Modeling Approaches for Assessing the Risk of Nonpoint-Source Contamination of Ground Water

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U.S. GEOLOGICAL SURVEY

Open-File Report 98–531

Denver, Colorado
1998

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Abstract

A review of modeling approaches to assess the risk of ground-water contamination indicated that stochastic solute-transport models can be effectively used to analyze uncertainty associated with the wide spatial variability of soil-hydraulic properties. Whereas deterministic models predict a unique outcome for a given set of conditions, stochastic models yield many outcomes based on the statistical distributions of model-input parameters. The resulting output probability distribution indicates the likelihood of contamination of ground water. Deterministic models can be used in a stochastic context if input parameters are sampled repeatedly. Additional uncertainty analysis involves evaluation of model, data, and parameter errors. Compared with more theoretical mechanistic models, functional deterministic models involve simplified treatments of water and solute transport, require less data, and can provide comparable results. Geostatistics can be used to predict values of model-input parameters at unsampled locations, to evaluate parameter uncertainty, to analyze solute-transport model residuals, and to create maps of model output. Geographic information systems (GIS's) can be used to organize soils and land-use data prior to contaminant-transport modeling. GIS-based comparison of contamination risk for different land uses and soil types can help identify areas for implementation of best management practices. A GIS map of model output can readily communicate to lay persons the risk of ground-water contamination by nonpoint-source pollutants.

INTRODUCTION

Ground water provides drinking water for more than half the Nation's population (Solley and others, 1993) and is the sole source of drinking water for many rural communities and some large cities. In 1990, ground water accounted for 39 percent of water withdrawn for public supply for cities and towns and 96 percent of water withdrawn by self-supplied systems for domestic use (Solley and others, 1993). Nonpoint-source contamination is considered the single greatest threat to the quality of ground water and surface water (Corwin and others, 1997). Knowing where the risk of ground-water contamination is greatest will alert water-resources managers and users of the need to protect water supplies.

The unsaturated zone is the "conduit" through which nonpoint-source contaminants must travel to reach ground water (Corwin and others, 1997). Characterization of soil properties permits use of unsaturated-zone solute-transport models to simulate leaching of nonpoint-source contaminants to ground water. Mapping model output in a geographic information system (GIS) can effectively convey the risk of ground-water contamination to policy makers, managers, and the general public. The spatial variability of physical soil properties that influence solute transport, however, profoundly affects the amount and timing of solute travel and, hence, the accuracy of model predictions. (Soil texture, volumetric water content, and soil hydraulic conductivity are examples of soil properties commonly used as model inputs.) Soil-coring studies have shown that up to 40 percent of pesticides were found twice as deep as predicted by a deterministic model (Jury, 1996). The variability of physical soil properties can cause extreme flow variations within an agricultural field, so that large

amounts of chemicals can quickly flow through relatively small areas. Preferential flow paths can develop from macropores in the root zone created by animal burrows, plant roots, dessication, freezing, and/or tillage (Michael J. Friedel, USGS, unpub. data, 1997). These pathways "short circuit" the infiltration process, causing water and solute to move through soil much faster than would be explained by the hydraulic conductivity of the soil matrix alone. The amount and timing of solute travel also are affected locally by variations in the hydraulic conductivity of the soil matrix and by focused recharge caused by topographic depressions.

Deterministic solute-transport models commonly predict that travel by chemicals through the unsaturated zone will take years. Field experiments, however, indicate that preferential flow paths dramatically reduce chemical travel time. In one experiment, water was applied to a field continuously until the water ponded at the land surface. A chloride tracer in the infiltrating water required only 5 minutes to arrive at a drain 0.4 meters below land surface (Jury, 1996). A dye tracer indicated that flow took place through root and worm channels and, in some instances, along fracture planes. Thus, preferential flow profoundly affects the "lag time" between chemical loading at the land surface and solute arrival at depth.

Better understanding of transient time in the unsaturated zone would help scientists in the National Water-Quality Assessment (NAWQA) Program to correlate changing land-use patterns with observed contaminant concentrations in ground water. The NAWQA Program is designed to enhance understanding of natural and human factors that affect water quality. NAWQA ground-water "land-use studies" evaluate the quality of recently recharged ground water for regionally extensive combinations of land use and hydrogeologic conditions (Gilliom and others, 1995). Wells are randomly sampled within the land-use study area, which represents the intersection of a targeted land use and an aquifer of interest. Land-use data must be compiled for a timeframe that is compatible with ground-water travel time, however, to produce a meaningful correlation between land use and ground-water quality. For example, if the lag time required for agricultural chemicals applied to the land surface to reach the water table in a given area is 20 years, as might be predicted with a deterministic model, Anderson land-use data collected in the 1970's (Anderson and others, 1976) are relevant to current concentrations of contaminants in ground water; but if preferential flow results in a lag time of 1–2 years, then more recent land-use data are needed. Physically based modeling approaches that address preferential flow are needed to derive realistic lag times, which can be used as a basis for selecting land-use data sets for interpretation of ground-water-quality data by NAWQA.

Purely deterministic models cannot incorporate the spatial variability existing at the field scale and larger. Jury (1996) wrote that stochastic modeling

> "is virtually the only viable option to pursue in making large-scale simulations of chemical movement. A fully deterministic model would require soil property data for every point in three-dimensional space over which the simulation is to be run. Since no one is now or ever will be using such an approach...everyone in the business of representing water and solute transport at a larger scale than a small plot is using a stochastic approach of one kind or another."

Stochastic models, which include a random component to address the spatial variability of soil properties, can predict a wide range of solute-leaching outcomes for a given area. Additionally, coupling of stochastic models with a GIS permits organization of model-input parameters and mapping of model results at large spatial scales typical of NAWQA ground-water studies.

