

Critical Review

Modeling Nonpoint Source Pollutants in the Vadose Zone with GIS

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Nonpoint source (NPS) pollutants are recognized as the single greatest threat to surface and subsurface sources of drinking water throughout the world. The vadose zone serves as the conduit through which NPS pollutants travel through surface soil to groundwater supplies. Because of increased dependency on groundwater supplies, the ability to model groundwater vulnerability to the leaching of NPS pollutants through the vadose zone has grown in significance. Geographic information systems (GIS) have emerged as a useful tool in environmental modeling, particularly for NPS pollutants. A review is presented concerning the modeling of NPS pollutants in the vadose zone with GIS. Areas discussed include the significance of NPS pollutants as a global environmental problem, the justification for the modeling of NPS pollutants in the vadose zone with GIS, the basic components of environmental modeling with GIS, a review of existing GIS-based NPS pollutant models, the application of geostatistics to GIS-based NPS pollutant modeling, the influence of scale, the reliability of NPS pollutant models based on model error and data uncertainties, and the future direction of GIS-based NPS pollutant modeling. The proliferation of GIS-based NPS pollutant models holds promise, yet caution is needed to avoid misuse of a potentially valuable environmental assessment tool for decision makers.

Introduction

Background. The information age of the 1990s is a time of global consciousness and competition where science and technology are at the forefront. For example, the application of science and technology is crucial in the solution of current and future global environmental problems. The world faces a wide variety of complex environmental threats: the loss of biodiversity; the depletion of the ozone layer; global climate change; the degradation of soil and water resources essential for food production; and the accumulation of widespread, health-threatening pollution.

Among the foremost global problems facing mankind is how to satisfy the ever-growing need for natural resources to meet living-standard and food demands, while minimizing

impacts upon an environment that already shows signs of serious levels of biodegradation. Over the past 25 years, the world has recognized that environmental problems are inseparable from those of human welfare and from the process of economic development and that many present forms of development erode the environmental resources on which human livelihood and welfare ultimately depend. This awareness has fostered the concept of sustainable agriculture as a means of meeting the world's future food demands.

The goal of sustainable agriculture is to meet the needs of the present without compromising the ability to meet the needs of the future. This presents a formidable dilemma because agriculture remains as the single greatest contributor of nonpoint source (NPS) pollutants to soil and water resources (1). Concomitantly, NPS pollutants are globally recognized as the single greatest threat to surface and subsurface sources of drinking water.

Characteristically, NPS pollutants do not recognize the political boundaries separating nations; are widespread in nature, making remediation efforts extremely complex and difficult; have the potential for maintaining a relatively long active presence in the global ecosystem; and may result in long-term, chronic effects on human health and aquatic degradation. Historically, NPS pollutants have received less attention than point source pollutants (i.e., pollutants isolated to a single "point") because point source pollutants are usually highly toxic, which poses an immediate threat to health. However, public concern has recently shifted to NPS pollutants because point source pollutants are easily identifiable (i.e., their location and identity are usually known), which makes them less of an unknown threat, whereas NPS pollutants originate from multiple sources and can have a cumulative effect that persists for several years or decades later.

Like the shift in concern from point source pollutants to NPS pollutants, public concern over the presence of NPS pollutants in different environmental compartments has also changed. In the past, NPS pollutants in surface waters were the primary environmental concern because the detection of low-level concentrations of NPS in subsurface water could not be confirmed. However, lower detection limits of analytical equipment and increased reliance upon groundwater as a water source for drinking and agriculture have brought public attention to the leaching of NPS pollutants through soil and into groundwater supplies.

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The reasons for the increased concern over the degradation of soil and groundwater resources are the result of the alarming rate of their degradation and the increased dependency upon these resources. The degradation of soil resources by human activities occurs at an unprecedented rate. It is estimated that globally 30–50% of the land is affected by NPS pollutants (2). Currently, an area approximately the size of China and India combined suffers moderate to extreme soil degradation caused by agricultural activities, deforestation, and overgrazing that has occurred over the past half century (3). This represents 11% of the world's vegetated surface, i.e., 1.2 billion ha. Of the 1.2 billion ha, approximately 12% are the consequence of chemical degradation resulting from salinization, acidification, and pollution (3). The concern over NPS pollution of the vadose zone is not only because of the degradation of the soil but also as a potential source of contamination to groundwater supplies due to the process of leaching. As surface water supplies have diminished in quantity and quality, greater demands have been placed upon groundwater supplies to meet domestic, agricultural, industrial, and recreational demands. In fact, 50% of the drinking water and 40% of the irrigation water used in the United States come from groundwater supplies. Because of the uneven distribution of available surface water supplies worldwide, the demand is even greater for groundwater supplies in countries such as Mexico. The awareness of the importance of groundwater supplies in meeting drinking and agricultural water demands has brought the concern over the degradation of groundwater to the forefront of public attention particularly in the United States and in European countries.

The ability to model NPS pollutants in the vadose zone provides a tool to optimize the use of the environment by sustaining its utility for food production while minimizing detrimental impacts and preserving esthetic qualities. The spatial complexity of the earth's surface and subsurface makes the problem of modeling NPS pollutants a data-intensive task. The volume of information needed to temporally and spatially characterize the physical, chemical, and biological parameters and variables needed in even the simplest functional models of solute transport in the vadose zone is tremendous. The ability to retrieve, manipulate, and display this onerous volume of information is a task perfectly suited for a geographical information system (GIS). The coupling of GIS to a model of solute transport in the vadose zone is a marriage designed to address the spatial problem of simulating NPS pollutants at various scales: field, basin, regional and global.

Assessing NPS Pollutants with GIS

Assessing the environmental impact of NPS pollutants at local, regional, and global scales is fundamental to achieving sustainable agriculture. Assessment involves in-situ quantification of a NPS pollutant and/or the determination of change of some NPS pollutant over time. This change can be measured in real time or predicted with a model. Real-time measurements reflect the activities of the past, whereas model predictions are glimpses into the future based upon a simplified set of assumptions. Both real-time measurement and model prediction are valuable. However, the advantage of prediction is that it can be used to alter the occurrence of detrimental conditions before they develop. Predictive models provide the ability to get answers to "what if" questions. Due to the expense and labor intensiveness of long-term field studies to quantify NPS pollutants, computer model simulations are increasingly more appealing. Forecasts from model simulations can be used in decision-making strategies designed to sustain agriculture. Such forecasts permit alteration in management strategy prior to the development of conditions that detrimentally impact either the agricultural productivity of the soil or the quality of the groundwater.

A GIS characteristically provides a means of representing the real world through integrated layers of spatial information. To model NPS pollution within the context of a GIS, the spatial heterogeneity of each transport parameter or variable of the deterministic transport model is represented by layers of spatial information formulating a three-dimensional distribution. The three-dimensional spatial distribution of each transport parameter/variable must be measured or estimated. This creates a tremendous volume of spatially indexed information due to the complex spatial heterogeneity exhibited by the numerous physical, chemical, and biological processes involved in solute transport through the vadose zone.

Basic Components of Modeling NPS Pollutants with GIS.

In their simplest form, GIS-based environmental models are comprised of three basic components (4): data, GIS, and environmental model. An understanding of the application of GIS to the modeling of NPS pollutants in the vadose zone requires a cursory understanding of each component and the interrelationship between these components.

(A) Data. All models require input data from which simulated output is generated. The significant feature of environmental models related to the simulation of NPS pollutants is the spatial and temporal variability of the input data.

The single greatest challenge to modeling NPS pollutants is to obtain sufficient data to characterize the temporal and spatial distribution with a knowledge of its uncertainty. Soil is an extremely heterogeneous medium that exhibits considerable spatial variability in many of its properties. The physical, chemical, and biological properties that influence the fate and movement of NPS pollutants in the vadose zone vary tremendously over very short distances and often vary independently of one another. Furthermore, virtually all of the properties characterizing transport processes vary both laterally and vertically. Maidment (5) insightfully points out that the most limiting factor to hydrologic modeling is not the ability to mathematically characterize the processes but to accurately specify the values of model parameters and input data.

Significance of Spatial Variability. The spatial variability of soil has been the focus of numerous books (6–8), review articles (9–14), and a compendium of Pedometrics-92 Conference papers (*Geoderma*, 1996, 60) ever since the classic paper by Nielsen et al. (15) concerning the variability of field-measured soil water properties.

The nature of soil variability is dependent on one's perspective or scale of resolution. For example, when viewed from the moon, the spatial diversity of the earth's surface appears as land and water. Whereas, low-level aerial photography yields tonal patterns of soils, landforms, geomorphic features, erosion, and vegetative patterns. If soil is observed at still greater resolution and in vertical cross section, spatial variability is seen in three dimensions as a succession of soil horizons and features not evident at the soil surface. Therefore, spatial variability can be recognized to varying degrees within two or three dimensions at microscopic, plot, field or landscape, regional, and global scales. Spatial variation is recognized as a continuum from short-range to long-range order.

Since the inception of the Soil Survey, the users of soil maps, most notably solute transport modelers, have desired to know to what extent they could assume that all the soil mapped as one class had equal potentialities. Users want and need confidence limits, probabilities, and frequency analyses on the composition of map units and information on how inclusions within a given map unit influence interpretations and behavior. The obvious question for a soil scientist to ask is how many samples are needed to characterize soil spatial variability? The response to this question depends on the magnitude of variability within the

TABLE 1. Sample Sizes Required for a 95% Probability of Detecting Change of 20, 40, and 100% in Mean of Solute Transport Parameters Using *t*-Test with $\alpha = 5\%$ (14)^a

parameter	no. of studies	no. of samples			av CV $\pm$ SD	capacity or rate parameter
		20%	40%	100%		
bulk density or porosity	13	6			10 $\pm$ 6	capacity
% sand or clay	10	28	9		28 $\pm$ 18	capacity
0.1 bar soil-water content	4	9			14 $\pm$ 7	capacity
15 bar soil-water content	5	23	7		25 $\pm$ 14	capacity
K_{sat}	13	502	127	22	124 $\pm$ 71	rate
infiltration rate content	8	135	36	8	64 $\pm$ 26	rate
$K(\theta)$	4	997	251	442	25 $\pm$ 14	rate
ponded solute velocity	1	1,225	308	51	194	rate
unsaturated solute velocity	5	127	33	7	62 $\pm$ 9	rate

^a K_{sat} is the saturated hydraulic conductivity. $K(\theta)$ is the unsaturated hydraulic conductivity as a function of water content θ .

population for the parameter in question and the probability level placed on the confidence limits (10).

