GIS Applications of Deterministic Solute Transport Models for Regional-Scale Assessment of Non-Point Source Pollutants in the Vadose Zone

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ABSTRACT

In recent years, worldwide attention has shifted from point source to non-point source (NPS) pollutants, particularly with regard to the pollution of surface and subsurface sources of drinking water. This is due to the widespread occurrence and potential chronic health effects of NPS pollutants. The ubiquitous nature of NPS pollutants poses a complex technical problem. The areal extent of their contamination increases the complexity and sheer volume of data required for assessment far beyond that of typical point source pollutants. The spatial nature of the NPS pollution problem necessitates the use of a geographic information system (GIS) to manipulate, retrieve, and display the large volumes of spatial data. This chapter provides an overview of the components (i.e., spatial variability, scale dependency, parameter-data estimation and measurement, uncertainty analysis, and others) required to successfully model NPS pollutants with GIS and a review of recent applications of GIS to the modeling of non-point source pollutants in the vadose zone with deterministic solute transport models. The compatibility, strengths, and weaknesses of coupling a GIS to deterministic one-dimensional transport models are discussed.

BACKGROUND IN NON-POINT SOURCE POLLUTANTS

Non-point source pollutants (e.g., sediment, fertilizers, pesticides, salts, or trace elements) in terrestrial systems refer to those contaminants in surface and subsurface soil and water resources that are diffuse, or rather are spread over large areas. NPS pollutants can not be directly traced to a point location and are generally low in concentration. A characteristic feature of NPS pollutants is their
ubiquitous nature. In contrast, point source pollutants are associated with a point location such as a toxic-waste spill. In the past, point source pollutants have received the greatest attention due to their conspicuous environmental impact at a localized point and to their association with acute health effects; however, even though point source pollution is generally highly toxic, it is relatively easily controlled and identifiable; consequently, concern has shifted in recent years to NPS pollutants that are low in concentration, and widespread in distribution.

Even though the threat varies throughout the world, contamination of soil and water resources by NPS pollutants is a major global environmental issue (Duda, 1993). NPS pollutants do not recognize boundaries between nations nor are they necessarily limited by physical geographic features such as lakes, rivers, mountains, or even oceans; herein lies the source of the concern for NPS pollutants. The extent of the contamination by NPS pollutants, the resultant difficulties in their removal, and the associated chronic health effects are the features that make NPS pollutants a major environmental threat.

Historically, the concern for the quality of surface water resources preceded that of subsurface resources due to greater reliance upon surface water to meet demands. The widespread occurrence of NPS pollutants in surface waters has been well documented. The USEPA (1990) identified agricultural non-point runoff of sediment and agricultural chemicals to cause impairment of 55% of the surveyed river length and 58% of the surveyed lake. The primary sources of NPS pollutants to surface waters are from agriculture and include surface runoff and erosion.

Often, NPS pollutants are naturally occurring such as salts and trace elements already present in soil and/or irrigation water, or are the consequence of direct application by man (i.e., pesticides and fertilizers). Regardless of their source, the buildup of NPS pollutants is usually the direct consequence of man’s activities including agriculture, urban runoff, feedlots, atmospheric pollution, and resource extraction.

Agriculture is recognized as the single greatest contributor of NPS pollutants to surface and subsurface waters on a national scale followed by urban runoff, and resource extraction (Humenik et al., 1987; USEPA, 1994). Throughout the world, 30 to 50% of the earth’s land is believed affected by NPS pollutants including erosion, fertilizers, pesticides, organic manures, and sewage sludge (Pimental, 1993). NPS pollution is associated with agriculture primarily because of the potential movement of materials from the land surface into rivers and streams via runoff and erosion, and into groundwater via leaching. NPS pollutants in the groundwater can be the result of (i) direct application of chemicals by man (e.g., pesticides and fertilizers) on the soil surface that subsequently enter groundwater by leaching, or (ii) evapotranspiration of applied irrigation water that leads to the accumulation of naturally-occurring residual salts and trace elements in the soil profile, and eventually to their transport into groundwater. Research on NPS impacts from agriculture has focused on erosion, pesticide losses in surface and groundwater, $\text{NO}_3^-$-N movement to groundwater, P loss in surface runoff, and salt and trace element accumulations in soil and groundwater (Sharpley & Meyer, 1994).
Recently, a shift in public concern from surface to subsurface water resources has developed out of the increased demand for groundwater to meet constantly increasing domestic, agricultural, and industrial demands for water. Already, groundwater accounts for one-half of the drinking water and 40% of the irrigation water used in the USA. The degradation of groundwater particularly by NPS pollutants is an issue of growing public interest primarily because of concerns related to long-term health effects.

