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Project Summary

Evaluation of Unsaturated/Vadose Zone Models for Superfund Sites

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Mathematical models of water and chemical movement in soils are being used as decision aids for defining groundwater protection practices for Superfund sites. Numerous transport models exist for predicting movement and degradation of hazardous chemicals through soils. Many of these require extensive input parameters that involve uncertainty due to soil variability and unknown future weather. The impact of uncertain model parameters upon the model output is not known. Model users require an understanding of this impact so appropriate parameters are measured at a site and model prediction uncertainty is incorporated into decisions. This report summarizes research findings that address the sensitivity and uncertainty of model output due to uncertain input parameters.

The objective of the research was to determine the sensitivity and uncertainty of travel time, concentration, mass loading and pulse width of contaminants at the water table due to uncertainty in soil, chemical, and site properties for four models, RITZ, VIP, CMLS, and HYDRUS. The models, which are all designed to estimate movement of solutes through unsaturated soils, span a considerable range in detail and intended use. Model parameters investigated include soil properties such as organic carbon content, bulk density, water content, and hydraulic conductivity. Chemical properties examined include organic carbon partition coefficient and degradation half-life. Site characteristics such as rooting depth, recharge rate, weather, evapotranspiration and runoff were examined when possible in the models. Model sensitivity was quantified in the form of sensitivity and relative sensitivity coefficients.

The study found that large uncertainty exists in many model outputs due to the combination of sensitivity and high parameter variability. In addition, predicted movement of contaminants was greater when the natural variability of rainfall was incorporated into the model than when only average fluxes were used. This is because major rainstorms that result in large fluxes of water and high leaching are essentially ignored when average flux values are used. The study reaffirms that uncertainty is pervasive in natural systems and that results of modeling efforts presented in a deterministic fashion may be misleading.

This Project Summary was developed by EPA's Robert S. Kerr Environmental Research Laboratory, Ada, OK, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

Mathematical models of water and chemical movement in soils are used as decision aids for defining remediation practices for Superfund sites. To use models in making decisions about remediation practices appropriate for Superfund sites, the model must predict the future behavior of the contaminant. Numerous transport models exist for predicting movement and degradation of hazardous chemicals through soils. Many of these require extensive input parameters that are often not measured and that include uncertainty due to inherent variability associated with the soil and weather conditions. Minimal information exists on the impact of uncertain input data on the outputs from these models. Given these conditions, guidelines regarding the selection and use of models are needed. This report summarizes research findings

addressing two issues of uncertainty in vadose modeling: (1) model sensitivity and (2) incorporating uncertainty into decisions using model predictions.

Model sensitivity refers to the change in model output resulting from a specified change in an input parameter. Sensitivity is observed by examining differences in graphs of the model outputs for different inputs in the expected range. If differences in output are large, the output is sensitive to these changes in inputs; if differences in output are small, the output is not sensitive to these changes in inputs.

The use of models in a predictive manner introduces uncertainty. For example, chemical leaching depends upon water movement through the unsaturated soil. This water movement is dependent upon the amount and distribution of water entering the soil and hence upon future weather. Since future weather is unknown, uncertainty exists in the model input. As a result, there is inherent uncertainty in the model output. Natural variability of the soil parameters is an additional source of input parameter uncertainty. The second part of the full report computes the uncertainty in model outputs due to uncertainty in one or more model inputs.

Results of the sensitivity and uncertainty analyses are presented for four models: RITZ, VIP, CMLS, and HYDRUS. RITZ, VIP, and CMLS were written as management tools, whereas HYDRUS is more appropriately suited for detailed research use by scientists. The models differ substantially in their intended use, assumptions and processes, input data requirements, computer requirements, and ease of use.