The purpose of this literature review is to identify risk-assessment methods that are transferable to NAWQA ground-water studies and to national synthesis. Emphasis is placed on methods that employ GIS and that apply to large spatial scales. Modeling approaches that can be applied at regional and national scales are relevant from a national-synthesis perspective, whereas the watershed scale seems appropriate for NAWQA study units. Stochastic modeling at large spatial scales, however, might dampen the variability of predictions—thereby reducing the effectiveness of the risk assessment—because of "averaging" of local environmental factors used as model inputs (such as soil texture data in the USDA's State Soil Geographic database). On the other hand, a contaminant-transport model developed for an extremely small area (such as a single agricultural field) would be so tightly calibrated to a specific set of soil and land-use conditions that it would lack transferability to watershed or regional scales. Modeling approaches used in

NAWQA study units and in national synthesis activities should be versatile and appropriate for the scale of the study. Statistical approaches such as logistic regression might have greater applicability at the national scale, and stochastic models might better reflect local variability in environmental and anthropogenic conditions such as soil type, land use, and climate.

Stochastic transport modeling in NAWQA would involve multiple simulations (called "realizations") of the subsurface environment; each realization is generated from a common statistical distribution, based on observations of the physical system. Thus, effective risk assessment uses a statistical framework, rather than trial-and-error or deterministic approaches commonly used in solute-transport modeling. (For the purpose of this literature review, "stochastic" refers to model simulations involving multiple sets of input conditions, as shown in figure 1.)

The most useful aspect of stochastic transport modeling within NAWQA might be to evaluate different management scenarios (while acknowledging the spatial variability of model-input parameters) rather than attempting to explicitly model preferential flow through macropores. Modeling flow through macropores remains problematic even for highly theoretical models. For example, Richard's equation (which describes changes in water flow in time and space) "does not apply directly to flow in nonhomogeneous soils, which are characterized by nonmatrix water flows...Many field soils are characterized by large voids, or macropores, that provide the opportunity for flow to bypass the small pores of the bulk soil matrix. This short-circuiting of the matrix microporosity is difficult to describe quantitatively" (Wagenet, 1993). A more common approach, recommended here, is to use a contaminant-transport model in a stochastic context to simulate a wide range of water and chemical fluxes in the soil matrix.

Recent literature on evaluating ground-water vulnerability to nonpoint-source contamination favors risk assessment using a stochastic framework. NAWQA should consider using such a framework with the following components:

1. Organization of model-input data and mapping of aquifer vulnerability in a GIS that is compatible with recommended modeling approaches;
2. Use of physically based models to enhance understanding of the processes controlling water and solute transport in the unsaturated zone, with emphasis on preferential flow;
3. A stochastic component that reflects the wide spatial variability (uncertainty) of soil properties and contaminant distributions in real-world, field environments;
4. Additional uncertainty analysis to evaluate errors associated with source data, model-input parameters, and the transport models themselves; and
5. Validation of vulnerability predictions with independent data sets describing actual ground-water quality conditions.

In particular, NAWQA provides a unique opportunity to achieve step (5), model validation. In most of the risk-assessment studies reviewed, no ground water-contaminant data existed for comparison with model output.

LITERATURE REVIEW

The following is an overview of the current status of modeling the transport of nonpoint-source contaminants in the unsaturated zone. Case studies will be reviewed after discussion of concepts, which include model types, data variability, prediction uncertainty, model validation, and geostatistics.

Concepts

Model Types and Scale Considerations

Modeling approaches for assessing the risk of nonpoint-source contamination of ground water include GIS overlays, index methods, statistical models, and deterministic and stochastic solute-transport models (table 1). (Modeling approaches in table 1 are shown in generally increasing order of complexity.) Solute-transport models are emphasized in this "Concepts" section because extensive information on the other, more familiar methods is available from other sources.

Solute-transport models can be classified as deterministic or stochastic. *Deterministic* models assume that, given a set of conditions, a solute-transport process yields a uniquely definable outcome (Wagenet, 1993). In contrast, *stochastic* models