The focus of this chapter is the contamination of soil and water resources within the vadose zone (i.e., the combination of saturated and unsaturated soil located between the soil surface and the groundwater table) by NPS pollutants and the entrance of NPS pollutants into the groundwater from leaching. This chapter will review the application of geographic information systems (GIS) to the subsurface modeling of NPS pollutants with deterministic models and will discuss the components required to successfully model NPS pollutants in the vadose zone with GIS.

**JUSTIFICATION FOR MODELING NON-POINT SOURCE POLLUTANTS WITH GIS**

As the world’s population continues to grow, mankind is faced with the onerous task of meeting the world’s food demand. This only can be accomplished with sustainable agriculture. Sustainable agriculture requires a delicate balance between crop production, natural resource use, environmental impacts, and economics. The goal of sustainable agriculture is to optimize food production while maintaining economic stability, minimizing the use of finite natural resources, and minimizing impacts upon the environment. Yet, agriculture remains as the single greatest contributor of NPS pollutants to soil and water resources (Humenik et al., 1987; USEPA, 1994).

Assessing the environmental impact of NPS pollutants at a global, regional, and localized scale is a key component to achieving sustainable agriculture. Assessment involves the determination of change of some constituent 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 means of assessment 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. Forecasting information from model simulations is used in decision-making strategies designed to sustain agriculture. This information permits an alteration in the management strategy prior to the development of conditions which detrimentally impact either the agricultural productivity of the soil or the quality of the groundwater.
Modeling the fate and movement of NPS pollutants in the vadose zone is a spatial problem well suited for the integration of a deterministic solute transport model with a GIS. A GIS characteristically provides a means of representing the real world through integrated layers of constituent spatial information. To model NPS pollution within the context of a GIS, each transport parameter or variable of the deterministic transport model is represented by a three-dimensional layer of spatial information. The three-dimensional spatial distribution of each transport parameter or variable must be measured or estimated. This creates a tremendous volume of spatial information due to the complex spatial heterogeneity exhibited by the numerous physical, chemical, and biological processes involved in solute transport through the vadose zone. GIS serves as the tool for organizing, manipulating, and visually displaying this information efficiently.

The ability to model environmental contaminants such as NPS pollutants provides a means to optimize the use of the environment by sustaining its utility without detrimental consequences while preserving its esthetic qualities. Some of the greatest interest in the use of GIS for environmental problem solving is to apply the technology to translate the results of models into environmental policy. Specifically, GIS-based models of NPS pollutants provide diagnostic and predictive outputs that can be combined with socioeconomic data for assessing local, regional, and global environmental risk; or natural resource management issues (Steyaert, 1993).

GIS-BASED NON-POINT SOURCE POLLUTANT MODELING IN THE VADOSE ZONE

A generic procedure for the development of most deterministic models involves (i) formulation of a simplified conceptual model consisting of integrated processes characterizing the system, (ii) representation of each individual process by an algorithm consisting of mathematical expressions of variables and parameters, (iii) verification of the algorithm(s) to ascertain if the conceptual model is truly represented, (iv) sensitivity analysis to determine the relative importance of the variables and parameters, (v) model calibration, (vi) model validation, and (vii) application of the model for simulation. Figure 5-1 shows a schematic of the deterministic modeling procedure illustrating the interrelationship between the different steps. Table 5-1 provides a compilation of definitions for many of the aforementioned modeling terms.