Model Descriptions

The four models selected in the analysis are RITZ, VIP, CMLS, and HYDRUS. All four models include sorption of the contaminant by soil and advection or movement of the contaminant with water. RITZ and VIP include sorption on an immobile oil phase as well as a vapor transport component. In addition, RITZ and VIP assume uniform soil properties and steady water flow. CMLS and HYDRUS can simulate layered soils and unsteady, unsaturated water flow. HYDRUS also includes hydrodynamic dispersion. Each of the models are described in greater detail below.

RITZ Model: The Regulatory Investigative Treatment Zone (RITZ) Model (Nofziger, *et al.*, 1988) was developed to predict the fate of contaminants mixed with oily wastes and applied to land treatment units. RITZ conceptualizes the vadose zone as consisting of two zones: (1) the plow zone where the sludge containing contaminant and oil occurs uniformly mixed within the soil and (2) the treatment zone, which contains no oil. The model simulates movement of the contaminant through both zones. In this study, the plow zone represents the portion of soil containing the contaminant at the beginning of the simulation. The bottom of the treatment zone represents the water table depth.

RITZ contains many simplifying assumptions: (1) Soil properties are assumed to be uniform throughout the profile. (2) The flux of water through the soil is assumed to be constant with depth and time. (3) Oil is assumed to be immobile and remains in the plow zone. (4) Both oil and contaminant degrade as first-order processes. (5) Partitioning of the contaminant between phases is linear, instantaneous, and reversible. (6) Dispersion in water phase is small and can be ignored. (7) The soil water content and unsaturated hydraulic conductivity can be described by the Clapp and Hornberger equation (Clapp and Hornberger, 1978),

$$\theta_w = \phi \left[\frac{q}{K_s} \right]^{\frac{1}{2b+3}} \qquad (1),$$

where θ_w is the soil water content, K_s is the saturated conductivity, q is the average recharge rate, θ is the soil porosity or saturated water content and b is the Clapp-Hornberger constant (that depends on soil properties).

VIP Model: The Vadose Interactive Processes (VIP) Model (Stevens, *et al.*, 1989) is similar to RITZ in the conceptualization of the vadose zone but consists of more complex chemical interactions. For example, VIP considers the dynamics of sorption rather than assuming instantaneous equilibrium between phases. It also simulates oxygen diffusion in the air-phase and oxygen-limited degradation of the contaminant, and diffusion of contaminant in the air phase. When oxygen is not limiting, sorption is instantaneous, and diffusion of contaminant is negligible. VIP solves the differential equations numerically. As a result, the recharge rate or flux of water passing through the soil can change with time on a monthly basis.

CMLS Model: The Chemical Movement in Layered Soils (CMLS) Model (Nofziger and Hornsby, 1986) was originally developed as a management tool to simulate the movement and degradation of pesticides in layered soils. In CMLS, the soil profile is composed of up to 20 layers. Soil and chemical properties are constant within a layer but may change from layer to layer. Water balance is computed on a daily basis to account for infiltration and evapotranspiration.

The following simplifying assumptions are made in CMLS: (1) Chemicals move only in the liquid (soil water) phase, and movement in the vapor phase can be ignored. (2) Partitioning of chemicals between the soil solids and water is described by the linear, reversible model with instantaneous equilibrium. (3) Dispersion and diffusion of the chemical are ignored. (4) Degradation is described as a first-order process. The degradation constant can vary with depth but not with time. (5) Water moves through the soil system in a slug-like manner. All water in the soil is pushed ahead of new water entering the soil. (6) The soil drains instantly to the "field capacity" water content after each infiltration event. (7) Water is removed from each layer in the root zone in proportion to the available water stored in that layer. (8) Chemicals move downward in the soil system; upward movement of chemicals is ignored. (9) No oil is present in the soil system.

The CMLS model estimates the amount of chemical at a particular position as a function of time. It does not calculate concentrations. If concentrations are needed, the user must estimate the mass of water in which the chemical is mixed and then calculate the concentration from this mass of water and the mass of chemical leached.