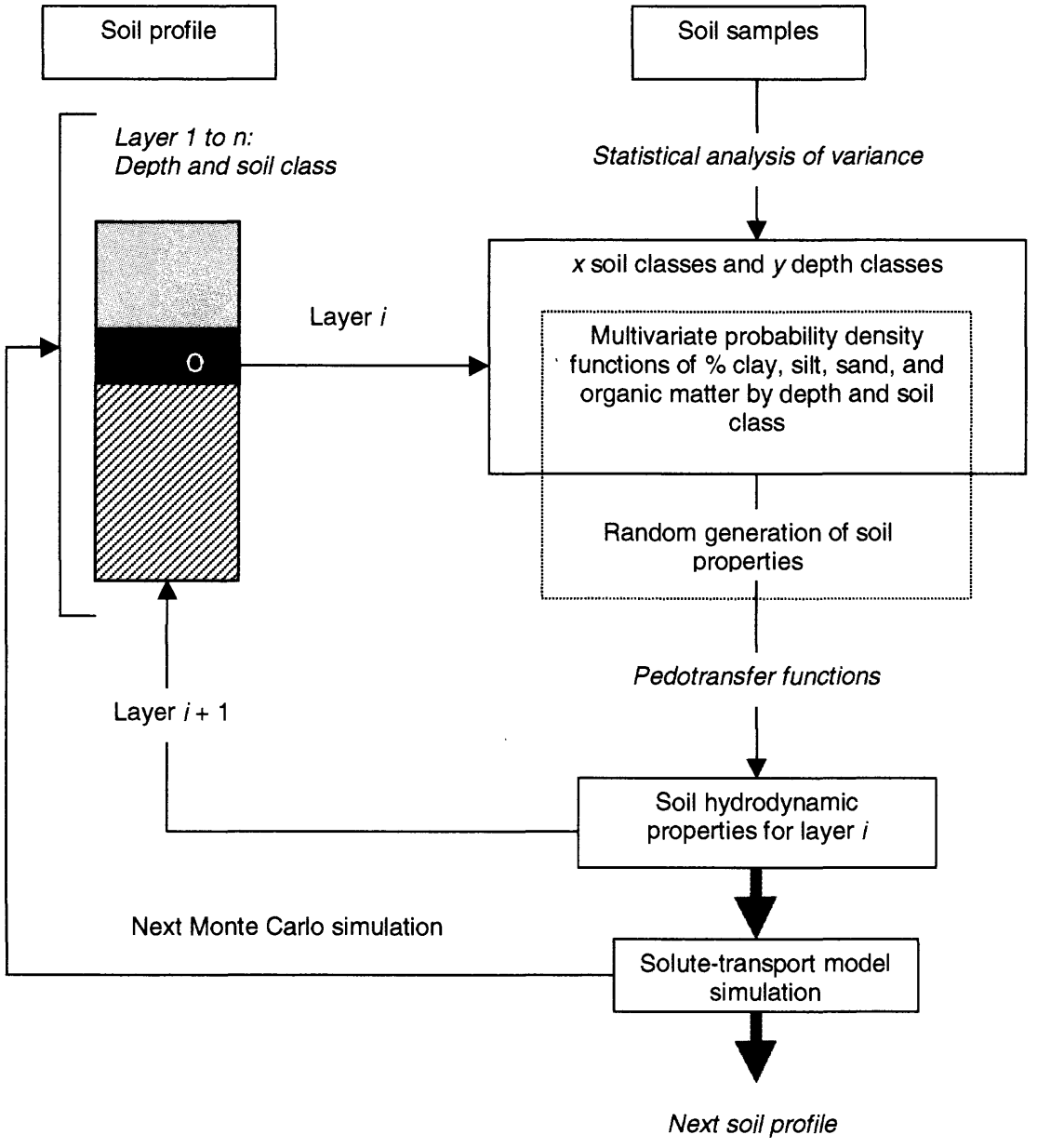

Figure 1. Monte Carlo simulation involves random generation of soil variables to yield multiple realizations of hydrodynamic properties for input to a solute-transport model (modified from Soutter and Pannatier, 1996).

Table 1. Model types and examples for risk assessment of nonpoint-source contamination of ground water

Model type	Example	Reference
GIS overlay	Nitrate risk map	Nolan and others, 1997.
Index	DRASTIC	Zhang and others, 1996.
	Deterministic	
Statistical	Logistic regression	Eckhardt and Stackelberg, 1995.
Functional solute-transport	CMLS	Wilson and others, 1996.
Mechanistic solute-transport	UNSATCHEM	Vaughan and others, 1996.
	Stochastic application of deterministic type	
Functional solute-transport	Monte Carlo application of GLEAMS	Wu and others, 1996.
Mechanistic solute-transport	Monte Carlo application of LEACH-P	Soutter and Pannatier, 1996.

presuppose that the outcome of a process is uncertain. Because deterministic models commonly use a single set of conditions, the resulting prediction might be of little value if the parameters describing the system are ill-defined or if they vary significantly in time and space. Deterministic models can be used in a stochastic mode, however, if input parameters are sampled randomly many times. For example, *Monte Carlo* simulation involves multiple modeling trials with randomly selected model-input parameters (fig. 1). Thus, stochastic models use multiple sets of conditions that reflect the randomness (as described by the statistical distributions) of model-input parameters. Each set of input conditions (realization) is equally likely to occur and generates a corresponding model output. The collection (*ensemble*) of outputs commonly is expressed as a cumulative probability distribution. In a typical application, the probability distribution indicates the likelihood that a contaminant will exceed a given concentration at a given depth.

Deterministic models include mechanistic and functional types (table 1). *Mechanistic* models incorporate the mathematics of fundamental solute-transport processes and commonly use equations to describe solute flow as a function of convection and diffusion-dispersion (Wagenet, 1993). Mechanistic models also are called *rate* models because they use parameters having rate dimensions (length or mass per time), such as hydraulic conductivity, to calculate changes in water content. Although mechanistic models are more amenable to simulating complex processes such as preferential flow through the unsaturated zone, data requirements are intense because model-input parameters must be adequately characterized throughout a study area. Mechanistic models commonly are used for research conducted at small spatial scales, such as a portion of a single agricultural field.

Functional models use simplified treatments of water flow and solute transport and require less data and expertise than mechanistic models (Wagenet, 1993). Functional models also are called *capacity* models because they emphasize capacity factors (e.g., volumetric water content at field capacity) in calculations of water and solute transport.

Functional models can provide results similar to those obtained with more rigorous mechanistic models and might be better suited to regional-scale assessments of solute transport. Hutson and Wagenet (1993) discussed the need for pragmatic, yet accurate, descriptions of water and solute flow for water-resource management. They compared functional (LEACHA) and mechanistic (LEACHP) pesticide-transport models and also compared model predictions to measured bromide and atrazine leaching profiles. The overall leaching pattern for the bromide tracer was similar for both models over a simulated 10-year period. Compared with measured bromide data, LEACHA predicted more retention at the land surface, until matric potential (used by the model to divide water between mobile and immobile phases) was reduced to –1000 kPa. In comparisons involving measured atrazine data, differences between the two models were less pronounced. The authors concluded that the need for multiple, long-term simulations in large-scale assessments using GIS makes functional models such as LEACHA a viable alternative to more theoretical models.

Görres and Gold (1996) used a fast, capacity-based model (LEACHA/N) to simulate nitrate transport in the recharge area of a production well. During extended periods, the capacity-based version compared favorably with the rate-based version of the model that uses Richard's equation. Additionally, the capacity-based version was ten times faster than the mechanistic version.

Jury (1996) described a stochastic-convective stream tube (SCST) model that simulates numerous one-dimensional soil columns in the area of interest. Soil properties are assumed locally homogeneous but vary from column to column. Taken together, the group of stream tubes represents the field, watershed, or region of interest. The collection of model predictions yields a probability distribution function that indicates the average loading for a given spatial scale. Model output, however, is not spatially registered. Although the column with the fastest flow has the earliest contaminant breakthrough, the column's location on the field is unknown. Linkage of the SCST model to a GIS requires more information than that provided by the output probability density function alone.