Deterministic models of environmental pollutants in the vadose zone are mathematical constructs of complex natural processes including transient-state water flow, chemical reactions (i.e., kinetic reactions and transformations), biotransformations, evapotranspiration, volatilization, diffusion (i.e., vapor and liquid), hydrodynamic dispersion, and mass flow. The basic reasons for developing models of unsaturated soil ecosystems are (i) to increase the level of understanding of the cause-and-effect relationships of the processes occurring in soil systems, and (ii) to provide a cost-effective means of synthesizing the current level of knowledge into a usable form for making decisions in the environmental policy arena (Beven, 1989a; Grayson et al., 1992).
Fig. 5-1. Schematic of the deterministic modeling procedure (based on Donigan & Rao, 1986; Loague, 1993).


<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Calibration</th>
<th>Model</th>
<th>Parameter</th>
<th>Sensitivity</th>
<th>Uncertainty</th>
<th>Validation</th>
<th>Verification</th>
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<tr>
<td>A sequence of statements of computer code comprising the numerical technique representing an individual process of an environmental system.</td>
<td>A test of a model with known input and output information that is used to adjust or estimate parameters for which measured data are not available.</td>
<td>An assembly of concepts in the form of a mathematical expression comprised of variables, and parameters that portrays understanding of a natural phenomenon.</td>
<td>A constant with variable values.</td>
<td>The degree to which the model result is affected by changes in a selected input parameter or variable.</td>
<td>Error associated with mathematical modeling resulting from the selection of an incorrect model with correct (deterministic) parameters/variables and/or the use of a perfect model with parameters/variables that are characterized by a degree of uncertainty (Bobba et al., 1995).</td>
<td>Comparison of model results with numerical data independently derived from experiments or observations of the environment.</td>
<td>Examination of the algorithm to ascertain that it represents the conceptual model and that there are no inherent numerical problems.</td>
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Prior to the emergence of GIS, the incorporation of spatial processes into the modeling of solute transport in the vadose zone was accomplished with numerical techniques such as finite elements. Even with today’s supercomputers, the application of finite elements to regional-scale problems such as NPS pollutants is impractical primarily because of the astronomical input data requirements and the limited availability of supercomputer time. GIS is currently used as a practical tool for incorporating a spatial capability into one-dimensional models that are more widely used and generally more easily understood than the multi-dimensional finite-element models.

The philosophy of modeling NPS pollutants in the vadose zone with a one-dimensional deterministic model of solute transport is based upon the integration of GIS into the simulation model. The physical, chemical, and biological properties influencing transport in the vadose zone are represented using a distributed parameter structure. By solving the equations of the deterministic model that are based on an understanding of the small scale processes, the parameters have a physical meaning and must be measured in the field or estimated. Burrough (1996, this publication) identified three components of GIS-based environmental models (see Fig. 5-2): data, GIS, and model. To clearly review the application of GIS to the problem of modeling NPS pollutants in the vadose zone, a review of each component and their interrelationship in the context of NPS pollution is presented.

**Data**

**Spatial Variability**

All models require input data. In the case of NPS pollutant models of the vadose zone, the measurement or estimation of physical, chemical and biological properties influencing solute transport is needed. Furthermore, the distribution of these transport parameters or variables as defined by their spatial variability and spatial structure must be known because of their influence on the efficacy of model discrimination and parameter estimation strategies. Ellsworth (1996, this publication) presents a comprehensive review of the influence of spatial variability and spatial structure upon parameter estimation and model discrimination.