The following discussion utilizes the coefficient of variation as a measure to compare soil property variation. The coefficient of variation (% CV) is defined as sample standard deviation expressed as a percentage of the sample mean. Some of the input variables and parameters needed for solute transport models of the vadose zone are dominated by the bulk characteristics of the solid matrix of the soil; consequently, the spatial variability of these properties are relatively small, which reflects the uniformity of soil genesis processes (14). These properties include porosity, bulk density, field capacity (i.e., soil-water content after free drainage has occurred, approximately 0.3 bar), and wilting point (i.e., soil-water content when plants begin to wilt, approximately 15 bar). Characteristically, these variables/parameters are associated more often with functional, deterministic models of solute transport (see Models subsection). Properties dominated by the bulk characteristics of the soil matrix are low to moderate in variability irrespective of field size or soil type. This is reflected in the low coefficients of variation as tabulated by Jury (14): porosity (CV = 7–11%), bulk density (CV = 3–26%), 0.1 bar soil-water content (CV = 4–20%), and 15 bar soil-water content (CV = 14–45%). In contrast, water transport parameters including saturated hydraulic conductivity, infiltration rate, and hydraulic conductivity–water content, or hydraulic conductivity–matric potential relations are characterized by a high variability of at least 100% or greater. These parameters are associated most often with mechanistic models of solute transport (see Models subsection). Finally, the calibration and validation of NPS pollutant models depend upon the comparison of predicted and measured solute concentrations. Solute transport experiments tabulated by Jury (14) have shown coefficients of variation of 60–130% for observed and simulated solute concentrations.

Not only do many model input variables and parameters vary considerably across a field, but substantial local-scale variability can also be found. It is common to find 50% of the variation in many soil properties within a 1–2 m radius. Local-scale variability occurs because soils vary significantly from one location to the next in their structural properties, textural composition, and mineralogical constituents. Human influence also has considerable effect. For instance, on agricultural lands salinity can vary significantly over short distances merely due to variations in surface topography and how water infiltrates into the soil. On soils with bed-furrow flood irrigation, the salinity within the bed can be an order of magnitude higher than the salinity below the furrow, which is just a few centimeters away. The increased salinity is due to the lateral and upward flow of irrigation water into the bed from the furrow that causes the accumulation of salts in the bed, while the salts directly below the furrow are continuously leached downward.

The local-scale structure is a feature that must be considered in relation to its influence upon the overall scale of interest. In other words, are local-scale influences in relation to the dominant processes of the “big picture” inconsequential or must they be taken into account? This is a relevant question useful in determining whether a sophisticated mechanistic or a simple functional model should be applied to a given NPS pollutant problem. Qualitatively, it is recognized that as the spatial scale increases, the complex local patterns of solute transport are attenuated and are dominated by macroscale characteristics. Furthermore, a knowledge of the local-scale structure not only is needed for model discrimination but also is of value in estimating the minimum volume of the soil sample necessary to represent a property at a given location. This will allow an estimation of the minimum spatial scale at which the field-scale parameters dominate solute transport behavior.

The scale of the averaging process becomes very important. Replicated measurements of representative variables/parameters where large field areas are involved must be substantial enough so that their mean values give a representative average. The type of model, functional or mechanistic, can be a factor in determining the scale of the averaging process. Table 1, which was originally presented by Jury (14), shows sample sizes necessary to have at least a 95% probability of detecting a relative change of 20, 40, and 100% in the value of the mean of various field-scale solute transport model parameters when using a one-sample two-tailed *t*-test with a probability of type 1 error set at $\alpha = 5\%$. The last column, which has been added to show whether the parameter is a capacity or rate parameter, indicates the type of model, functional or mechanistic (see Models subsection), with which the parameter is associated. Capacity parameters are found in functional models, while rate parameters are associated with mechanistic models. Table 1 clearly shows that when using functional models of solute transport the sample size necessary to represent the parameters is significantly less than for mechanistic models. Furthermore, the uncertainty of the measurement as indicated by the sample variance is as important as the mean value because it indicates the precision of the mean and uniformity of the measurement. Because most models of NPS pollutants in the vadose zone are one-dimensional, uniformity is particularly significant to illustrate the extent of validity of the assumption of one dimensionality for a defined volume of soil.

There is a need to quantify soil variability and to determine the scale or scales of its occurrence. Such information is increasingly needed for modeling of water flow and contaminant transport in GIS applications and for environmental impact assessment. Different approaches have been proposed for quantifying variability in soil map unit delineations. Traditionally, map unit composition has been quantified by transecting selected delineations of the map unit and determining at each point on the transect whether or not the

soil is the same as or similar to the selected series. Confidence intervals were calculated using either the Student's *t*-distribution or a binomial method (16). The major advantage of the *t*-statistic for calculating map composition is that it allows an estimate of the amount of variability within delineations, provided that more than one set of samples is taken for each delineation, as well as the amount of variability between delineations. The primary disadvantage of this approach is that it can result in biased estimates if care is not taken to account for differences in the size of the delineations, and the associated difference is the number of samples taken within each delineation. Care should be taken to ensure that the sampling density is the same for all delineations.

Although the two methods just described have been the most commonly used in the past, the recent proposed use of geostatistical methods (17) and fuzzy set theory (18–22) to incorporate variability and imprecision, respectively, into soil map unit delineations has gained recognition and favor. The obvious advantage of using geostatistics is that it not only provides an estimate of a value of a property at a given point or over a given area but also provides an estimate of the error associated with that estimated value. However, there are disadvantages that have precluded its routine application: (1) the method is sample intensive, requiring a large number of samples within the area being described to accurately estimate the semivariogram, and (2) the method is site specific, so the results have limited use outside of the sampled area. Geostatistics are useful in characterizing variability that exists due to random processes within the spatial system, and hence statistical and probabilistic models are appropriate. However, there are certain aspects associated with variability (i.e., imprecision or vagueness in data) that cannot be attributed to randomness whether due to complexity, missing information, imprecision, and/or the use of natural language. Because soil variation is more continuous than discrete and consequently calls for a continuous approach, fuzzy set theory (23) offers an appropriate means of modeling the imprecision or vagueness in a continuous system by allowing the matching of membership on a continuous scale rather than on a Boolean binary or an integer scale. Fuzzy set theory is a generalization of classical Boolean algebra to situations where zones of gradual transition divide classes rather than conventional crisp boundaries. Fuzzy sets are especially useful when insufficient data exist to characterize variability using standard statistical measures (e.g., mean standard deviation and distribution type). The central concept of fuzzy set theory is the membership function. The membership function is a mathematical relationship that defines the grade of membership with 1 representing full membership, 0 representing nonmembership, and a suitable function defining the flexible membership grades between 0 and 1. Aside from the representation of imprecision occurring within a map unit, fuzzy set theory also has been applied to represent the imprecision of boundary location and the gradual changes that actually occur between map unit boundaries on thematic maps (24).

The implications of soil and climatic variability on broad-scale modeling of NPS pollutants has been studied by Jury and Gruber (25), Fousseureau et al. (26), and Wilson et al. (27). The findings of Jury and Gruber show that soil and climatic variability can introduce a small probability that some mass of even relatively immobile NPS pollutant will migrate below the soil surface even when the projected mass is negligible as determined from models neglecting variability by using average values for soil and climatic properties. This is significant in lieu of the fact that some regulatory decisions have established a compliance surface below which pesticides may not migrate (28). Fousseureau et al. (26) demonstrated a means of replicating soil variability by using bootstrapping to generate pseudo-profiles of soils from pedon characterization data. Their approach permitted an assessment of the

uncertainty associated with model output due to the variability of soil input data. Wilson et al. (27) explored a means of capturing real-world soil variability through the use of existing databases (i.e., the USDA-NRCS State Soil Geographic Database, STATSGO; the county-level Soil Survey Geographic Database, SSURGO; and the Montana Agricultural Potential System, MAPS). Their findings revealed that the higher resolution of the SSURGO database was needed to identify those areas where potential chemical applications are likely to contaminate groundwater.

Though not as extensively studied as the spatial variability of soil, the aspect of temporal variability particularly of soil hydraulic properties is of concern. Temporal variation is attributed to both intrinsic factors (i.e., natural processes) such as freezing and thawing, root growth and exudates, wetting and drying cycles, carbon turnover and biological activity and extrinsic factors (i.e., man-related activities) such as tillage operations. Temporal changes have been demonstrated to occur for total porosity (29, 30), bulk density (29, 30), water retention (29, 31, 32), saturated hydraulic conductivity (30), macroporosity (29, 33, 34), and infiltration (35–37). Tillage affects both the magnitude and the variability of soil properties because it physically disrupts the structure of the soil and causes changes in water and solute flow patterns, which may change again with time as soil settles and continuous macropores develop through active soil biota and/or physical processes of nature (e.g., freezing and thawing, wetting and drying). To handle temporal data within existing soil survey databases, Grossman and Pringle (38) provided a description of a record to join together the use and time invariant information from soil survey documentation with use-dependent temporal quantities. From the GIS standpoint, Langran (39) reviewed temporal research in information processing, contrasted various proposed temporal designs, and summarized the problem of adapting it to GIS requirements.