HYDRUS Model: HYDRUS: One-Dimensional Variably Saturated Flow and Transport Model, Including Hysteresis and Root Water Uptake (Kool and van Genuchten, 1991) is a finite element model and is the most computationally demanding of the selected models. In HYDRUS soil and chemical properties are assigned as a series of points, and these properties can vary from one point to another. As a result, the user has great flexibility to define initial conditions to represent the site of interest. Assumptions incorporated into HYDRUS include (1) partitioning of chemical between solid and water is described by a linear, reversible model with instantaneous equilibrium between phases; (2) movement in the vapor phase is ignored; and (3) no oil is present in the system.

Sensitivity and Uncertainty

The sensitivity of a model refers to the change in a selected model output resulting from a specified change in a single input parameter. Mathematically the sensitivity coefficient, S, is defined as

$$S = \frac{\partial f}{\partial x} \qquad (2),$$

where f represents the output of interest and x represents the input parameter (McCuen, 1973). If the model output can be written in a nice symbolic form, the sensitivity can be applied by differentiating f symbolically. However, models are often too complex for this approach; in this case the sensitivity can be calculated using the difference equation

$$S = \frac{\Delta f}{\Delta x} \qquad (3).$$

Model sensitivity, S, as defined by Equations 2 and 3 is the change in model response per unit change in the input parameter. The change in model output due to a small change in input parameter is given by

$$\Delta f = S \Delta x \qquad (4),$$

where Δf is the change in output f due to a change of Δx in the input parameter. That is, the product of the sensitivity, S, and the change in input parameter is the change in model output.

The value of S calculated from these equations has units, which makes it difficult to compare sensitivities for different input parameters. This problem is overcome by using the relative sensitivity, S_r, given by

$$S_r = \frac{\partial f}{\partial x}\frac{x}{f} = S\frac{x}{f} \qquad (5),$$

or

$$S_r = \frac{\Delta f}{\Delta x}\frac{x}{f} = S\frac{x}{f} \qquad (6),$$

where f is the value of the model output and x is the value of the input parameter. The relative change in model output, $\Delta f / f$, can then be estimated from the relative change in input parameter, $\Delta x / x$, and the relative sensitivity using the equation

$$\frac{\Delta f}{f}\frac{x}{f} = S_r\frac{\Delta x}{x} \qquad (7).$$

Hence, the relative sensitivity is a measure of the relative change in model output corresponding to a relative change in the input parameter. In short, S_r gives the percentage change in model response for each one percent change in the input parameter. If the absolute value of S_r is greater than 1, the absolute value of the relative change in model output will be greater than the absolute value of the relative change in input parameter. If the absolute value of S_r is less than 1, the absolute value of the relative change in model output will be less than the absolute value of the relative change in input.

Uncertainty analysis is used to incorporate simultaneous changes in more than one parameter and variability of the parameters. Two approaches are frequently used for defining model uncertainty. The first approach, a deterministic approach, is most applicable to models in which explicit equations can be written for model outputs as functions of input parameters. The first-order second-moment uncertainty analysis is a widely used technique in this approach. It provides a method of calculating the mean, variance, and covariance of model outputs from means, variances, covariances and sensitivity coefficients for the model inputs. First-order second-moment analysis is most appropriate when the model is not strongly nonlinear in its parameters and the coefficients of variation of the parameters are small.

The second approach is a stochastic method, which is often used when the explicit formula for a complex system cannot be obtained or the equations are cumbersome. The Monte Carlo technique, which is an example of this approach, requires knowledge of the frequency distribution of each input parameter and the correlations among these parameters. Input parameters are generated at random from the parameter populations so that means and correlations are preserved. Each set of inputs is used in the model to compute the outputs of interest. This process is repeated many times until the probability distribution of the model outputs is defined. Summary statistics of the outputs are then computed or the entire distribution is used in the analysis.