Even though soil scientists have been aware of the spatial variability of the physicochemical dynamics of soils, the extent of that variability was not clearly demonstrated until Nielsen et al.’s. (1973) classic paper concerning the variability of field-measured soil water properties. At present, the single greatest challenge in cost-effectively modeling NPS pollutants is to obtain sufficient transport parameter data to characterize the spatial distribution of the data with a knowledge of their uncertainty. Maidment (1993) points out that the factor most limiting to hydrologic modeling, in general, is not the ability to characterize hydrologic processes mathematically, or to solve the resulting equations, but rather the ability to specify the values of the model variables and parameters representing the flow environment accurately. The complex spatial heterogeneity of soil necessitates the collection of tremendous volumes of spatial data. This makes data collection for large areas prohibitively expensive due to labor cost.
Components of GIS-Based Environmental Models

Fig. 5-2. Components and subcomponents of GIS-based environmental models (based on Burrough, 1996).
Because of the natural heterogeneity of soils, scientists no longer expect to extrapolate solute transport models developed from single-dimensional laboratory soil columns to field situations. Current research has relied upon field-scale tracer experiments to demonstrate the significant spatial variability of parameters of the convection-dispersion equation (Biggar & Nielsen, 1976; van der Pol, 1977). Such studies prompted the development of probability models of solute transport (Dagan & Bressler, 1979; Jury, 1982; Simmons, 1982). The impracticality of characterizing the transport parameters needed for mechanistic models of solute transport for every point within a spatial domain has made the application of stochastic models more appealing. Nevertheless, GIS by its nature is most intuitively juxtaposed with a one-dimensional deterministic model of solute transport.

The fundamentals of spatial variability of soil properties and their influence upon transport modeling in the vadose zone are succinctly and lucidly reviewed by Jury (1986). Jury (1986) points out that, “any hope of estimating a continuous spatial pattern of chemical emissions at each point in space within a field must be abandoned due to field-scale variability of soils.” The spatial variability of a parameter or variable should generally be represented by its sample mean with its associated sample variance; however, lateral correlations are known to exist for samples taken near to one another; consequently, a knowledge of the spatial structure of each transport parameter or variable is needed to determine the intensity or resolution at which a parameter or variable must be measured to characterize its field-scale spatial variability. It is here that spatial statistics is potentially valuable. Spatial correlation can be determined. The maximum sample spacing of a parameter or variable can be estimated that will capture the parameter’s spatial variability. Various techniques of spatial interpolation can be used to increase resolution while maintaining the integrity of the spatial variability patterns (Journel, 1996, this publication).

Actually, there may not always be a need to construct highly accurate representations of the field average of each transport parameter or variable as long as a sensitivity analysis is conducted to determine the effect that a variation in each parameter or variable has upon the simulated results. Those parameters or variables with the greatest effect are obviously the parameters or variables to know more accurately. Furthermore, as Jury (1986) points out, an estimate of the variation of each parameter or variable to construct a crude sample frequency diagram may be of greater value than an accurate arithmetic average.

Scale Dependency

With the integration of GIS into simulation models of soil and water processes there is an ability to dynamically describe solute transport processes at spatial scales ranging from micro to macroscale (Wagenet & Hutson, 1996). The ability to readily translate scales up or down requires careful consideration of potential incompatibilities where knowledge or data at one spatial scale is translated to a spatial scale either larger or smaller than the scale intended. For example, the use of a one-dimensional solute transport model and transport parameters from a single soil profile to describe leaching at a field scale (i.e., up-scaling), or
the use of satellite remote sensing data to initialize a mechanistic model of solute transport (i.e., down-scaling). Nowhere is scale dependency more cogently discussed with regards to GIS applications of NPS pollutant modeling in the vadose zone than in a paper by Wagenet and Hutson (1996) and in a similar paper by Grayson et al. (1993) concerning surface hydrologic modeling.