Sources of Data. The thirst for parameter and input data by models that simulate NPS pollutants in the vadose zone is met from three sources: (1) measurement methods, (2) estimation methods, and (3) existing databases. Each source of data carries distinct advantages and limitations.

(A) Measurement Methods. A review of current physical measurements to determine flow-related properties of subsurface porous media and soil physical properties is provided by Dane and Molz (40) and Topp et al. (41), respectively. The measurement of variables and parameters related to solute transport along with characterization of initial and boundary conditions necessary for model simulation, calibration, and validation constitutes a considerable investment of time and labor because of the tremendous volume of data required. Although direct measurement of transport parameters and variables is probably the most reliable means of obtaining accurate information for modeling purposes, it is also the most labor intensive and costly. A quick and easy means of obtaining these measurements is crucial to the cost-effective modeling of NPS pollutants. Remote sensing and non-invasive techniques potentially offer the most cost-effective means of measuring crucial transport-related data.

Corwin (42) provides a cursory review of some of the instrumental techniques recently developed for the remote/non-invasive measurement of variables and parameters found in transport models for the vadose zone. Table 2 shows a summary of some of the methods currently in use and the parameters they have been used to study. Even though considerable progress has been made over the past decade in the area of remote sensing, Corwin (42) concluded that “the array of instrumentation needed to measure all the parameters and variables in even the simplest of transport models for the vadose zone is not available and in most cases is not even on the drawing board”; consequently, “the greatest progress [in the modeling of NPS pollutants] needs to be

TABLE 2. Representative List of Remote Sensing and Non-invasive Techniques Used To Study Properties and Parameters Useful in Solute Transport Models for Vadose Zone

measurement method	property or parameter studied	cited refs
Geophysical resistivity methods: electromagnetic induction	salinity soil-water content saturated hydraulic conductivity clay content depth to claypan herbicide partition coefficients	43–50 51, 52 53 54 55, 56 57
electrical resistivity tomography	water flow in fractures	58
aerial photography (B&W and color)	geomorphological and structural details	59–61
X-ray tomography	soil bulk density soil-water content	62–64
ground-penetrating radar	preferential flow paths	65
magnetic resonance imaging	water flow paths	66
microwaves	surface soil moisture	67, 68–72
multispectral scans (SPOT & Landsat TM)	textural variation	73
thermal infrared	surface temperature for soil moisture and evapotranspiration estimation	74, 75
advanced very high resolution radiometry (AVHRR)	canopy resistance, albedo, leaf area index and fraction of vegetative cover for evapotranspiration	76

TABLE 3. Referenced List of Parameter Estimation Methods for Common Parameters Used in Solute Transport Models for Vadose Zone

estimated parameter	cited refs
soils parameters	
bulk density	77, 78
diffusion coefficients	79
effective porosity	80
field capacity	78, 80–83
hydraulic conductivity (K) vs matric potential (h)	84–106
hydrodynamic dispersion	107–111
organic matter	112
pore water velocity	107–111
residual saturation	80
saturated hydraulic conductivity (K_{sat})	80, 83, 113–117
total porosity	80
water content (θ) vs matric potential (h)	77, 80, 81, 84, 85, 89, 92, 94, 97, 98, 106, 115, 118–133
wilting point	78, 80–83, 119, 134, 135
volatilization rate	79
chemical parameters	
cation-exchange capacity	135, 136
partition coefficient	78, 79, 137–145
pesticide decay rates	79, 107, 138, 140, 146
plant uptake	78
crop parameters and data	
emergence and maturity	147
maximum root zone depth	78
hydrologic parameter	
minimum evaporation depth	78

made in the area of instrumentation". Aside from the fact that remote sensing/non-invasive methods are still in their infancy, in most cases the parameters measured are often not directly applicable to solute transport models. For instance, the use of electromagnetic induction to measure soil salinity is not a direct measure of salinity in the soil solution, but rather measures the bulk electrical conductivity of the soil including the conductivity of both the solid and liquid phases.

(B) *Estimation Methods.* The inability of remote measurement techniques and instrumentation to meet the demand for spatial and temporal input data needed by NPS pollutant models has resulted in the development of transport parameter estimation techniques that are based upon the formulation of transfer functions.

Transfer functions relate readily-available and easy-to-measure soil properties to more complex transport variables/parameters needed for simulation. Table 3 provides a referenced list of the estimation methods for many of the commonly used parameters in solute transport models of

the vadose zone. The most common of the transfer functions, the pedo-transfer function (PTF), uses particle-size distribution, bulk density, and soil organic-carbon content to yield soil-water retention or unsaturated hydraulic conductivity functions (148). Rawls et al. (149) provides a review of soil-water retention estimation methods. Reviews of methods of estimating soil hydraulic parameters for unsaturated soils have been written by van Genuchten and Nielsen (150), van Genuchten et al. (151), and Timlin et al. (152).

PTFs have been developed to predict the hydraulic characteristics of a textural class using more easily measured soil data. However, PTFs are limited in accuracy. For example, a recent evaluation of PTFs has shown that greater than 90% of the variability of simulations for a map unit was due to the variability in the estimated hydraulic parameters with the PTFs, which brings the value of PTFs into question (153).

Although estimation methods are cheap and ease to use, their limited accuracy makes them less desirable than directly measured data. Nonetheless, if measured data is not avail-

TABLE 4. List of Some Existing Databases for Use in Modeling NPS Pollutants with GIS

database	source	description
soils databases:		
SOTER	ISRIC ^a	World Soils and Terrain Digital Database: global-scale database of soils, terrain, climate, vegetation, and land use data; scale 1:1 000 000
NATSGO	USDA-NRCS ^{b,c}	National Soil Geographic database: national-level soils database of USA; scale 1:7 500 000; application: national, regional, and multi-state resource appraisal, planning, and monitoring; linked to Soil Information Record (SIR) database for soil property data; soil mapping units contain many components with soil properties reflecting the percentage of the map unit having the queried properties
STATSGO	USDA-NRCS ^{b,d}	State Soil Geographic database: state-level soils database of USA; scale 1:250 000; application: state and regional studies of large watersheds, small river basins; linked to SIR; map units consist of 1–21 components with each component consisting of up to 25 physical and chemical properties
SSURGO	USDA-NRCS ^{b,e}	Soil Survey Geographic database: county-level (most detailed) soils database of USA; scale 1:12 000 to 1:63 360; duplicate of original soil survey maps; application: resource planning and management of private property, townships, and counties; linked to Map Unit Interpretation (MUIR) database for soil attribute data; map units consist of 1–3 components including over 25 physical and chemical soil properties
meteorologic databases:		
	NOAA	weather station data comprised of daily rainfall, daily min/max temperature, daily average temperature, relative humidity, etc.
SNOTEL	USDA-NRCS ^f	daily snow and precipitation amounts at specific locations within specified states and regions
miscellaneous databases:		
CIMIS	California Dept. of Water Resources ^g	seasonal crop evapotranspiration estimates
UNSODA	USDA-ARS ^h	database of measured unsaturated hydraulic properties (water retention, hydraulic conductivity, and soil water diffusivity) and basic soil properties (particle-size distribution, bulk density, organic matter, etc.)

^a International Soil Reference and Information Center, P.O. Box 353, 6700 AJ Wageningen, The Netherlands. ^b Technical Information: National Soil Survey Center; USDA-ARS; Federal Bldg., Room 152, 100 Centennial Mall, North; Lincoln, NE 68508–3866; Phone: 402–437–4149. Data Source: USDA-NRCS; National Cartography and Geospatial Center; 501 Felix St., Bldg. 23; P.O. Mail 6567; Fort Worth, TX 76115; Phone: 800–672–5559. ^c Web site: <http://www.ncg.nrcs.usda.gov/natsgo.html>. ^d Web site: <http://www.ncg.nrcs.usda.gov/statsgo.html>. ^e Web site: <http://www.ncg.nrcs.usda.gov/ssurgo.html>. ^f Web site: <http://www.ncg.nrcs.usda.gov/water.html>. ^g California Department of Water Resources, Office of Water Conservation, P.O. Box 942836, Sacramento, CA 94236–0001. ^h F. J. Leij, USDA-ARS, U.S. Salinity Laboratory, 450 West Big Springs Rd., Riverside, CA 92507–4617.

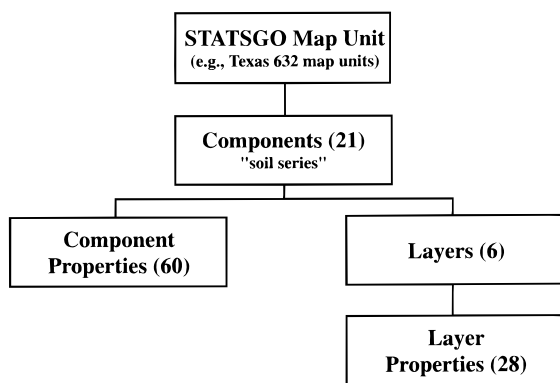


FIGURE 1. Structural hierarchy of the STATSGO soil database (154).

able, then estimations using transfer functions are usually the next best alternative.

(C) Existing Soils Databases. In most instances, limited resources do not permit the measurement or even estimation of needed input or parameter data. In these instances, the use of existing soil databases is crucial. SSURGO, STATSGO, and NATSGO are soil databases for the United States that are available from the Natural Resource Conservation Service, NRCS (see Table 4). SSURGO (Soil Survey Geographical Database; map scale ranges from 1:12 000 to 1:63 360) is a county-level database, and it is the most detailed GIS database available from NRCS. STATSGO (State Soil Geographical Database; map scale 1:250 000) is the state-level database designed for state, large watershed and small river basin purposes. The structural hierarchy of the STATSGO database is shown for the purpose of illustration in Figure 1. NATSGO (National Soil Geographical Database; map scale 1:7 500 000)

is the national soil database whose map units are defined by major land resource area (MLRA) and land resource region (LRR) boundaries. Even though considerable data are available through existing databases, most soil databases do not meet minimum data requirements for many of the distributed-parameter models used for NPS pollutants in the vadose zone nor do they provide useful statistical information concerning the uncertainty of the soil property data (155); consequently, there is a need for a re-evaluation of the types of information collected in soil surveys to meet the quantitative requirements of environmental and agricultural management models (156). An excellent example of the use of existing data sources in a GIS-based solute transport modeling application is the recent work of Wilson et al. (27). Table 4 provides a list of some of the existing databases.