Physical Setting

The sensitivity of a particular output to changes in model inputs depends upon the entire set of parameters used in the model and upon the total system being analyzed. The general scenario simulated was from a benzene release near Perdido, Alabama. The soil in the area was the Norfolk sand (fine-loamy, siliceous, thermic Typic Paleudult). At the beginning of the simulation, 100 g m^{-2} benzene was assumed to be uniformly distributed in the top 0.5 m of soil. A water table was assumed to be present at a depth of 2 m. Soil properties for the top 2 meters of the Norfolk sand were obtained from Quisenberry, *et al.* (1987) for the same soil in Blackville, South Carolina. Data on the organic carbon content (OC) of the soil were not available, and, as a result, percent organic carbon content was assumed to decrease with depth according to the equation

$$OC(d) = 1.35e^{-4.0d} \qquad (8),$$

where d is the soil depth (m). The organic carbon content determined for the middle of each soil layer was used for that entire layer. The initial water content throughout the soil profile was internally calculated by the RITZ and VIP models from the specified recharge rate, the saturated conductivity, and the Clapp-Hornberger constant. CMLS assumes the initial water content of each soil layer is the field capacity value. An initial water content of 0.15 $cm^3\ cm^{-3}$ throughout the soil profile was used as the initial condition in HYDRUS. The parameters for the van Genuchten closed-form hydraulic functions (van Genuchten, 1980) were obtained from the soil water retention and unsaturated hydraulic conductivity data using the RETC software (van Genuchten, *et al.*, 1991). Soil porosity was computed from the bulk density. The Clapp-Hornberger constant (Clapp and Hornberger, 1978) required in the RITZ and VIP models was determined by regression.

Climatological data from the Perdido area of Alabama were obtained for the nearby sites of Fairhope from the SE Regional Climate Center. The only evaporation (ET) data available were from Fairhope. Daily weather data from the Fairhope site were used in the simulation runs for HYDRUS and CMLS models. Average recharge rates required for RITZ and VIP were calculated from total rainfall and total evaporation data at these sites. Average rainfall and evaporation rates for the area were 5 and 4 mm per day, respectively. Daily weather data from Caddo County, Oklahoma, were also used for some of the analyses using CMLS since the data available for Perdido were not sufficient for the Monte Carlo simulations.

The organic carbon partition coefficient and degradation rates for benzene were obtained from values in the literature. A value of 80 $cm^3\ g^{-1}$ was used as the organic carbon partition coefficient and a half-life of 100 days was used as the rate of degradation.

Sensitivity Results

Sensitivity analyses based on the physical setting described above were conducted for the selected models. In particular, the sensitivity analysis focused on four primary model outputs: (1) the time at which the

contaminant reaches the water table, (2) the amount of contaminant entering the saturated zone, (3) the width of the contaminant pulse at the water table, and (4) the concentration of the contaminant entering the ground water.

The results of the sensitivity analysis for each of the models (RITZ, VIP, CMLS, and HYDRUS) are summarized below. It should be recognized, however, that although these results reflect the specific model's parameter sensitivity, the results are also dependent upon the total system (physical setting) that is conceptualized.

RITZ Model

Results of the sensitivity analysis for the RITZ model indicate that the output describing the total amount of pollutant leached to ground water has the highest relative sensitivity parameter values with respect to the other model outputs. This indicates that a relative change for most of the parameters will result in a larger change in the model result for amount of pollutant leached than travel time or pulse width. Specifically, for the amount of pollutant leached, organic carbon content, saturated water content, treatment zone depth, partition coefficient, and degradation half-life are sensitive parameters as these exceed 2.0 relative sensitivity. In contrast, the travel time relative sensitivities range from -0.72 to 0.76 with organic carbon content, bulk density, saturated water content, treatment zone depth, recharge rate, partition coefficient, and half-life of oil being the principal sensitive parameters. The relative sensitivities for the pulse width model output were the lowest values ranging from -0.46 to 0.60. The primary sensitive parameters for this model output were recharge rate, sludge application rate, oil-water partition coefficient, Henry's law constant, concentration of oil in sludge, density of oil, and half-life of oil.