The essential feature of combining a deterministic model of solute transport to a GIS is a knowledge of the spatial scale dependency of each physical, chemical, and biological process influencing solute transport. For instance, two limiting horizontal spatial scales are known for the dispersion process in solute transport modeling: the local-scale dispersion and the field-scale dispersion. The local-scale dispersion is the solute spread associated with local measurements (i.e., a single solution sample). Field-scale dispersion is the solute spread associated with the field-scale dispersion process (i.e., global or field-averaged measurements). Studies by Schulin et al. (1987) and Butters et al. (1989) revealed similar results in calculating values of local and field-scale dispersion with field-scale dispersivities four times and two times greater than the average local-scale dispersivity, respectively. Van Wesenbeeck and Kachanoski (1991) developed a method for measuring the transition from the local-scale to the field-scale solute travel-time variance as a function of the spatial scale during unsaturated flow conditions. This provides an estimation of the minimum horizontal spatial scale or rather the minimum plot size at which the field-scale dispersion dominates solute transport behavior. Van Wesenbeeck and Kachanoski (1994) later determined the depth dependence of the lateral scale relationships and showed a distinct range at a scale of 1 to 1.5 m, which is similar to the scale of the pedon for the soil used. Similar studies are needed to determine the spatial distribution of other transport-related parameters.

The spatial structure of each significant transport parameter is needed to determine the transition from the local scale to the field scale as a function of spatial scale. This will allow an estimation of the minimum spatial scale at which the field-scale parameters dominate solute transport behavior. It is for this reason that parameters exhibiting a scale dependency must be measured at the scale for which the application is intended. A dispersion coefficient determined from a laboratory experiment is of no value as input into a model intended for field-scale application.

The issue of scale dependency poses basic questions regarding the compatibility of models with input and validation data, and the relevance of the model to the spatial scale of applied interest (e.g., molecular, pedon, field, watershed, regional, or global scales). The effect of scale on hydrologic response has been recognized in rainfall-runoff modeling since the early 1960s (Minshall, 1960; Amorocho, 1961), and more recently in vadose zone modeling (Schulin et al., 1987; Butters et al., 1989; Van Wesenbeeck & Kachanoski, 1991; Wagenet, 1993; Wagenet & Hutson, 1995, 1996). 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. Wagenet and Hutson (1996) pointed out several scale-related factors that must be considered to ameliorate the ambiguities that otherwise plague the assessment of model performance: (i) sampling and measurement approaches for input-output data and parameter determi-
nation must be consistent in scale with the models being used, (ii) the type of simulation model (e.g., functional or mechanistic) employed must consider the scale of application and the nature of available data at that scale, and (iii) measurement and monitoring methods also must be used that are relevant at the temporal domains being modeled.

**Measurement and Estimation Methods**

Even simple functional deterministic models of transient-state solute transport (e.g., TETrans by Corwin & Waggoner, 1991a,b; Corwin et al., 1991; CMLS by Nofziger & Hornsby, 1986; and others) require a dozen or more input parameters and variables. More sophisticated numerical models (e.g., LEACHM by Wagener & Hutson, 1989; PRZM by Carsel et al., 1985; and others) require significantly more parameters or variables that are usually extremely difficult and time consuming to measure. A review of physical measurements currently in use to determine flow related properties of subsurface porous media is provided by Dane and Molz (1991). The measurement of the necessary transport parameters along with initial and boundary conditions constitute a considerable investment of time just to model a single point location. Multiple this information by a spatial factor and in some cases by a temporal factor, and the volume of data becomes tremendous.

Because of the volume of data required, it is not difficult to see how a quick and easy means of measuring each model input parameter and variable is crucial to the cost-effective modeling of NPS pollutants. Remote sensing offers a possible solution to the problem. Remote sensing techniques have been reviewed with respect to their application in hydrology and soil processes (Johannsen & Sanders, 1982; Hobbs & Mooney, 1990; Wessman, 1991; Schultz, 1993; Rango, 1994). The use of GIS with remote sensing has been most successfully applied to the determination of land use to estimate NPS pollution of surface waters (Pelletier, 1985; Oslin et al., 1988; Jakubauskas et al., 1992; Myhre et al., 1992; Myhre and Shih, 1993).

