With high biodegradation rates the minimum concentrations can be greatly reduced (compare row a and b and row c and d in column 3) in either scenario.

Table 2. Model results for four scenarios showing a comparison of best and worst cases for the four outputs (first arrival time, maximum concentration, duration and risk).								
	First Arrival Time		Maximum Concentration		Duration		Risk Factor	
	Earliest (1)	Latest (2)	Lowest (3)	Highest (4)	Shortest (5)	Highest (6)	Best (7)	Worse (8)
High Conductivity Scenario								
(a) Low Biodegradation	20	1140	6.4	30	1580	8310	2.01e5	1.95e6
(b) High Biodegradation	20	1760	0.0081	28.3	1340	7210	562	1.54e6
Low Conductivity Scenario								
(c) Low Biodegradation	7.9	604	6.9	30	1580	9210	1.71e5	1.76e6
(d) High Biodegradation	7.9	740	0.079	30	1580	7610	3330	1.55e6

Table 3 shows a comparison of the parameters across the scenarios. This comparison was made to determine if the extreme cases were generated by the same sets of parameters, despite changes in the average values of the parameter. These results imply that it is possible to determine a generic set of worst case parameters for three of the outputs (first arrival time, maximum concentration and duration above the threshold). In some cases the results are insensitive to a given parameter and either parameter could generate the worst case. For example, the first arrival is independent of release duration in these cases, because the release duration was much greater than the arrival times. Generally the results were consistent for the first arrival, maximum concentration and duration. Definition of the worst case for risk, however, was less clear as the parameter sets were not the same for each simulation. The porosity, fraction organic carbon, dispersivity and half life were different for the scenarios and suggested that a generic set of parameters did not exist for risk.

Conclusions

Uncertainty in model inputs results from spatial variability and incomplete or imperfect sampling methods. Running all combinations of input parameters gives bounds on the plausible outputs of the model. For each individual parameter set selected for analysis, the worst case parameters varied with the output of interest (i.e., first arrival time, maximum concentration, duration, and risk). Given the chosen output, however, the worst case parameter sets were the same for each combination of hydraulic conductivity and biodegradation rate for the first three outputs. In contrast, the risk output, perhaps because it depends strongly upon both the concentrations and the duration of the breakthrough curve, had no consistent set of worst case parameters. For risk the uncertainty analysis must be performed individually for each parameter set, while for the others this analysis showed that a generic set of worst case parameters existed.

Table 3 Comparison of data sets giving the worst cases for each of four model outputs.									
Scenario	Hydraulic Conductivity	Porosity	Gradient	Fracture on organic carbon	Koc	Dispersivity	Half Life	Source concentration	Source Duration
<i>Earliest First Arrival</i>									
Low Conductivity, Low Biodegradation	H	L	H	L	L	H	E	H	E
Low Conductivity, High Biodegradation	H	L	H	L	L	H	E	H	E
High Conductivity, Low Biodegradation	H	L	H	L	L	H	E	H	E
High Conductivity, High Biodegradation	H	L	H	L	L	H	E	H	E
<i>Highest Maximum Concentration</i>									
Low Conductivity, Low Biodegradation	H	L	H	E	E	H	H	H	E
Low Conductivity, High Biodegradation	H	L	H	E	E	H	H	H	E
High Conductivity, Low Biodegradation	H	L	H	E	E	E	H	H	E
High Conductivity, High Biodegradation	H	L	H	E	E	H	H	H	E
<i>Longest Duration</i>									
Low Conductivity, Low Biodegradation	L	H	L	H	H	H	H	H	H
Low Conductivity, High Biodegradation	L	H	L	H	H	H	H	H	H
High Conductivity, Low Biodegradation	L	H	L	H	H	H	E	H	H
High Conductivity, High Biodegradation	L	H	L	H	H	H	H	H	H
<i>Highest Risk</i>									
Low Conductivity, Low Biodegradation	L	H	H	H	H	L	L	H	H
Low Conductivity, High Biodegradation	L	H	H	H	H	L	L	H	H
High Conductivity, Low Biodegradation	L	E	L	E	E	H	E	H	H
High Conductivity, High Biodegradation	L	L	L	H	L	H	H	H	H
H = high value, L = low value, E = either value									

Disclaimer

This paper has been reviewed in accordance with the U.S. Environmental Protection Agency's peer and administrative review policies and approved for presentation and publication. The authors express their appreciation to John Stephenson and the staff of the Pennsylvania Department of Environmental Protection and the Ohio Bureau of Underground Storage Tank Regulations.

References

ASTM, 1995, Standard Guid for Risk-Based Corrective Action Applied at Petroleum Release Sites, American Society

for Testing and Materials, ASTM Designation E 1739095.

Buscheck, T.E. and C.M. Alacantar, 1995, Regression Techniques and Analytical Solutions to Demonstrate Intrinsic Bioremediation, Intrinsic Bioremediation, Hinchee, R.E., J.T. Wilson, D.C. Downey, eds., Battelle Press, 3(1).

Eggleston, J.R. and S. A. Rojstaczer, 2000, Can We Predict Subsurface Mass Transport?, Environmental Science and Technology, 34, 4010-4017.

Leij, F.J. and S.A. Bradford, 1994, 3DADE: A computer program for evaluating three-dimensional equilibrium solute transport in porous media, Research Report No. 134, U.S. Salinity Laboratory, Riverside, CA.

Miller, C.T. and W.G. Gray, 2002, Hydrological Research: Just Getting Started, Ground Water, 40(3), 224-231.

Oreskes, N., K. Shrader-Frechette, K. Belitz, 1994, Verification, Validation, and Confirmation of Numerical Models in the Earth Sciences, Science, 263, 641-646.

United States Environmental Protection Agency, 1989, Risk Assessment Guidance for Superfund Volume 1, Human Health Evaluation Manual (Part A), Interim Final, Office of Emergency and Remedial Response, Washington, DC, EPA/540/1-89-002.

van Genuchten, M. T. and W. J. Alves, 1982, Analytical Solutions of the One-Dimensional Convective-Dispersive Solute Transport Equation, United States Department of Agriculture, Agricultural Research Service, Technical Bulletin Number 1661.

Xu, M., and Y. Eckstein, 1995, Use of weighted least-squares method in evaluation of the relationship between dispersivity and scale, Groundwater, 33(6), 905-908.