VIP Model

VIP was written to model movement of a chemical in a system similar to that used in RITZ. VIP includes oxygen transport, oxygen exchange, and oxygen loss that are not present in RITZ. It also incorporates chemical movement in the vapor phase for the pollutant.

The conditions modeled in this study represent conditions for which vapor movement is minimal and oxygen is not limited so the two models would be expected to agree. The time at which the pollutant reaches 2 m and the concentration in water at that time are in good agreement between the models. However, the end of the contaminant pulse is much more gradual for VIP than for RITZ. Also, the concentration of pollutant in water during the duration of the pulse decreases more rapidly in VIP than in RITZ. These results show that the travel time and pulse width increase as the recharge rate increases as was observed in the analysis of RITZ. The impact of these parameters upon concentration is nearly identical to those discussed for RITZ with the following exceptions:

1. The rate of decrease in concentration as a function of time during the duration of the pulse is greater than that predicted by RITZ.
2. The pulse width predicted by VIP is somewhat greater than that predicted by RITZ due to the gradual decline in concentration at the trailing edge of the pulse.
3. When model parameters are such that substantial movement takes place in the vapor phase, radically different concentration functions are predicted by VIP. VIP predicts low concentrations of pollutant at the 2-m depth at very small times for simulations with Henry's constants exceeding 0.005. RITZ does not predict this early arrival of the contaminant. Also, although VIP predicts the end of the pulse will occur at an earlier time, the change is not as large as that predicted by RITZ. While VIP shows a rapid increase in concentration at 2 m to a concentration of 0.01 g m^{-3}, RITZ predicts the pollutant never reaches that depth.

These results imply that sensitivity coefficients for VIP are approximately those of RITZ for conditions when vapor movement is of minor importance and oxygen-limiting conditions do not exist. A thorough examination of the sensitivities under oxygen-limiting conditions was not carried out in this study.

CMLS Model

When totally uniform systems are simulated using CMLS, the predicted positions of the bottom of the chemical pulse are in good agreement with RITZ. CMLS predicts that the top of the chemical moves more rapidly through the shallow soil layers than does RITZ. Hence the duration of the pulse entering the water table is less for CMLS than for RITZ. This difference is because RITZ assumes that the flux of water at every depth in the soil is the same, and therefore the top and bottom of the chemical slug move at the same velocity (assuming no oil is present). In CMLS the flux of water passing any depth on a particular day is the difference between the flux entering the soil surface and the amount of water stored in the soil profile above that depth. Therefore, the flux of water in the root zone decreases with depth so chemicals near the soil surface move more rapidly than chemicals below the root zone. (CMLS predicts that the top and bottom of the chemical pulse move at the same speed when the root zone depth is zero and the soil properties are uniform with depth.)

CMLS allows the user to model movement through layered soils where soil-water and chemical properties change with depth. When layers are simulated, the chemical reaches the 2-m depth approximately 150 days earlier than when average soil properties are used. The duration of the chemical pulse entering the water table is greater for the layered soil than for the uniform soil. This is primarily due to a lower velocity of chemical in the shallow soil layers where the sorption coefficient is greater than in the uniform case. For this soil, the use of uniform soil properties causes CMLS to overestimate the travel time and to underestimate the amount leached with respect to the layered simulation. The simulations described above for CMLS and RITZ assumed daily infiltration and evapotranspiration rates equal to the long-term average values derived from measurements taken at Fairhope, Alabama, between 1983 to 1991. Additional simulations were conducted using daily water fluxes from the same time period, January 1, 1983 to 1990. Results are shown in Table 1. In particular, layered soils and daily fluxes resulted in a mean travel time that was 47% slower than the uniform soil - uniform flux case. The amounts leached for the layered soil with uniform flux and the layered soil with daily flux are 4 and 18 times greater than the uniform case, respectively. These leaching amounts are based on a half-life of 100 days. If the half-life were less than 100 days these factors would be larger. When average infiltration and evapotranspiration rates are used in CMLS, solute leaching is underestimated due to the impact of large rainfall events and the resulting large water fluxes being essentially ignored.