As spatial scale increases, processes controlling solute transport at the local scale become less important, and macroscale characteristics predominate. Whereas mechanistic models are commonly used at molecular, soil aggregate, ped, and soil-horizon scales, functional models commonly are used at scales ranging from a single field to global (Corwin and others, 1997). Stochastic models are used at the field and watershed scales, whereas statistical models (another type of deterministic model) are used at state, regional, national, and global scales. Functional models are used at larger spatial scales because sampling requirements are less intense for capacity parameters than for rate parameters. Fewer samples are required to determine representative values for capacity parameters, which have lower coefficients of variation (CV's) than rate parameters. Stochastic models based solely on capacity parameters, however, might inadequately simulate extreme events resulting from the wide spatial variability of water-transport parameters.

Data Variability and Sources

Solute-transport models can rely solely on *bulk-soil* (capacity) model parameters (e.g., bulk density, percent sand, soil-water content) or can include *water-transport* (rate) parameters (e.g., infiltration rate; unsaturated hydraulic conductivity) (Corwin and others, 1997). The spatial variability of both types of model-input parameters results in prediction uncertainty. (Spatial data gaps in a study area also cause prediction uncertainty—see section entitled "Prediction uncertainty and sources of error.") Water-transport properties, however, vary considerably more than bulk-soil properties. Corwin and others (1997) reported that water-transport properties had CV's as high as 194 percent (ponded solute velocity), whereas the highest CV for a bulk-soil property was 45 percent (15-bar soil-water content). Additionally, soil properties vary significantly within even small portions of an agricultural field. Fifty percent of the variation of many properties can occur within 1–2 m (Corwin and others, 1997). Given the extreme variability of water-transport properties, the range of outcomes from stochastic models based solely on bulk-soil properties might be unrealistically narrow. Further, stochastic models based on *measured* water-transport properties, as opposed to water-transport properties calculated from bulk properties such as soil texture, should better simulate extreme events such as water and solute transport through preferential flow paths.

Sources of soil data commonly used in nonpoint-source contamination studies include the USDA's State Soil Geographic (STATSGO) and Soil Survey Geographic (SSURGO) databases. STATSGO is 1:250,000 scale and applies to state and regional studies of large watersheds (Corwin and others, 1997). SSURGO data are 1:12,000–1:63,360-scale duplicates of soil survey maps and apply to smaller areas such as private property, townships, and counties. Although SSURGO data are more detailed, related GIS coverages are unavailable for many areas of the Nation, limiting its use in NAWQA.

Prediction Uncertainty and Sources of Error

Prediction uncertainty is caused by (1) model error, (2) input error, and (3) parameter error (Loague and others, 1996). *Model error* results when an inappropriate model incorrectly simulates a process (even though data input and parameter estimates are correct), or when a model is not properly calibrated. *Input errors,* which include measurement error, are errors in source terms such as soil-water recharge and chemical application rates. *Parameter error* occurs

when model parameters are highly interdependent, or when areal distributions of parameters have been inadequately characterized by a small number of point measurements. For example, the inability to characterize soil and solute-transport properties everywhere in a study area (e.g., for a mechanistic model) causes uncertainty in predictions of solute travel time and concentration. In an extreme case, inadequate characterization of the subsurface environment can create more uncertainty than that caused by the spatial variability of the subsurface properties themselves (Lynn J. Torak, USGS, unpub. data, 1998). Uncertainty associated with mechanistic solute-transport models, which require thorough characterization of the subsurface environment, arises from the need to fill data gaps by interpolating measured values of model inputs. The sum of model, input, and parameter errors is called the *total* or *simulation* error (Loague and others, 1996).

Loague and others (1996) used first-order uncertainty analysis (FOUA) to evaluate errors associated with simple models used to screen pesticides in ground waters of the Pearl Harbor Basin in Oahu, Hawaii. FOUA is a "method of evaluating error propagation when mathematical operations are performed to calculate values of some variable of interest..." (National Research Council, 1993). The objective is to estimate the uncertainty (e.g., variance) in the dependent variable, given the error associated with the independent variable. The pesticide screening models in the Oahu study were based on attenuation factors (AF) and retardation factors (RF), and yielded five risk classes (Loague and others, 1996). FOUA yielded a standard deviation ("total uncertainty") for each screening method. Data uncertainty was sufficiently high that changes in risk class occurred more than 50 percent of the time when a single standard deviation was added or subtracted from each risk index value.

AF model error was preliminarily assessed by comparing AF rankings of pesticide mobility with output from PRZM, a functional pesticide-transport model (Loague and others, 1996). AF compared well with PRZM, but PRZM uses an empirical fluid-transport algorithm, and transient pesticide concentration profiles at sites in the Pearl Harbor Basin were inadequately represented. Therefore, AF model error was inadequately addressed by comparison with PRZM alone.

Model Validation

Model "validation is the complement of calibration; model predictions are compared to field observations that were not used in model development or calibration...validation is an independent test of how well the model (with its calibrated parameters) is representing the important processes occurring in the natural system" (National Research Council, 1993). Validation of nonpoint-source contamination models is hampered by large uncertainties that arise from simulation errors associated with large spatial scales (Corwin and others, 1997). Preliminary validation can include (1) comparison of summary statistics (mean, variance) for model output and observed values, (2) calculating differences between observed and predicted values, and (3) qualitative assessment of compared results (Poiani and Bedford, 1995). These comparisons require observed concentrations of ground-water contaminants.

Validation comparisons also can include hypothesis testing of simulated and observed data groups, and statistical analysis of residual errors calculated in step (2) to characterize possible systematic over- or under-prediction by the model (Loague and others, 1996). Comparisons can be enhanced by graphical displays of, for example, ranges and medians of predicted and observed values.

Role of Geostatistics and Other Interpolation Methods

Geostatistics has a potentially broad role in risk assessment for nonpoint-source contamination of ground water. Geostatistics can be used to (1) analyze the spatial variability of model-input parameters, (2) predict values of model-input parameters at unsampled locations, (3) evaluate the adequacy of the data-collection network, (4) evaluate parameter uncertainty using standard deviation maps of model inputs, (5) evaluate model calibration and prediction uncertainty, and (6) map model output for presentation to lay audiences. In geostatistical theory, the experimental semivariogram relates sample spacing to spatial variability (Corwin and others, 1997). The semivariogram is used to evaluate the spatial correlation structure of a variable, a preliminary step to applying geostatistical methods such as *kriging* or *conditional simulation* (see descriptions below). Semivariograms of some variables reveal nested structures that indicate scale effects on spatial variability

(Lynn J. Torak, unpub. data, 1998). For example, "microscale" variation is manifested as a "nugget effect"—purely random variation within the smallest sampling interval—in some semivariograms; and larger variations at larger sample spacings sometimes are superimposed on the nugget semivariance. For more information on geostatistics, see Clark (1987), Delhomme (1978), and Journel and Huijbregts (1978).