Remote sensing methods such as electromagnetic induction (DeJong et al., 1979; Rhoades & Corwin, 1981; Williams & Baker, 1982; Oluic & Kovacevic, 1983; Wollenhaupt et al., 1986; Palacky, 1987; Williams & Hoey, 1987; Kachanoski et al., 1988; Mazac et al., 1988; Corwin & Rhoades, 1990; Slavich & Petterson, 1990; Diaz & Herrero, 1992; Greenhouse & Slaine, 1983; Sudduth & Kitchen, 1993; Doolittle et al., 1994; Jaynes et al., 1995; Lesch et al., 1995) electrical resistivity tomography (Mazac et al., 1988; Daily et al., 1992), near-IR measurements (Sudduth & Hummel, 1993), x-ray tomography (Tollner, 1994) thermal-IR measurements (Ottle et al., 1989; Jupp et al., 1990; Shih & Jordan, 1993; Moran et al., 1994b), NOAA advanced very high resolution radiometry (Huang et al., 1995) microwave measurements (Jackson & Schmugge, 1986; Jupp et al., 1990; Wood et al., 1993; Schmugge et al., 1994) ground penetrating radar (Topp et al., 1980; Doolittle, 1987; Truman et al., 1988; Raper et al., 1990; Kung & Donohue, 1991; Kung & Lu, 1993), and multispectral scanning (Everitt et al., 1977; Chaturvedi et al., 1983; Agbu et al., 1990a,b; Hick & Russell, 1990; Bobba et al., 1992; Jakubauskas et al., 1992; Csillag et al., 1993; Moran et a,
1994a; Rahman et al., 1994) have recently been used in an attempt to reduce the labor intensiveness of directly or indirectly determining some subsurface transport parameters or variables and NPS pollutant levels. Unfortunately, most of the aforementioned remote sensing techniques are still in their infancy with regards to direct applications in subsurface solute transport modeling; consequently, they are limited in their current usefulness.

The use of remotely sensed data for land use and resource surveys is not new; however, the applications of remote sensing to near and subsurface processes influencing NPS pollution distribution within the vadose zone are less well understood. The inherent problems associated with the complexity of soils have resulted in few definitive subsurface applications. Nevertheless, there is evidence that remote sensing applications for quantitative and temporal analysis of near and subsurface processes will be a future possibility. Geophysical resistivity methods (e.g., electromagnetic induction, electrical resistivity tomography, and others) have been used to study the spatial variability of the electrical properties of soils as a substitute for the variability of various soil physical properties such as soil water content (Kachanoski et al., 1988) saturated hydraulic conductivity (Mazac et al., 1988), soil salinity (DeJong et al., 1979; Rhoades & Corwin, 1981; Williams & Hoey, 1987; Lesch et al., 1992), clay content (Williams & Hoey, 1987), depth to claypan (Sudduth & Kitchen, 1993), herbicide partition coefficient (Jaynes et al., 1995), forest soil quality (McBride et al., 1990), and water flow in a hydrogeologic environment (Dailey et al., 1992). The nondestructive quantification of soil bulk density and water content with x-ray computed tomography has shown some promise particularly for determining bulk density, but is less accurate for water content (Tollner, 1994). The intended use of near infrared light reflectance has been primarily the sensing of soil organic matter and moisture (Shonk et al., 1991; Sudduth et al., 1991; Sudduth & Hummel, 1993). Because remote sensing measures spatial information rather than point data, it can help to correct errors for input data such as precipitation or evapotranspiration (ET) resulting from point measurements. Satellite data can be used to improve the definition of soils and land covers that are needed to determine regional distributions of infiltration, ET and runoff coefficients. The most important remotely sensed satellite information for surface and subsurface hydrologists is probably the estimation of soil moisture and ET derived from satellite thermal-infrared images and/or NOAA advanced very high resolution radiometer (AVHRR) satellite data used in combination with energy balance models at the land-atmosphere interface (Carlson, 1985; Engman, 1986; Taconet et al., 1986; Ottle et al., 1989; Carlson et al., 1990; Shih & Jordan, 1993; Moran et al., 1994b; Huang et al., 1995) and the determination of effective meso-scale hydraulic properties using the inverse modeling approach combined with remotely sensed data from surface reflectance, surface temperature, and multifrequency microwave techniques (Feddes et al., 1993). Microwave techniques, particularly passive microwave measurements, have shown good correlation with ground data of surface soil moisture (Jackson & Schmugge, 1986; Wood et al., 1993; Chaturvedi et al., 1983; Schmugge et al., 1994). Ground-penetrating radar has been demonstrated to be a potential tool to nondestructively map soil layers with textural discontinuities, and also may have potential in mapping certain types of
preferential flow (Kung & Donohue, 1991; Kung & Lu, 1993). Multispectral scanning satellite data including the high spatial resolution data of SPOT and Landsat thematic mapper (TM) digital imagery have been used to diagnose general salinity problems (Everitt et al., 1977; Csillag et al., 1993; Rahman et al., 1994), differentiate general textural variation (Agbu et al., 1990b), and delineate subsurface flow systems such as recharge and discharge areas (Bobba et al., 1992; Obyedkov & Zektser, 1993).