(B) GIS. A GIS is defined by Goodchild (157) as a “general-purpose technology for handling geographic data in digital form with the following capabilities: (1) the ability to preprocess data from large stores into a form suitable for analysis (reformatting, change of projection, resampling, and generalization), (2) direct support for analysis and modeling, and (3) postprocessing of results (reformatting, tabulation, report generation, and mapping)”. Even more recently, at the January 1996 NCGIA Conference in Santa Fe, NM, Goodchild is quoted as saying that GIS has come to mean “the wide range of activities within the broad rubric of digital geographic information” (158). This broadened definition reflects the rapidly expanding capabilities and applications of GIS. In the context of NPS pollutant modeling, a GIS is a tool used to characterize the full information content of the spatially variable data required by solute transport models. GIS is characterized by its capability to integrate layers of spatially-oriented information. The advantages of GIS in its

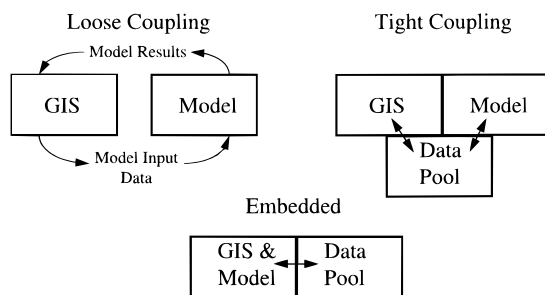


FIGURE 2. Three of the most common types of coupling of GIS to an environmental model: (a) loose, (b) tight, and (c) embedded.

application to general spatial problems include “the ease of data retrieval; ability to discover and display information gained by testing interactions between phenomena; ability to synthesize large amounts of data for spatial examination; ability to make scale and projection changes, remove distortions, and perform coordinate rotation and translation; and the capability to discover and display spatial relationships through the application of empirical and statistical models” (159).

The use of geographic information systems in environmental modeling has proliferated over the past two decades. In its infancy GIS was primarily used to create inventories of natural resources. However, over the past 10–15 years modeling and analysis applications with GIS have become more prevalent, especially in the environmental assessment arena. In particular, the past half decade has produced three NCGIA International Conferences on Integrating GIS and Environmental Modeling that have resulted in three significant texts covering the timely topic (160–162). The principal benefit of coupling GIS to environmental models is to enable the models to deal with large volumes of spatial data that geographically anchor many environmental processes. This is especially true of hydrologic processes. GIS applications to hydrologic modeling have been used in the past most widely and effectively by surface hydrologists and to a lesser extent by groundwater hydrologists for NPS pollutant applications. Only within the past decade have soil scientists begun to utilize GIS as a tool in data organization and spatial visualization of NPS pollution model simulation. Recently, emphasis has been placed upon the application of GIS to NPS pollutant problems associated specifically with the vadose zone. An example of the burgeoning interest in this area is reflected in the papers presented at the 1995 SSSA Bouyoucos Conference entitled “Applications of GIS to the Modeling of Non-Point Source Pollutants in the Vadose Zone”. This conference resulted in a compendium of papers published in a special symposium section of the *Journal of Environmental Quality* (163) and in the SSSA Special Publication *Applications of GIS to the Modeling of Non-Point Source Pollutants in the Vadose Zone* (164).

Coupling GIS to an Environmental Model. Currently, no generalized GIS system has the data representation flexibility for space and time together with the algorithmic capability needed to construct process-based models internally; consequently, environmental models and GIS must be coupled. There are a spectrum of strategies for linking models to GIS. A continuum exists ranging from loose through tight coupling to an embedded system approach in which the GIS and the model are fully-integrated into a single software system (Figure 2). A loose coupling involves data transfer from one system to another by storage of data in one system and subsequent reading of the data by the other. For example, the GIS could create external text files consisting of input data for the model and, possibly at some later time, the model could read these files and perform the necessary calculations. The important characteristic of loose coupling is the separate functionality of the programs that implement the GIS and those imple-

menting the models. A majority of the applications described in the literature represent this approach because it requires little software modification. Usually, only the file formats of the corresponding input and output routines require changes. In tight coupling, the data management is integrated into the system. Characteristically, a tight coupling will provide a common user interface for both the GIS and the model, and the information sharing between the respective components is transparent. Thus, the tightly-coupled model and the GIS must share the same database (Figure 2). For certain tightly-coupled models, transactions between the model and the database are handled separately from the transactions controlled by the GIS (165). In this situation, a possibility of conflicts arises if the model is run while the GIS is also accessing the same data. This problem can be avoided by implementing software control of the environmental model within the GIS. As the degree of coupling between the GIS and the model increases to the point where the model’s functions are essentially part of the built-in functionality of the GIS, then the model is termed embedded (Figure 2). An example would be the RAISON model that integrated a GIS, hydrologic models, a spreadsheet, and an expert system (166). In embedded systems, the coupling of software components occurs within a single application with shared memory rather than sharing the database and a common interface. Embedded systems require a substantial amount of time and money to develop and may be difficult to modify when changes are needed. There is unlikely to be any universally optimal strategy as individual applications and resource constraints will determine precise forms (167).

Another important operation in coupling a GIS to any model is the categorization of data. For example, Vaughan and Corwin (168) describe a coupled one-dimensional functional model that requires parameter data (e.g., field capacity) for each soil layer within each soil column, but the model also requires boundary condition specifications at the soil surface. If the boundary condition at the surface is determined by irrigation delivery, for example, then boundary conditions for all points within a single irrigated field would, by assumption, be identical. Thus, storage of these boundary condition data can be done for the entire field rather than duplicating them for each location. The design of a spatial database should be hierarchical and take advantage of standard procedures to eliminate any unnecessary duplication (169).

(C) Models. By definition, mathematical models integrate existing knowledge into a framework of rules, equations, and relationships for the purpose of quantifying how a system behaves (170). As long as models are applied over the range of conditions from which they were initially developed, they serve as a useful tool for prognostication. Models can range in complexity from the simplest empirical equation to complex sets of partial differential equations that are only solvable with numerical approximation techniques.

Since the 1950s, numerous models have been developed to simulate the one-, two-, and three-dimensional movement of solutes through the vadose zone. Addiscott and Wagenet (171) discussed a categorization of these models based upon conceptual approach. Their categorization distinguished between deterministic and stochastic and between mechanistic and functional. According to Addiscott and Wagenet (171), the key distinction between deterministic and stochastic models is that deterministic models “presume that a system or process operates such that the occurrence of a given set of events leads to a uniquely definable outcome” while stochastic models “presuppose the outcome to be uncertain”. Stochastic models consider the statistical credibility of both input conditions and model predictions, whereas deterministic models ignore any uncertainties in their formulation. The second level of model distinction is between mechanistic and functional models. As stated by Addiscott and Wagenet

TABLE 5. General Characteristics of Regression Type of GIS-Based NPS Pollutant Models of Vadose Zone^a

cited ref	model name	GIS	pollutants	focus of study	area (size)
Corwin et al. (173)	not specified	ARC/INFO	salinity (TDS)	salinization potential	Wellton–Mohawk Irrigation Dist., AZ (170 mi ²)
Skop (174)	not specified	not specified	nitrate	nitrate leaching potential	Denmark (42 900 km ²)
Teso et al. (175)	PSCLR	ARC/INFO	pesticides	groundwater pollution potential	San Joaquin Val., CA (15 298 mi ²)
Wang et al. (176)	not specified	ARC/INFO	salinity	salinization potential	Broadview Water District, CA (9.25 mi ²)

^a Abbreviations: AZ, Arizona; CA, California; TDS, total dissolved solids.

(171) “mechanistic is taken [here] to imply that the model incorporates the most fundamental mechanisms of the process, as presently understood”, whereas the term functional is used for “models that incorporate simplified treatments of solute and water flow and make no claim to fundamentality but do thereby require less input data and computer expertise for use”.

Because of lateral and vertical variation of soil, it is not reasonable to expect that three-dimensional models capable of describing point-to-point variability could be calibrated by any conceivable combination of measurements at field scales (i.e., hundreds or thousands of hectares); consequently, field-scale models of processes in which large surface and subsurface areas are treated relatively uniformly will need to be one-dimensional (14). For this reason, the vast majority of models that have been coupled to a GIS to simulate NPS pollutants in the vadose zone have been one-dimensional. Because modeling NPS pollutants in the vadose zone is a spatial problem well suited for the integration of a deterministic solute transport model with a GIS, deterministic models of solute transport have almost exclusively been used in combination with GIS to simulate NPS pollutants.

GIS-Based Deterministic Models for NPS Pollution Simulation. Corwin (42) provided a review of GIS applications of one-dimensional, deterministic solute transport models to field-, basin- and regional-scale assessment of NPS pollutants in the vadose zone. Prior to the review by Corwin (42), Poiani and Bedford (172) presented a review of selected GIS-based NPS modeling studies that emphasized wetlands applications. Their review included a particularly useful table summarizing each GIS-based model. Tables 5–7 are an enhancement of the original table presented by Poiani and Bedford, but are restricted to a summarization of GIS-based NPS pollutant models for the vadose zone.