Clearly the water fluxes or the weather sequences used to drive the model have a large impact upon the predictions. Therefore, weather will have a large impact upon the sensitivity coefficients. Since it is desired to get an understanding of the sensitivity for any weather sequence, the model was run many times for different weather sequences characteristic of a site. Results from all of the different simulations were summarized and used in the sensitivity analysis. The site chosen is near Fort Cobb, Oklahoma. Annual rainfall there varied from 398 to 1034 mm during the 1948 to 1975 time period. Average

Table 1. *Comparison of Predicted Travel Time, Duration of Loading, and Amount Leached for Benzene the Norfolk Soil with Different Levels of Simplification. Weather for Fairhope, Alabama. Model Used was CMLS.*

	Travel Time (Days)	Duration (Days)	Amount Leached (%)
Uniform Soil/Uniform Water Fluxes	699	70	1.0
Layered Soil/Uniform Water Fluxes	541	115	3.8
Layered Soil/Daily Water Fluxes			
Beginning Year			
1983	327	242	32.9
1984	573	152	3.6
1985	374	72	9.9
1986	423	5	5.4
1987	224	87	29.9
1988	276	28	16.3
1989	370	58	9.6
1990	395	320	33.0
Mean	370.2	120.5	17.6

annual rainfall was 709 mm during that time period. Weather sequences were generated using the weather generator developed by Richardson and Wright (1984), which is incorporated into the current version of CMLS. Probability distributions of travel time and amount leached to ground water were obtained and used in the sensitivity analyses.

Results of the sensitivity analysis for the designated model outputs indicate that all CMLS parameters are important as the lowest maximum value of the relative sensitivity coefficients for any given parameter and probability range was 0.54. In particular, the relative sensitivities for the amount leached are generally negative since the amount leached decreases as the parameter value increases, and the magnitudes of these relative sensitivities are much greater than those for travel time or pulse width. Since the magnitudes of these relative sensitivities are greater than 1, the relative change in predicted amount leached will be greater than the relative change in the parameter itself. In addition, the relative sensitivity values generally increase by at least a factor of two, which indicates that daily weather is a major component of the total uncertainty in a predicted value for amount leached. In contrast to the sensitivities for the amount leached, the sensitivity coefficients for travel times and pulse width are generally positive and of much lower magnitude. Further, relative sensitivities are generally constant or decrease as probability levels increase.

HYDRUS Model

Simulations using HYDRUS were run using three rainfall data sets, 1983, 1985, and 1987. The percent of the total pollutant predicted to be leached below the 2-m depth was 27%, 3%, and 10% for 1983, 1985, and 1987, respectively. Clearly, weather variability significantly impacts the predicted pollutant leaching results. The results for 1983 agree well with those of CMLS. However, for 1985 and 1987, CMLS predicts faster contaminant transport to the groundwater table and greater amounts leached.

As with the other models, results of the sensitivity analysis for the HYDRUS model indicate that the output describing the total amount of pollutant leached to ground water has higher relative sensitivity parameters than travel time and pulse width. Specifically, for this model output, HYDRUS is sensitive to the values for the partition coefficient, saturated water content, and the van Genuchten ß parameters. In contrast, the travel time relative sensitivities are lower in magnitude and differ in sign from the amount leached output sensitivity values. Travel time is quite sensitive to van Genuchten ß, saturated water content, partition coefficient, root uptake potential, and bulk density. Relative sensitivities for pulse width are high for saturated water content, bulk density, dispersivity, and the van Genuchten ß coefficient. All three output parameters are quite insensitive to residual water content and diffusion coefficient.