Kriging, a weighted local interpolator, can be used to predict the values of model-input parameters at unsampled locations within an area. Advantages of kriging over other interpolation methods are that (1) it provides a variance of the kriged prediction (Collins, 1996), and (2) it is an "exact" interpolator—it returns the observed value at sampled locations. Kriging also can be incorporated into two-dimensional stochastic simulations to develop multiple realizations of random variables used as inputs to a solute-transport model. The randomly selected (unconditionally simulated) values are combined (conditioned) with kriged estimates using a method called conditional simulation (Delhomme, 1978; Varljen and Shafer, 1991).

Geostatistics also can be used to test data-collection adequacy, evaluate parameter uncertainty, and to ascertain model performance. For example, maps of kriging standard deviations associated with model-input parameters and predicted solute concentrations can indicate areas of uncertainty. Semivariogram analysis can be used to evaluate scale effects on model uncertainty by analyzing the spatial correlation structure of solute transport-model residuals. Spatially correlated residuals indicate that the solute-transport model has been poorly calibrated (Lynn J. Torak, unpub. data, 1998). In contrast, uncorrelated residuals (indicated by a "pure-nugget" semivariogram) indicate proper model calibration.

Finally, output from solute-transport models applied at discrete locations can be interpolated by kriging to produce a grid for mapmaking in a GIS. The resulting map can be used to communicate to lay audiences the areas at risk of nonpoint-source contamination of ground water.

Besides kriging, other interpolation methods that have been evaluated in conjunction with GIS include inverse distance-weighted averaging, polynomial regression, splining, and the lapse rate method (Collins, 1996). Weber and Englund (1992) compared inverse distance, inverse distance squared, kriging, and other interpolation methods using a large data set consisting of 19,800 computed, local variances of land elevations from a digital elevation model. The elevation variances were sampled using random, cellular-stratified, and regular-grid designs. The inverse distance-squared and inverse-distance methods had the lowest linear loss score (LLS) and mean square error (MSE). Log kriging had the next lowest LLS and rank kriging had the next lowest MSE. The authors speculated that kriging might have performed better than inverse-distance methods had the data exhibited strong anisotropy and had the samples been clustered (several of the data sets were randomly sampled). Anisotropy and sample clustering, mostly absent in the data set, tend to favor kriging. More importantly, solute-transport data tend to be clustered. Kriging automatically declusters data through the weights that are used in the prediction process (Lynn J. Torak, unpublished data, 1998).

Coupling GIS to a Solute-Transport Model

A GIS can be used to organize and analyze model-input data and to map model predictions. Additionally, solute-transport models can be loosely or tightly coupled to a GIS or embedded within it. *Loose coupling* refers to transfer of data from the GIS to an environmental model with little or no software modification (Corwin and others, 1997). Usually only the formats of input and output files require modification. In contrast, *tightly coupled* models feature user interfaces, and the functionality of *embedded* models is incorporated into the functionality of the GIS. Although tightly coupled and embedded systems are more efficient from a user standpoint, loose coupling is all that is required to organize data within a GIS for subsequent use in a solute-transport model, and to map model results.

Case Studies

Case studies on the modeling of nonpoint-source contamination of ground water include the use of aquifer-vulnerability index methods such as DRASTIC, statistical models, and physically based, deterministic models with and without a stochastic component. These methods are discussed below in order of generally increasing complexity.

GIS Overlay and Index Methods

GIS overlay and index methods (table 1) have been used in regional screening assessments of aquifer vulnerability. These methods often result in inaccurate predictions of local water quality, however, because model-input data commonly are small-scale (low-resolution), and the modeling process is subjective.

Dubrovsky and others (1995) used a GIS to evaluate ancillary data, randomly select wells for sampling, and to stratify ground-water-quality data by overlying land use for statistical analysis. For example, potential sampling sites were identified based on well depth and percentage of land use within a 0.8 km radius around a well. This is not an aquifer vulnerability study per se, but is included to show a practical and effective way of using GIS to organize and analyze ground-water quality data. Vineyards and almond orchards in the San Joaquin-Tulare Basins NAWQA study unit were delineated in the GIS. Ground-water nitrate data stratified by these land uses were compared using nonparametric statistics. Nitrate concentration and exceedances of the U.S. Environmental Protection Agency's maximum contaminant level (MCL) of 10 mg/L nitrate as nitrogen were greater in the almond orchards than in the vineyards. The rate of fertilizer application in the almond orchards is more than three times that in vineyards, so input of nitrate to the water table likely explains the observed difference in nitrate concentration.

Nolan and others (1997) used GIS overlays to map the risk of nitrate contamination of shallow ground water for the conterminous United States. Risk categories were created by GIS analysis of the following variables: nitrogen loading from fertilizer, manure, and atmospheric deposition; population density (surrogate for nitrogen loading in densely populated areas); soil drainage characteristic; and extent of woodland compared with cropland in agricultural areas (surrogate for nitrate attenuation processes such as denitrification, dilution, and plant uptake in the southeastern United States). Areas with high nitrogen input, well-drained soils, and less extensive woodland relative to cropland had the highest potential for nitrate contamination of shallow ground water (wells 100 feet deep or less). Statistical verification of the national risk map indicated that median nitrate concentration was 4.8 mg/L in wells representing the high-risk group, and the MCL of 10 mg/L was exceeded in 25 percent of the wells. In contrast, median nitrate concentration was only 0.2 mg/L in wells representing the low-risk group, and the MCL was exceeded in 3 percent of the wells.