Three categories of deterministic models have been coupled to GIS to simulate NPS pollution in the vadose zone: regression models, overlay and index models, and transient-state solute transport models. Regression models (Table 5) have generally used multiple linear regression techniques to relate various causative factors to the presence of a NPS pollutant. Various soil properties or conditions are related to groundwater vulnerability or to the accumulation of a solute in the soil root zone (173–176). For instance, Corwin et al. (173) related soil salinization factors (i.e., soil permeability, irrigation efficiency, and groundwater quality) to the development of salinity in the root zone for the entire Wellton–Mohawk Irrigation District (170 mi²). More recently, logistic regression techniques have been utilized to identify areas of groundwater vulnerability to pesticides (175) and the development of soil salinity (176). Overlay and index models (Table 6) refer to those models that compute an index of NPS pollutant mobility from either a simple functional model of steady-state solute transport (177–184) or a steady-state mechanistic model (187). Two types of overlay and index models have been developed: property-based and process-based. Property-based index models are established upon hydrogeologic setting (e.g., DRASTIC) or NPS pollutant properties (e.g., GUS). Process-based index models are founded upon the characterization of transport processes

(e.g., Rao’s Attenuation Factor model). Overlay and index models have been used largely to assess groundwater pollution vulnerability to pesticides and nitrates. Transient-state, process-based solute transport models (Table 7) include deterministic models capable of handling the movement of a pollutant in a dynamic flow system. Transient-state, process-based models describe some or all of the processes involved in solute transport in the vadose zone: water flow, solute transport, chemical reactions (adsorption–desorption, exchange, dissolution, precipitation, etc.), root growth, plant–water uptake, vapor phase flow, degradation, and dispersion/diffusion. The most recent progress has occurred in the coupling of transient-state solute transport models to GIS (194–198, 202, 209, 210).

GIS-Based Stochastic Models for NPS Pollution Simulation. Jury (14) pointed out that the difficulty of constructing a three-dimensional model of chemical transport as a consequence of field variability has two significant implications: (1) any hope of attempting to estimate a continuous spatial pattern of chemical transport must be abandoned, and (2) there exists a possibility of extreme deviations from average movement so that significant concentrations of chemical may flow within relatively small fractions of the total cross-sectional area which may be nearly impossible to detect from point measurements. The latter implication has fostered the development of stochastic solute transport models for the vadose zone as opposed to deterministic models.

Two distinct stochastic approaches are currently in use for dealing with the spatial variability encountered in modeling NPS pollutants in the vadose zone: geometric scaling and regionalized variables. Jury (14) indicates that geometric scaling uses specific “standardized variables to scale the differential equations describing transport and relates the standardized variables to some measurable or definable property of each local site of a heterogeneous field”. Once the variables are defined, the onerous task of characterizing the variability is reduced to determining the statistical and spatial distribution of these scaling parameters. In contrast, Jury (14) explains that the regionalized variable approach regards the “various parameters relevant to a field-wide description of transport as random variables characterized by a mean value and a randomly fluctuating stochastic component”.

In comparison to deterministic models, the coupling of a stochastic solute transport model to GIS is relatively unexplored. In a recent paper discussing the potential compatibility of stochastic transport models with GIS, Jury (213) suggested that stochastic-convective stream-tube modeling seems the most compatible with GIS because it “utilizes a relatively simple local process driven by parameters that might be associated with soil morphological features, and could be integrated up to a large scale by simple arithmetic averaging over the local sites”. A stochastic stream-tube model is made up of parallel, non-interacting one-dimensional soil columns whose properties are locally homogeneous but vary from one soil column to the next. The collection of all stream tubes constitutes the field-, basin-, or regional-scale area being represented. This approach is in essence the same approach that has been undertaken in the past

TABLE 6. General Characteristics of Overlay and Index Type of GIS-Based NPS Pollutant Models of Vadose Zone^a

cited ref	model name	GIS	pollutants	focus of study	area (size)
Merchant et al. (177) Corwin and Rhoades (178, 179)	DRASTIC Threshold Model	ERDAS ARC/INFO	non-specific salinity (TDS)	groundwater pollution potential salinization potential	Harvey County, KS (800 mi ²) Wellton–Mohawk Irrigation Dist., AZ (170 mi ²)
Khan and Liang (180) Evans and Myers (181) Regan (182)	Attenuation Factor Index DRASTIC DRASTIC	ARC/INFO ERDAS pcARC/INFO	pesticides non-specific non-specific	groundwater pollution potential groundwater pollution potential groundwater pollution potential	Oahu, HI (1500 km ²) 100 mi. ² in DE Pima and Santa Cruz Cnty., AZ
Halliday and Wolfe (183) Rundquist et al. (184) Pincus et al. (185)	DRASTIC LPI	ERDAS ARC/INFO	nitrogen non-specific pesticides	groundwater pollution potential groundwater pollution potential agrichemical impact on surface and subsurface waters	TX NE Walnut Creek Watershed, IA (15 mi ²)
Rogowski (186) Wylie et al. (187) Lo Porto et al. (188)	Leaching Index and QAT NLEAP DRASTIC	not specified GRASS IDRISI	nitrate nitrate	groundwater pollution potential nitrate leaching potential	Mahantango Creek Watershed, PA (100 km ²) South Platte River, CO Lucca Plain, Italy (200 km ²)
Zhang et al. (189) Navulur et al. (190, 191) Bui et al. (192) Mulla et al. (193)	PCI and Goss Model (1992) DRASTIC SWIM Attenuation Factor Index and Leaching Fraction Index	ARC/INFO ARC/INFO SEEPAGE not specified not specified	pesticides nitrate salinity pesticides	groundwater pollution potential salinization groundwater pollution potential	Tulare County, CA IN Dalrymple Shire, Australia (68000 km ²) Washington State Univ., WA (0.14 ha)

^a Abbreviations: AZ, Arizona; CA, California; CO, Colorado; DE, Delaware; HI, Hawaii; IA, Iowa; IN, Indiana; KS, Kansas; NE, Nebraska; PA, Pennsylvania; TX, Texas; WA, Washington; TDS, total dissolved solids.

TABLE 7. General Characteristics of Transient-State Type of GIS-Based NPS Pollutant Models of Vadose Zone.

cited ref	model name	GIS	pollutants	focus of study	area (size)
Bleecker et al. (194, 195) Petach et al. (196)	LEACHM LEACHM	ARC/INFO not specified	pesticides pesticides	groundwater pollution potential spatial variability of soil leaching potential	NY, CT, RI, MA, NH, VT, ME 7 × 10 km area, Albany, NY
Corwin et al. (197–199) Hutson (200) Khakural and Robert (201) Wilson et al. (202) Geleta et al. (203)	TETrans LEACHA LEACH-N and NLEAP CMLS GLEAMS and EPIC	ARC/INFO not specified SSIS ARC/INFO EARTHONE	salinity (TDS) pesticides nitrate herbicides nitrate	groundwater pollution potential groundwater pollution potential nitrate leaching potential groundwater pollution potential agrichemical impact on surface and subsurface soil and water	Broadview Water Dist., CA (9.25 mi ²) NY, CT, RI, MA, NH, VT, ME Redwood, Stearns Sherburne Cnty., MN Teton County, MT panhandle counties of OK USA
Kellogg et al. (204) Hoogeweg and Hornsby (205) Reynolds and De Jong (206) Görres and Gold (207) Soutter and Pannatier (208) Tiktak et al. (209) Vaughan et al. (210) Wu et al. (211) Zhang et al. (212)	GLEAMS (GWVIP & GWVIN) CMLS and GLEAMS LEACHM LEACHA/N LEACH-P PESTRAS Unsatchem GLEAMS ^b modified HYDRUS/DRASTIC	not specified ARC/INFO not specified ARC/INFO not specified ARC/INFO ARC/INFO ARC/INFO not specified	pesticides and nitrogen pesticides pesticides nitrate pesticides pesticides salinity nitrate non-specific	groundwater pollution potential groundwater pollution potential groundwater pollution potential nitrate leaching potential groundwater pollution potential groundwater pollution potential nitrate leaching potential groundwater pollution potential	Lake Manatee watershed, FL Grand River watershed, Canada (680 000 ha) Beaver River watershed, DE (300 ha) Rhône Valley, Switzerland (20 km ²) The Netherlands Broadview Water District, CA (9.25 mi ²) 3 10-ha plots, Pike County, OH Goshen County, WY

^a Abbreviations: CA, California; CT, Connecticut; DE, Delaware; FL, Florida; MA, Massachusetts; ME, Maine; MN, Minnesota; MT, Montana; NH, New Hampshire; NY, New York; OH, Ohio; OK, Oklahoma; RI, Rhode Island; VT, Vermont; WY, Wyoming; TDS, total dissolved solids. ^b Stochastic application of GLEAMS.

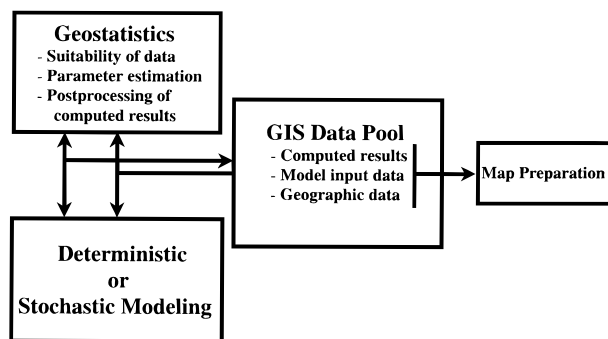


FIGURE 3. Data flow diagram showing how geostatistics interface with the GIS database and model.

where deterministic piston-flow local transport models have been coupled to soil survey information only now there is an associated stochastic component of information. Jury (213) warns that the challenge of this approach will be “to develop a reasonable local-scale model whose parameters can be related to identifiable local-scale features”.

Role of Geostatistics in the Modeling Process. Geostatistics can provide support for the modeling process by (1) determination of the suitability of a particular data set for use as input data for a model; (2) estimation of data values required by models at locations where actual measured values are not available; and (3) post-processing of computed results (Figure 3). The GIS data pool provides data for both geostatistical analysis and modeling. Results of either geostatistical analyses or modeling are also returned to the data pool (Figure 3).