Uncertainty Analysis

Monte Carlo simulations were conducted using RITZ for estimating uncertainty with respect to soil and chemical properties. The probability distributions of the soil parameters were determined using soil data from 87 soil profiles and 10 soil series of sand from Florida. The bulk density, saturated conductivity, organic carbon content, saturated water content, and Clapp-Hornberger constant were best described by log-normal distributions. The range of values for the partition coefficient and half-life of benzene were found in the literature. Normal distributions were assumed for these two parameters. Soil properties and chemical properties were assumed to be uncorrelated. If the generated saturated water content exceeded the soil porosity based on the generated bulk density, the set of generated parameters was rejected and another set was generated. One hundred sets of input parameters were generated for Monte Carlo simulation.

Results of incorporating the variability and uncertainty of soil parameters into RITZ for the standard scenario were defined for three probability levels. At any instant of time, the predicted concentration of pollutant at the 2-m depth was less than the value for 95% of the simulations. These results indicate that the maximum concentration has values in the range of 0.06 to 0.64 g m^{-3} for 90% of the simulations. Five percent of the predicted values are greater than 0.64 g m^{-3} and 5% are less then 0.06 g m^{-3}. In addition, the uncertainty analysis indicates that the travel time for the pollutant ranges from approximately 940 to 1460 days with 90% of the values falling in the 980 to 1370 day range. The computed pulse width varies from 950 to 1050 days with 90% of the values between 960 and 1020 days. The predicted leaching varies from 0.009% to 0.2% of the amount applied with 90% of the values in the range of 0.02% to 0.2% of the amount applied. Clearly, there is a large uncertainty in model predictions due to only soil properties.

The results of the uncertainty analysis due to uncertainty in the partition coefficient and half-life of the pollutant indicate the maximum concentrations on the 95%, 50%, and 5% probability curves are 0.7, 0.21, and 0.008 g m^{-3}, respectively. This range is slightly larger than those for soil properties. Specifically, the travel time varies from 970 to 1310 days for these simulations with 90% of the values in the range of 1050 to 1220 days. Pulse width takes on values of 950 to 1010 days due to uncertainty in these chemical properties. Ninety percent of the values are in the range of 970 to 1000 days. The amount leached varies over more than

4 orders of magnitude with 90% of the leaching amounts in the range of 0.004 to 0.4 % of the amount applied. In this case the uncertainty in amount leached due to chemical properties exceeds that due to soil properties.

Simulations for systems incorporating uncertainty in both soil and chemical properties produced results that exceeded those for soil and chemical properties individually. Large differences in predicted concentrations have nearly 150-fold differences in concentration between the 5% and 95% probabilities. Travel times take on values from 950 to 1540 days with 90% of the values in the 960 to 1350 day range. Pulse widths vary from 950 to 1060 days with 90% of the simulations between 955 to 1020 days. Calculated amounts leached beyond the 2-m depth have values of 0.0003 to 0.8%. Ninety percent of the values lie in the range of 0.004 to 0.5%.

The results of the uncertainty analysis indicate that uncertainties exist and must be incorporated into the use of models. In particular, it is more realistic to think in terms of the probability that a certain type of behavior will take place rather than attempting to say whether or not that behavior will occur. Moreover, the fact that soil properties vary spatially within a mapping unit must be acknowledged. Further, modelers are better served to simulate movement in that unit for the many different sets of properties expected and to summarize the model predictions than to attempt to derive some representative set of parameters for the region hoping that the model output for that set will describe the entire region. By simulating results for many sets of parameters expected in the area, it is possible to determine the contaminant leaching for the area and gain knowledge of the likely range of leaching possible. All of this information can then be used in the decision-making process. Uncertainties must also be included when validating models experimentally.

Finally, the uncertainty in model predictions due to uncertainty in input parameters represents only part of the overall uncertainty. This analysis does not incorporate uncertainty due to model simplifications of real phenomena, errors in understanding that phenomena, or errors in solving the simplified problem.

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The complete report, entitled "Evaluation of Unsaturated/Vadose Zone Models for Superfund Sites," (Order No. PB 94-157765; Cost: $27.00, subject to change) will be available only from
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