DRASTIC and SEEPAGE were modified to assess aquifer vulnerability to nitrate contamination in Indiana (Navulur and Engel, 1996). DRASTIC and SEEPAGE both assign dimensionless weights and ratings to factors assumed to affect solute transport in the unsaturated zone. The weights are different for SEEPAGE, however, depending on whether contaminant sources are concentrated or dispersed. STATSGO soils data were used in the analysis, and land use and fertilizer loading data were combined with the rating schemes to develop vulnerability indices that were mapped in a GIS. Vulnerability indices were compared with nitrate data from 380 wells using the Pearson correlation coefficient, which was 0.67 for the modified DRASTIC method. Both DRASTIC and SEEPAGE tended to underestimate contamination potential by describing areas with high nitrate concentration as low-risk.

A modified DRASTIC method was used to evaluate ground-water vulnerability in Goshen County, Wyoming (Zhang and others, 1996). A GIS was used to organize soil and hydrologic data, assign aquifer vulnerability rating values, and to create vulnerability maps. The authors modified DRASTIC by weighting all factors equally and incorporated a map of irrigation-related recharge to show aquifer vulnerability. HYDRUS, a finite-element solute-transport model, was used to evaluate uncertainties in the aquifer vulnerability map. Soil hydraulic properties (volumetric water content and unsaturated hydraulic conductivity) were estimated from literature values, based on soil texture. Using HYDRUS, the amount of solute leached was computed at 130 locations within the study area. An interpolated map of model output closely matched the aquifer vulnerability map produced by GIS overlays. Neither map, however, was compared with actual ground-water quality data.

Statistical Models

Statistical models are a type of deterministic model (table 1), but are less physically based than models that use equations to describe water flow and solute transport. Thus, they are incapable of explicitly simulating complex processes such as preferential flow. Logistic regression is a multivariate method that yields contamination probabilities suitable for mapping in a GIS.

Eckhardt and Stackelberg (1995) found that nitrate concentrations in ground-water samples from suburban and agricultural areas of Long Island, New York, were elevated compared with samples from forested areas. Nitrate was detected in water samples from 83 of 90 wells in the study area. Logistic-regression equations were developed to predict the probability of exceeding 3 mg/L of nitrate in ground water. Explanatory variables consisted of population density, percent medium-density residential land use, percent agricultural land use, and depth to the water table. The chi-squared statistic, Akaike Information Criterion, and rank correlations between predicted probabilities and observed responses were used to evaluate model performance. Rank correlation coefficients range from zero (no fit) to one (perfect fit). Logistic-regression models developed for nitrate had rank correlation coefficients of 0.87–0.88. The logistic-regression equations indicated that nitrate concentration generally increased as population density and percent residential and agricultural land use increased, and as the depth to the water table decreased.

Teso and others (1996) used a logistic-regression model to predict the probability of occurrence of DBCP (a nematicide) in ground water beneath land sections of eastern Fresno County, California. Soil particle-size classes (e.g., sandy, loamy) were used as independent variables in the stepwise development of the model. A nonparametric test was used to assess model prediction accuracy, based on the presence or absence of DBCP in at least one well sample from each section. Predicted probabilities were converted to a point coverage that was used to create gridded probability surfaces of the study area. The stepwise procedure resulted in a significant ($p = 0.017$) model that included sandy and fine particle-size classes. Although the model correctly predicted the contamination status of *contaminated* sections 89.7 percent of the time, the overall success rate (considering both contaminated and uncontaminated sites) was only 53.2 percent. The overall success rate might have been affected by the number of samples used to determine the contamination status of a section. More than 91 percent of the incorrect model predictions occurred for uncontaminated sections, most of which had only a single well sample.

Deterministic Solute-Transport Models

A functional, Chemical Movement through Layered Soils (CMLS) model was used with two sets of soil and climatic data to evaluate the effect of spatial scale on predicted pesticide transport (Wilson and others, 1996). Soil data were obtained from STATSGO and SSURGO, and climate data were obtained from a Montana statewide database (20 km^2 cell size) and from fine-scale surfaces (0.55 km^2 cell size) interpolated with thin-plate splines. The SSURGO database was prepared by scanning, where necessary, USDA-NRCS map sheets and converting them to GIS coverages. The CMLS model was used to predict the fraction of applied chemical remaining in the soil profile, and the position of the solute front at specified times. The four sources of soils and climate data yielded different numbers of GIS polygons, which increased with increasing spatial resolution. The depth of the pesticide solute front was predicted for each polygon, then averaged over all polygons (weighted by area) and all years. For soils data, pesticide mobility and spatial variability (expressed as the mean solute-front depth and standard deviation) increased when fine-scale SSURGO data were used, compared with STATSGO data. Differences between the two sources of soil data were statistically significant at the 0.01 level. Use of fine-scale, interpolated climate data resulted in less pesticide mobility and spatial variability, however, compared with statewide data. The smoothed, interpolated climate data apparently were more spatially uniform than the statewide data.

Vaughan and others (1996) coupled a mechanistic, variably saturated flow model (UNSATCHEM) to a GIS to calculate unsaturated-zone carbon dioxide (CO_2) flux in the San Joaquin Valley, California. UNSATCHEM calculates diffusive and convective chemical transport in the air and water phases. The GIS was used to generate "sectors" with uniform cropping and irrigation practices. Whereas volumetric water content (required by the pesticide transport model) was calculated from the bulk density and gravimetric moisture content of soil samples, hydraulic conductivity and water retention were determined from literature values, based on soil texture. CO_2 flux was simulated for 74 locations within the land-use sectors using UNSATCHEM, and cumulative daily fluxes were interpolated throughout the study area by kriging. The kriged map indicated that the less

irrigated areas had the highest CO_2 flux, suggesting that CO_2 might have been trapped in soil layers by irrigation water.