Any attempt to model NPS pollutants with directly measured input and parameter data beyond a few thousand hectares is virtually impossible. At this scale, conventional means of measuring transport-related data are too burdensome and remote measurement techniques are currently too unreliable. The inability of remote measurement techniques to meet the demand for spatial input data by NPS pollutant modelers has resulted in the development of transport parameter estimation methods. Estimation methods include the development of transfer functions and the establishment of effective parameters.

Transfer functions relate more readily available or easy-to-measure soil properties often assembled during soil surveys to more complex, difficult-to-measure transport parameters that are needed for simulation. The most common of these pedo-transfer functions (PTFs) has as arguments basic soil data (e.g., particle-size distribution, bulk density, and organic C content) and yields as a result the water retention function or the unsaturated hydraulic conductivity function (Bouma & van Lanen, 1987). Two subdivisions of PTFs are made: class and continuous. A class PTF predicts the hydraulic characteristics of a textural class, whereas a continuous PTF predicts the hydraulic characteristics using actual measured soil data (Wosten et al., 1995). Generally speaking, class PTFs are cheap and easy to use, but their accuracy is limited. As an alternative to measured field data, the spatial distributions of input data and parameters have been estimated with the use of soil survey data in conjunction with a continuous PTF approach and applied to a solute transport model (Petach et al., 1991). A recent functional evaluation of PTFs for the estimation of soil hydraulic properties, however, has shown that greater than 90% of the variability of simulations for a map unit was due to variability in the estimated hydraulic parameters using the PTFs (Vereecken et al., 1992).

The algorithms in a deterministic model are often based on an understanding of processes at the scale of laboratory soil columns where such characteristics as hydraulic conductivity and soil water retention are well known. When applied to field scales, these characteristics are measured at numerous points in the field. It is assumed that within a particular model element the parameter is constant (i.e., continuum assumption); however, as the element size increases the assumption that a parameter is representative of the whole element becomes questionable. This is because the spatial variability is too great to be represented by a single value. In fact, even though in principle it should be possible to take enough measurements to determine the distribution of each parameter, the practicality of obtaining the required number of measurements makes it infeasible; consequently, the parameter values are often effective parameters that result in the observed input-output relationship. Effective parameters represent the input-output relationships, but the internal estimates of transport by the model
are simply values that, at the scale of integration, provide satisfactory estimates of the transport process and are not true reflections of the actual behavior or the manifestation of a physically measurable quantity (Grayson et al., 1993).

Klemes (1986) very succinctly addressed the problem of the measurement of field-scale hydrologic variables in the statement “… the search for new measurement methods that would yield area1 distributions, or at least reliable area1 totals or averages of hydrologic variables such as precipitation, evapotranspiration, and soil moisture would be a much better investment for hydrology than the continuous pursuit of a perfect massage that would squeeze the nonexistent information out of the few poor anemic point measurements . . .”

In many or even 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. Reviews of some of the soil databases (e.g., SSURGO, STATSGO, and NATSGO) available within the USA have been provided by Reybold and TeSelle (1989), Lytle (1993), and Nielsen et al. (1996, this publication); however, most of these 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 data concerning the soil properties (Wagenet et al., 1991). Bouma (1989) insightfully recognized the need for a reevaluation of the types of information collected in soil surveys to meet the quantitative requirements of environmental and agricultural management models.