Tools for preliminary statistical examination of spatial data sets include *h*-scatterplots for analyzing actual data values and indicator maps as gray-scale plots of standardized ranks of the data (214). The GIS can support these operations by providing data selection and sorting in addition to map-making. These preliminary analyses assist in discovering features of the data such as spatial trends, spatial correlation, and specific data values that appear outside the general grouping of the data and may be questionable (termed erratic). For example, sets of *h*-scatterplots at varying values of *h* (the distance between points) show variation of spatial correlation with distance by plotting of data pairs for each distance. Erratic data values are quite noticeable in such plots. For analysis of relationships between different types of data, the data can be ranked using a uniform score transform for plotting and calculation of the rank correlation coefficient, which can be compared to the standard correlation coefficient. These two statistics are separate measures of the correlation between two types of data. They can aid in revealing potential influences of erratic values because the rank correlation coefficient is less sensitive to such values (215). Selective removal of erratic values from the data generates modified data sets for study using more refined geostatistical methods that are applied to all such data sets to assess the importance that the erratic data have for any conclusions or decisions.

Among the linear geostatistical methods of analyzing spatial data, a common tool is the experimental semivariogram (from now on referred to simply as semivariogram), which represents the effect of distance between sampling points on variability (216). There are several related measures of spatial correlation such as plots of spatial covariance, correlograms, and indicator semivariograms (217). A semivariogram indicates how the mean-squared variation between pairs of data values changes with spacing between the two measurement locations. Ideally, a semivariogram will show zero variability at a sample spacing of zero and semivariance increasing with increasing spacing up to a point where it levels off at a sill value. Real data seldom have such ideal behavior; normally there is a finite, but difficult to quantify,

semivariance at a spacing of zero known as the nugget effect. Also, the sill value is often not constant because, at continually greater spacing, new soil types are encountered causing further increases in the variation between pairs of measured values. This description of the semivariogram assumes that there is no directional dependence. In fact, such is probably not the case, and computation of the semivariogram should account for directionality by taking data pairs connected by lines that lie within some angular tolerance of a specified direction. Taking as principal directions the set of perpendicular directions that show the greatest difference between their respective semivariograms usually gives a reasonable representation of the directional character of the data.

Modeling of the spatial covariance is necessary for estimation of data values at unsampled points using any of the kriging-type techniques. The spatial covariances are obtained from modeling semivariograms using, for example, the spherical, exponential, or power models. Anisotropy can also be represented by defining an azimuth angle for rotation of the principal axes from north in addition to providing model parameters for each of the two principal directions (217).

Deterministic water flow and solute transport models require a complete data set at every site where simulations will be performed. However, sampling for measurement of data required by the model often cannot be carried out so extensively. Thus, flow and transport modeling in a GIS context usually requires local estimation of at least some of the input data. One approach is through PTFs as previously described. Alternatively, geostatistical techniques such as kriging can be employed in situations where the density of existing data points is sufficient to make spatial interpolation a practical method for estimating a parameter. Advantages of estimation by kriging techniques are as follows: (1) the spatial structure of the data, as represented by semivariogram modeling, will be integrated into the estimation; (2) for locations where data points are known, kriging estimates the data value exactly; (3) the data provide the starting point for determining the weighting as compared to other methods such as inverse-distance-squared weighting that rely on an assumption (218). Kriging estimates demand that the data conform to the requirements of second-order stationarity, meaning the semivariogram is independent of location, and there is no regional trend in the data (216, 219). For estimation at unknown points based on a normal distribution of data for a single parameter, the ordinary point kriging method is appropriate. If there are two or more parameters that are cross-correlated, then cokriging may make a more accurate estimation. Both the kriging and cokriging methods require preparation and modeling of semivariograms or some other measure of spatial covariance. Cokriging also requires computation of the cross-semivariogram and modeling of the individual semivariograms and the cross-semivariogram using a linear model of coregionalization (215, 220). A non-Gaussian distribution can be handled either by a transformation or by disjunctive kriging or cokriging (221, 222). Also, the sequential indicator simulation technique can handle non-Gaussian data that consist of both hard and soft data sets (223, 224). Measured values that are georeferenced are considered hard data whereas ranges in the value of a property such as those included in soil surveys are an example of soft data. Given the difficulty in obtaining hard measurements of soil properties, the sequential indicator simulation approach can substantially improve estimation through the addition of soil survey data (223). One problem with estimating soil properties from existing soil maps results from the narrow lines indicating transitions between soil types. Most transitions in soil type take place over a finite transition zone, and semivariogram modeling of soil properties can be improved by modeling only those data that are not located within such a transition zone (225).

Another possibility for generating data at unsampled locations is stochastic simulation. A simulation generates data values by drawing them randomly from a Gaussian distribution. Methods include turning bands (226, 227), spectral methods (228), sequential Gaussian simulation (217), and matrix decomposition (229). A conditional simulation ensures that those values are statistically consistent with a set of measured data (the conditioning data). Non-Gaussian distributions are common for many types of soil data, but transformation of conditioning data from such distributions into Gaussian form allows implementation of the simulation methods (230). Unlike regression or kriging, which produce a single estimation at unsampled points, stochastic simulation can generate many data sets known as realizations. Deutsch and Journel (217) advise "Inasmuch as a simulated realization honors the data deemed important, it can be used as an interpolated map for those applications where reproduction of spatial features is more important than local accuracy". For water flow and transport modeling, stochastic simulation of input data is useful for studying the propagation of uncertainty within the models. However, computational demands of these models may preclude running such a calculation for a large number of realizations. Some discretion is necessary because stochastic simulation is a rapidly evolving field, and some of the simulation methods have not yet been extensively tested with real data.

Finally, geostatistics can assist in post-processing model results. Maps are especially useful for representation of post-processed data because non-specialists are often familiar with interpreting maps whereas graphs and histograms frequently require more detailed knowledge. A map could simply represent computed values, for example, the TIN module of ARC/INFO [ARC/INFO was designed by ESRI, 380 New York, Redlands, CA 92373] can drape a surface representing computed values over an irregularly spaced set of locations (197). Kriging the computed data can estimate the results at locations on a grid for mapmaking by raster GIS methods. For example, a model calculation of CO₂ flux through the soil surface at points within an irrigated agricultural area was kriged to obtain a gridded set of estimated values that was plotted using the GRID module of ARC/INFO (165). Other geostatistical techniques can be applied to model results. For example, semivariograms of computed results might be compared with those representing initial conditions to determine whether the modeling is causing changes in the spatial variability. The raster maps from GIS systems provide a good way to plot data that represent a continuous surface as is the case with many model results.

Environmental applications of geostatistics frequently require more information than just spatial estimates of the results of modeling. In a regulatory framework, one might want a spatial estimate of the probability that the flux concentration of a contaminant entering the groundwater exceeds a trigger value. The application of soil treatments in a precision farming operation could be locally contingent on concentrations of specific chemical species in the soil falling below an acceptable level. For these problems, the desired result cannot be estimated from a linear combination of surrounding values as in kriging. Considering the precision farming example, the function that is needed will be zero in all areas not requiring treatment but will need to specify treatment quantity for the treatable areas. This kind of nonlinear function can be generated from weighted sums of the indicator functions produced by disjunctive kriging or cokriging (231). The conditional probability that a particular value is exceeded is known as the point conditional probability estimator and is also obtained from these indicator functions (221, 222, 232–234). However, this point estimator should be taken to apply to areas that are the same size as the sampled area. For many decision-making applications, the size of the area impacted by the decision is larger than the area

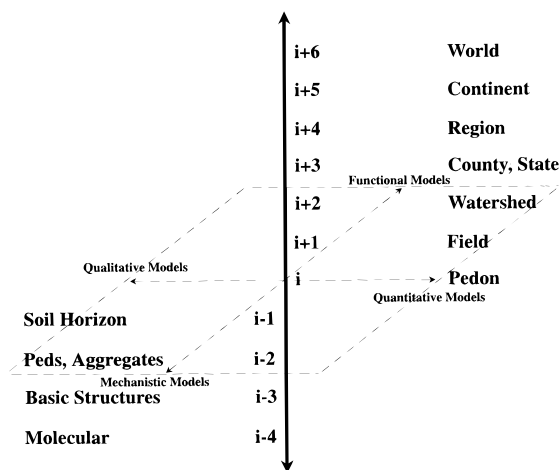


FIGURE 4. Organizational hierarchy of spatial scales pertinent to NPS pollutant models (238).

represented by a sample. Increasing the size of the affected area requires a change of support, and computation of conditional probabilities for such larger areas must be revised to deal with block rather than point values (235, 236).

Scaling Considerations. The integration of GIS into solute transport models of the vadose zone provides the ability to dynamically describe NPS pollutant transport at a range of spatial scales allowing the user to rapidly scale "up" and "down". However, this introduces incompatibilities between the model and data and raises basic questions regarding (1) the compatibility of the model with input and validation data and (2) the relevance of the model to the applied spatial scale. Wagenet and Hutson (237) addressed the issue of scale dependency and proposed three scale-related factors to consider when applying GIS-based solute transport models to the simulation of NPS pollutants in soils:

(1) The type of model (i.e., functional or mechanistic) must consider the scale of application and the nature of the available data at that scale.

(2) Sampling and measurement of input and validation data must be spatially consistent with the model.

(3) Measurement and monitoring methods must be relevant at the temporal domain being modeled.

A hierarchical depiction of the scales for the leaching of NPS pollutants shows a range in scale from molecular to global (Figure 4). Models of solute transport in the vadose zone exist at all scales. Qualitatively speaking, as spatial scale increases, the complex local patterns of solute transport are attenuated and dominated by macroscale characteristics. For this reason, mechanistic models are utilized more frequently at the (i) to ($i - 4$) scales, while functional models are more often applied to scales ranging from ($i + 1$) to ($i + 6$). The stochastic application of deterministic models is found at the ($i + 1$) scale, and stochastic models generally are used at the ($i + 1$) and ($i + 2$) scales. Statistical models are found to be applied most often at the larger scales, ($i + 3$) to ($i + 6$). A complete discussion of the application of models at different spatial and temporal scales is given by Wagenet (239).