Kumar and others (1998) used the Root Zone Water Quality Model (RZWQM), which includes a macropore flow component, to predict water flow and atrazine transport to subsurface drains. RZWQM is mechanistic and assumes that macropores are cylindrical in the top soil horizon and are planar cracks in bottom horizons. Continuous macropores are assumed to be vertical to any specified depth, and dead-end macropores are assumed to branch off horizontally from the continuous macropores in each soil horizon. The "average volume fraction of macroporosity" (macroporosity as a fraction of soil volume) and size of the macropores must be known to permit calculation by the model of the flow and solute transport through macropores. Assuming gravity flow, Poiseulle's law (which relates flow to hydraulic gradient and water density and viscosity) is used to calculate the maximum flow capacity of the macropores. After the onset of ponding conditions, RZWQM allows water and solutes at the soil surface to flow into simulated macropores at their maximum flow capacity. The "average volume fraction of macroporosity" was determined from Poiseulle's equation using data from infiltration measurements made in experimental plots representing moldboard plow (MP) and modified no-tillage (NT) practices. Other soil properties required by the model include soil-water content, unsaturated hydraulic conductivity, bulk density, porosity, particle-size distribution, and soil texture.

Subsurface drain flow and atrazine concentration were predicted with and without simulated macropore flow for each tillage practice (Kumar and others, 1998). Macropore flow slightly improved the accuracy of predicted, subsurface drain flows in NT plots, based on comparison of predicted and observed values. Macropore flow, however, did not improve prediction of subsurface drain flows for MP plots. Lateral saturated hydraulic conductivity was the most sensitive model parameter affecting flow to drain lines and was greater for the NT system. Predicted atrazine concentrations in NT plots were much greater with simulated macropore flow than without and fitted observed atrazine concentrations reasonably well. In contrast, RZWQM underpredicted atrazine concentration in NT plots when the macropore component of the model was disabled. Compared with the NT plots, predicted and observed atrazine concentrations for the MP plots were significantly lower, and atrazine concentrations with and without simulated macropore flow were similar.

Deterministic Solute-Transport Models With Stochastic Component

The above studies typically used single realizations of model-input parameters to produce simulations with a unique outcome. This approach cannot characterize uncertainty associated with the wide spatial variability of model-input parameters. The following studies add a stochastic component by repeatedly sampling model-input parameters for use in multiple simulations (figure 1, table 1).

Görres and Gold (1996) used Monte Carlo simulations with a rootzone nitrogen fate model to produce statistical distributions of nitrate leaching for different soil and land management combinations. A GIS was used to combine soil classes and agricultural management practices in a watershed in southern Rhode Island into "land strata." Percent organic matter, bulk density, and field capacity were measured for the different soil textural classes, and hydraulic conductivity was measured in the field using an inverse-auger hole method. A fast capacity-based leaching model (LEACHA/N) was used to predict solute transport. The model calculated unsaturated hydraulic properties with pedotransfer functions, based on the measured data. Using a Monte Carlo algorithm, model-input values were randomly selected from the statistical distributions of measured soil properties, and the LEACHA/N model was run 100 times for each land stratum. The Monte Carlo simulations generated cumulative distribution functions (CDF's) of nitrate concentration in leachate from the root zone. The CDF's indicated the degree of variability associated with intrinsic soil properties and agricultural management practices, for each stratum. CDF's also were calculated at a spatial scale equal to the entire recharge area. These had less variability than CDF's developed at the "point" support scale, which used a large number of small areas located within a given land use-soil type stratum. CDF's developed at the larger spatial scale, however, effectively identified land uses (e.g., conventionally managed silage corn on sandy soil) that had a higher probability of exceeding a threshold nitrate concentration in ground water. The

authors suggested that these CDF's could be used to identify sites within a recharge area for implementation of best management practices.

Holtschlag and Luukkonen (1997) used a steady-state unsaturated-zone transport model to compute the fraction of atrazine remaining (RM) at the water table. The pesticide transport model was applied to 5,444 wells in Kent County, Michigan, using county-based hydrologic and lithologic information. The county-based data were discretized into grid blocks for input to the solute-transport model. Infiltration and deep percolation, used to compute water flux in the leaching model, were estimated from precipitation, recharge, and streamflow data. Precipitation varied only slightly within the county. Considering all 5,444 wells, the computed time of travel between the land surface and the water table varied from 2.2 to 118 years, with a mean of 17.7 years. RM values were transformed and kriged to produce a map of aquifer vulnerability.

Monte Carlo simulations were performed to address uncertainties in hydrologic, lithologic, and pesticide data used by the leaching model (Holtschlag and Luukkonen, 1997). A total of 2,500 parameter values was randomly generated using probability density functions representing model-input parameters, and used to compute RM values for a subset of 100 wells. The standard deviation in RM at each well was used as a measure of prediction uncertainty. Kriging standard deviations at the well points were used to assess uncertainty associated with spatial interpolation.

Wu and others (1996) used a GIS to organize data for three hydrologic environments in Pike County, Ohio, into 34 subenvironments with unique soil, topography, and farming characteristics. Each subenvironment was considered a statistically independent "soil column." The Groundwater Loading Effects of Agricultural Management Systems (GLEAMS) model was used to predict unsaturated-zone nitrate transport in each soil column. GLEAMS considers leaching and nitrogen-transformation processes such as denitrification. Saturated hydraulic conductivity and other soil properties were determined in the laboratory from soil samples. Monte Carlo simulations were used to randomly generate 100 values of model-input parameters for each of three horizons in each soil column. GLEAMS was then used to predict total nitrate leaching below one meter for a 3-year period. The mean and standard deviation of simulated total nitrate leaching were calculated for each soil column and mapped in the GIS to depict aquifer vulnerability and the uncertainty of model predictions. An analysis of variance indicated that agricultural management practice, soil type, and their interaction had a significant effect on predicted nitrate leaching ($p = 0.0001$).

For three of the soil columns, ground-water nitrate samples were collected from field plots using suction lysimeters (Wu and others, 1996). Statistical tests indicated that predicted total nitrate leaching was not significantly different from the observed values. Predicted values, however, appeared to be much less than observed values for one of the plots.