The parameters and input variables found in functional and mechanistic models reflect the scale of the application of each category of model. Capacity parameters such as those listed in Table 1 are generally associated with functional models, while rate parameters are associated with mechanistic models. Characteristically, capacity parameters are less spatially variable than rate parameters and require fewer samples to determine a representative value (see Table 1). Generally speaking, sampling intensity requirements favor the application of functional models at larger spatial scales.

Aside from sampling intensity, there is also the consideration of the physical size of the sample volume used to

assess the value of the physical or chemical property. Sample volume is an important scale issue with regard to measurements used to develop input data or measurements needed for model validation (240). As stated by Wagenet and Hutson (237), "Until sampling and measurement approaches are consistent in scale with the models being used at that scale, our assessments of model performance will be plagued by ambiguity that arises from this lack of appreciation of scale-dependency".

The relevance of temporal domain is also a consideration not to be overlooked. Larger spatial scales appear more constant because the rapid dynamics of the lower scales are disregarded (241). For this reason, time steps of functional models can expand over days, such as the time between irrigation or precipitation events, while the time steps of mechanistic models characteristically extend over minutes.

Reliability of GIS-Based NPS Pollutant Models Based upon Model and Data Uncertainties. The uncertainties associated with assessing the vulnerability of groundwater to point source and NPS pollutants are cogently discussed in the National Research Council's *Ground Water Vulnerability Assessment: Contamination Potential Under Conditions of Uncertainty* (242). The reliability of a model is determined by the error associated with its simulated output and the intended use of the simulated output. Error is inherent in all models no matter how sophisticated or complex. There are three sources of error inherent to all NPS pollutant models (243): (i) model error, (ii) input error, and (iii) parameter error. Model error results in the inability of a model to simulate the given process, even with the correct input and parameter estimates. Model error can be due to the characteristic over-simplification of the complexities of the actual processes described within the model. Input error is the result of errors in the source terms (e.g., soil-water recharge and chemical application rates). Input error can arise from measurement, juxtaposition, and/or synchronization errors. Input (or data) error is inherent not only in estimated information but also in measured data as well; therefore, uncertainty is associated with all data. Parameter error has two possible connotations. For models requiring calibration, parameter error usually is the result of model parameters that are highly interdependent and non-unique. For models with physically-based parameters, parameter error results from an inability to represent aerial distributions on the basis of a limited number of point measurements. The combination of input and parameter errors is reflected in the quality of the model simulations (relative to ground truth) and in the reliability of the simulations for use in making decisions. The aggregation of model error, input error, and parameter error is the simulation (or total) error. Simulation error is complicated further, for multiple-process and comprehensive models, by the propagation of error between model components.

Different methods have been used to evaluate uncertainty in NPS pollutant models. These methods fall into two distinct categories: (i) sensitivity analysis, where the primary concern is assessing the propagation of error between model components; and (ii) uncertainty analysis, where the causes of simulation uncertainty are the focus of concern. Uncertainty analysis considers the inherent uncertainty in model input and parameter information and the subsequent effect this uncertainty has upon simulation results. Uncertainty analysis can be carefully designed to uncover information shortfalls and process misrepresentation. Sensitivity analysis, on the other hand, makes no use of information related to the sources or ranges of uncertainty in the model input, i.e., only considering the sensitivity of the model outputs to slight changes in an input variable/parameter. Uncertainty analysis methods for estimating data uncertainty fall into two general categories (244): (i) first-order variance propagation and (ii) Monte Carlo methods.

First-order techniques were used by Loague and his co-workers (e.g., refs 245–247) to characterize the impact of data errors in assessments of pesticide leaching, by Khan and Liang (180), for the Pearl Harbor Basin on the Hawaiian island of Oahu. Loague and his co-workers (e.g., refs 248 and 249) also characterized the impact of model error in the regional-scale leaching assessments for the Pearl Harbor Basin. A summary of the long-term effort to characterize simulation error, for the Khan and Liang pesticide leaching assessments, can be found in the recent review by Loague et al. (243). In a related study, Loague (250) attempted to quantify the worth of supplemental information in reducing the data error uncertainties for the GIS-driven groundwater vulnerability assessments for the Pearl Harbor Basin (also see ref 251). The general idea here is to cast NPS pollution assessments in terms of risk analysis (243). The cost of variance reduction for NPS pollution assessment models is illustrated in Figure 5.

The typical parameter surface maps (e.g., soil survey maps) used in NPS pollutant models are most often based upon point value measurement averages that are extrapolated to large unsampled regions without consideration for the variability (uncertainty) in the measured data. The impact of this is illustrated in Figure 6, where soil organic-carbon content for the Pearl Harbor Basin is presented, based upon extrapolation from soil taxonomy, for both mean estimates of the data and with consideration of the variability in the data. By not considering the variability in the data there is obviously, as seen in Figure 6, tremendous opportunity for error propagation (see ref 252).

The intended use of model simulations determines the level of error that can be tolerated for the simulations to be of value. There are generally three regional-scale uses for GIS-based NPS pollutant models: (i) assessment of existing conditions resulting from legacies, (ii) prediction of future impacts resulting from ongoing or future activities, and (iii) development of concepts for the design of future experiments to improve the understanding of processes. An important question to ask is whether the current generation of colored maps made from NPS pollutant models, designed to address (i)–(iii), are reliable enough for use in the decision-management arena? Currently, the honest answer to this question for (i) and (ii) is no, primarily because of uncertainties in data; for (iii) the answer is yes. However, there is fantastic potential for GIS-based NPS pollutant models to provide useful insights into the assessment, remediation, and prevention components of increasingly visible regional-scale contamination problems.

The major problem in applying simulated NPS vulnerability assessments to real problems is that it has not been possible to rigorously and unequivocally validate, based upon field observations, any regional-scale earth science modeling approach (e.g., refs 253 and 254). The model validation problem is directly linked to the uncertainties, which can be tremendous at regional scales, that are always associated with simulation errors. It should be pointed out that performance standards have not yet been established for any of the applied problems that NPS pollutant models are used. Future NPS simulation efforts will be greatly improved if well-defined model testing protocols, including model performance standards, are established.

Complete model evaluation requires both operational and scientific examination (255). The operational component of model evaluation is the assessment of accuracy and precision. Accuracy is the extent to which model-predicted values approach a corresponding set of measured observations. Precision is the degree to which model-predicted values approach a linear function of measured observations. The concept of scientific evaluation is the assessment of consistency between model-predicted results and the prevailing scientific theory (255). The concept of scientific evaluation

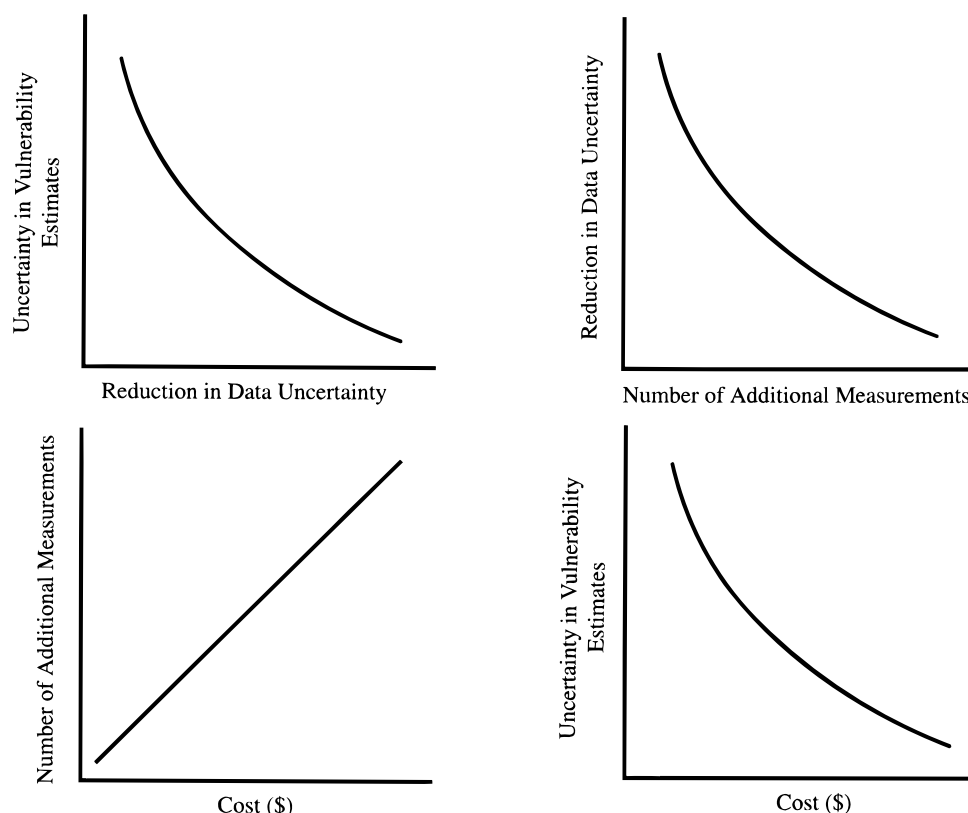


FIGURE 5. Schematic illustration of the general relationship between the cost of variance reduction and the efficiency of GIS-based NPS pollution models.

is well suited to evaluating deterministic-conceptual and stochastic-conceptual models; however, it is not appropriate for deterministic-empirical or stochastic-empirical models. The range of values over which established accuracy is expected to vary is a confidence interval. The magnitude of a confidence interval is a measure of reliability. The probability that a confidence interval is smaller or larger than some value is a significance test. Both parametric and nonparametric statistical procedures are available for significance tests (255). Evaluation of an NPS pollutant model's performance should include both statistical criteria and graphical displays (256). A combined assessment approach can be useful for making comparative evaluations of model performance between alternative/competing models.

There are several areas of concern related to uncertainty in GIS-based NPS pollutant models and the simulation maps they yield. A list of the guidelines addressing these concerns is presented (243):

(a) The location of field measurements should be included on all data overlay maps. Information imported from outside the region of interest should be tagged as such.

(b) The method(s) used for data extrapolation to unsampled sites should be described. The use of spatial interpolation techniques, such as geostatistics, will facilitate the characterization of data uncertainties.

(c) The uncertainty in data overlay maps should be presented as separate maps.

(d) The number of samples used to determine soil characteristics at a given classification (e.g., order) should be similar, relative to the size of the area being represented, for each taxonomic category.

(e) The correlation between and within the soil and chemical data sets should be considered to prevent redundant uncertainties.

(f) The depth to groundwater or a realistic compliance surface should be based upon field information and not set to an unrealistic over-conservative value. Recharge areas for

critical aquifer systems must also be identified to facilitate objective assessment of groundwater vulnerability.

(g) Serious consideration should be given to the grid size used in GIS overlays relative to soil and recharge data. One must also acknowledge that soils information accumulated over many years for purposes other than regional-scale groundwater vulnerability assessments will not always be adequate; additional sampling and analysis will almost certainly be required.

(h) Mobility indices and screening models used to generate groundwater vulnerability maps should be subjected to rigorous evaluation, based upon field observation and comparisons with physics-based simulations of coupled fluid flow and solute transport in unsaturated/saturated systems.

(i) Statistical criteria and graphical displays should be used to quantitatively evaluate the performance of models used to generate groundwater vulnerability assessments. The establishment of acceptable performance standards must be addressed.

(j) Supplemental data collection should be based upon reduction in assessment uncertainties and economic feasibility.

(k) The spatial and temporal variability in recharge (precipitation minus evapotranspiration) and land cover (a reasonable surrogate for pesticide application rates and dates) needs to be incorporated into groundwater vulnerability assessments.

(l) The heterogeneity of near-surface soil/geologic columns need to be accounted for in regional-scale groundwater vulnerability assessments.

Where Is GIS-Based Modeling of NPS Pollutants Headed?

Current trends in GIS-based NPS pollutant models involve the integration of the previously discussed components and analytical tools (i.e., measured/estimated/existing data, GIS,

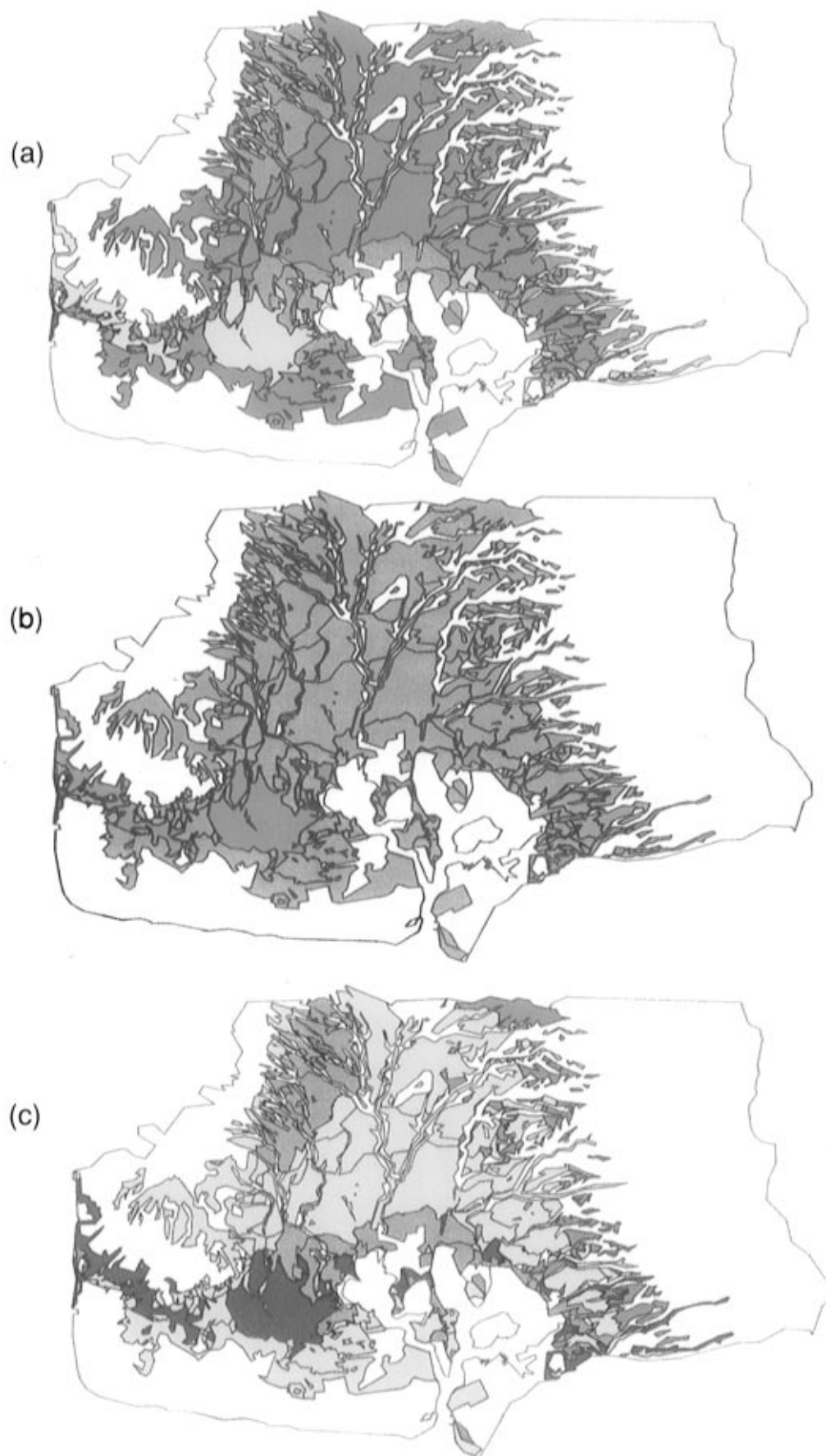


FIGURE 6. Soil organic carbon for the Pearl Harbor Basin based on soil classification at the order taxonomy category (243): (a) mean, (b) mean plus one standard deviation, (c) mean minus one standard deviation. Color key: light blue, $3.0\% \leq f_{oc}$; dark blue, $2.0\% < f_{oc} < 3.0\%$; yellow, $1.0\% < f_{oc} \leq 2.0\%$; red, $f_{oc} \leq 1.0\%$.

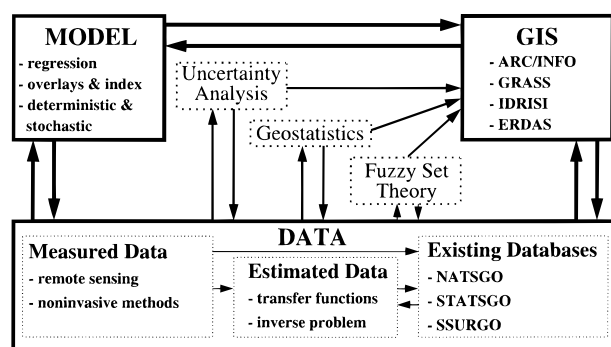


FIGURE 7. Integrated components of a GIS-based NPS pollutant model system. Arrows show the flow of information.

solute transport model, uncertainty analysis, geostatistics, and fuzzy set theory) into a system (Figure 7). Future trends in the development of GIS-based NPS pollutant models are best viewed from the perspective of the basic components: data, GIS, and solute transport modeling.

Developments in GIS related specifically to environmental modeling are most likely to occur in three areas: enhanced spatial servers, enhanced desktop GIS technology, and embedded spatial analysis and GIS technology. Enhanced spatial servers resting on extended relational database management systems (RDBMSs) are needed as a means by which the vast volumes of data necessary as input into the models can be efficiently supplied to end users. Enhanced desktop GIS technology, such as ESRI's commercially available ArcView [ArcView was designed by ESRI, 380 New York, Redlands, CA 92373], will enable users to customize a user-friendly GIS to fit their specific application. Finally, more embedded spatial analysis and GIS technology will be incorporated within NPS pollutant models, or alternatively, advanced modeling and simulation capabilities will be embedded in GIS to create an integrated, stand-alone application package.

Historically, the majority of regional-scale NPS pollutant models of the vadose zone have assumed a homogeneous soil profile when in actuality the profile is heterogeneous. As evidenced by the proliferation of transient-state, processed-based NPS pollutant models, the trend is clearly toward the coupling of GIS to more sophisticated mechanistic models that not only account for layering within the soil profile, but describe nonequilibrium physical flow (i.e., macropore and preferential pathway flow) and nonequilibrium chemical conditions (i.e., kinetic sorption). The continued modeling of existing and future knowledge regarding soil biology and its relationship to solute sorption, degradation, and sequestration at the field scale is needed particularly with respect to organic NPS pollutants. As suggested by Wagenet and Hutson (237), more experimental data, new theory, and improved operational models are needed in the areas of preferential flow, kinetic sorption, and degradation.

Aside from the computational burden, the most imposing barrier to the use of sophisticated mechanistic models for field-scale NPS pollutant applications is obtaining the data. Without question, the greatest advancements in modeling NPS pollutants are needed in the area of cheap and accurate measurements of scale-relevant input and parameter data where a statistical knowledge of measurement uncertainty is also provided. As mentioned, remote sensing and non-invasive measurement techniques offer the greatest promise in this area. However, because developments in GIS and solute transport modeling have far out paced those in data measurement as applied to NPS pollutant modeling, direction needs to be given to assure that the remote sensing/non-invasive techniques provide data that are directly applicable and usable by GIS-based NPS pollutant models. This will

help prevent the development of instrumentation that serves no direct service to environmental modeling.

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