Petach and others (1991) used LEACHM, a mechanistic model, to simulate pesticide and bromide leaching for a 7-km by 10-km region near Albany, New York. LEACHM uses relations between water content, matric potential, and hydraulic conductivity to describe water movement in soil. Although the model cannot explicitly simulate water movement through macropores, the authors were able to simulate a wide range of water fluxes. Data from soil surveys, land-use databases, and pesticide handbooks were integrated in a GIS to identify agricultural areas and related soil types. Land use, soil type, and related particle-size fractions in the study area were obtained from state databases. Soils with similar hydraulic properties throughout the soil profile were grouped, yielding six "hydrologic groups." The mean and standard deviation of saturated hydraulic conductivity and related soil properties were calculated for each of three soil layers (50–150 cm deep) in each hydrologic group using pedotransfer functions, based on the mean soil-texture properties of each group. The statistical distributions of soil-hydraulic properties in each hydrologic group were used to generate values of saturated hydraulic conductivity and related soil properties for input to LEACHM, resulting in 25 1-year simulations for each hydrologic group and 150 total simulations. Mean annual total precipitation and 90^{th} percentile values were used to evaluate both average and high precipitation inputs.

Mean year-end cumulative fluxes of water and chemicals were calculated for each layer of each soils hydrologic group for the two different precipitation scenarios (Petach and others, 1991). In general, substantial differences in chemical flux occurred as the chemicals moved through the soil profile. For example, EPCT flux varied by one order of magnitude

at 50 cm, but varied by 16 orders of magnitude at 150 cm, for the mean precipitation scenario. Variations in bromide flux at depth were significantly less, however. Chemical breakthrough curves (BTC's) of mean solute mass were influenced by soil and chemical properties. Whereas atrazine BTC's indicated loss of mass from degradation, losses of bromide mass in each soil layer were attributed solely to leaching. Coefficients of variation (CV's) of solute flux were 20–40 percent for both water and chemicals (less than reported in field studies in the literature), possibly because only variations in soil properties were included in the model. The authors speculated that allowing other model-input parameters to vary, such as sorption coefficients and soil organic matter content, would yield CV's closer to field values. The high and low extremes of atrazine and EPTC fluxes occurred in small areas of the region, which were readily identified in a GIS.

Soutter and Pannatier (1996) used LEACH-P, a mechanistic model, to predict pesticide transport for a 2-km by 10-km area in the upper Rhone Valley, Switzerland. Soil properties (e.g., soil texture and organic matter content) were determined at 196 locations from laboratory analysis of samples, and water-table fluctuations were measured using a network of 312 piezometers. Minimum and maximum water-table height was predicted at soil-sampling sites using co-kriging, after removing trend in the water-level data. The Monte Carlo method was used to repeatedly simulate (100 trials) pesticide transport to the water table for a 3-year period at each of the 196 soil profiles. Model-input parameters were obtained from randomly generated soil property data using pedotransfer functions (figure 1). Aquifer vulnerability was expressed as the ratio of cumulative pesticide flux to total applied pesticide. Medians of the 100 simulated vulnerability indices were interpolated with ordinary kriging to produce an aquifer vulnerability map with four risk classes. Because map features were not well correlated with water-table height, the vulnerability index was assumed to be significantly affected by soil spatial variability.

Comparison of Methods to Generate Multiple Realizations

The above studies demonstrate that the Monte Carlo method can be used to effectively generate multiple realizations of inputs to a solute transport model. Because the variance of the model output distribution is a function of the number of Monte Carlo realizations, large numbers (100–1,000) of realizations commonly are employed to ensure reasonable results. The large number of trials, however, can require excessive amounts of computer time. Alternative methods of generating multiple realizations rely on stratified sampling schemes that reduce the variance of the output distribution and, hence, require significantly fewer trials than the Monte Carlo technique.

McKay and others (1979) compared random sampling (e.g., Monte Carlo), stratified sampling, and Latin hypercube sampling (LHS) to generate multiple realizations for a model that simulates depressurization of a straight pipe filled with water. The LHS method divides each of the input variables X_k into N strata (e.g., 16) and randomly samples once from each stratum, to ensure that each input variable has all portions of its distribution represented by input values. The components of the various X_k input variables are matched at random to form N realizations (N = 16 in this example) of model inputs.

The sampling-modeling process was repeated 50 times to develop comparative statistics for the three sampling methods (McKay and others, 1979). The standard deviation of the estimated mean of model output responses was somewhat lower for stratified sampling than for random sampling. The standard deviation of the estimated mean was significantly lower for the LHS method, however, being about one-fourth that of the random-sampling estimator. Additionally, the standard deviation of the estimated variance of model output responses was significantly lower for the LHS method than for random-sampling and stratified-sampling estimators. The variance reduction associated with LHS means that fewer realizations are necessary to achieve the same precision obtained with random sampling methods such as Monte Carlo simulation.

CONCLUSIONS

Various modeling approaches for assessing the risk of nonpoint-source contamination of ground water are described in recent scientific literature. Compared with GIS-overlay methods and statistical models, deterministic models are more physically based because they commonly use equations describing

solute flow as a function of convection and dispersion-diffusion. Only one of the models reviewed here (Root Zone Water Quality Model) can explicitly simulate solute transport through macropores, but many deterministic models can be used in a stochastic context to simulate a wide range of solute fluxes. Stochastic models use multiple sets of conditions that reflect the uncertainty of model-input parameters. Deterministic models can be used in a stochastic mode if input parameters are sampled randomly many times by, for example, Monte Carlo simulation. Latin hypercube sampling, however, can achieve the same precision as random sampling with significantly fewer realizations. Functional deterministic models involve simplified treatments of water and solute transport, require less data, and can provide results similar to more theoretical models. Geostatistics can be used to predict values of model-input parameters at unsampled locations, to evaluate parameter uncertainty, to analyze residual errors during model validation, and to prepare model output for mapping. Geographic information systems (GIS's) can be used to delineate areas with unique soil and land-use characteristics prior to contaminant-transport modeling. GIS-based comparison of contamination risk for different land uses and soil types can help identify areas for implementation of best management practices. A GIS map of model output can readily communicate to lay persons the risk of groundwater contamination by nonpoint-source pollutants.

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