**Uncertainty**

Error is inherent, unavoidable, and sometimes undetectable in environmental modeling. The existence of various errors reflects upon the uncertainty and therefore the reliability of model predictions. Uncertainty has a significant practical implication. Uncertainty poses doubt about or affirms the use of predictive outputs as a basis for policy guidance and action. Commonly, uncertainty analysis quantifies the uncertainty of an important decision or policy variable that is estimated by a mathematical model. In contaminant fate and transport modeling uncertainty analysis estimates the reliability of the cumulative distribution of model outputs so that decisions can be based on the probability that concentrations of pollutants will exceed an established regulatory threshold level.

There are several potential sources of uncertainty. Uncertainty can be due to model errors resulting from characteristic simplification of the complexities of the actual processes being described by the model. Uncertainty may arise because the model does not capture the natural variability in a parameter or variable, both in space and in time. Uncertainty also may result because the techniques for measuring or estimating the value are inexact.

The propagation of error by models is evaluated with sensitivity analysis while causes of prediction error are assessed with error or uncertainty analysis methods. Unlike sensitivity analysis which considers the sensitivity of the model output to slight changes in an input parameter or variable, uncertainty analysis considers the inherent uncertainty in model input data and the subsequent effect this uncertainty has on model prediction. A number of uncertainty methods have
been developed and applied specifically to hydrologic and water resource problems (Dettinger & Wilson, 1981; Beck, 1987; Schanz & Salhotra, 1992; Summers et al., 1993). Recently, Loague et al. (1989, 1990) and Zhang et al. (1993a) used uncertainty analysis specifically for deterministic transport models in the vadose zone.

Methods for estimating the uncertainty of model predictions from deterministic models generally fall into two major categories: Monte Carlo methods and first-order variance propagation. Monte Carlo simulations (see Zhang et al., 1993a; Bobba et al., 1995) involve the repeated sampling of the probability distribution for model parameters, boundary conditions and initial conditions; and the use of each generated set of samples in a simulation to produce a probability distribution of model predictions. Monte Carlo simulations are computationally intensive, particularly if the contaminant transport model is numerically complex. An alternative approximate technique, the Rackwitz-Fiessler method, can be used when computation times prohibit the use of Monte Carlo simulation (Veneziano et al., 1987; Schanz & Salhotra, 1992). First-order variance propagation methods such as First-Order Second-Moment (FOSM) analysis require the calculation of a deterministic output trajectory for the model followed by the quantification of the effects of various small amplitude sources of output uncertainty about the reference trajectory (Burges & Lettenmaier, 1975; Argantesi & Olivi, 1976). The application of FOSM analysis is limited to simple models that are continuous with respect to model parameters and time. Furthermore, FOSM approximation deteriorates when the coefficient of variation is >10 to 20%, which, of course, is common for soil properties in solute transport modeling (Zhang et al., 1993a).

The problem with the use of generalized rather than measured data has been the associated uncertainties. Loague (1994) concluded in his uncertainty analysis of potential groundwater vulnerability simulations with a simple index-based model that the uncertainty in the data was so great that the resulting maps of potential groundwater vulnerability and leaching assessment were actually best used as guides for data collection strategies rather than the purpose of environmental impact assessment for which they were intended. In spite of this fact, there has been a proliferation of deterministically-derived GE-based groundwater vulnerability maps at regional scales that use soil survey data as input data.

GIS

General Background

A GIS is defined by Goodchild (1993) as a “general-purpose technology for handling geographic data in digital form with the following capabilities: (i) the ability to preprocess data from large stores into a form suitable for analysis (reformatting, change of projection, resampling, and generalization), (ii) direct support for analysis and modeling, and (iii) postprocessing of results (reformatting, tabulation, report generation, and mapping).” 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 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” (Walsh, 1988).

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, during the past 10 to 15 yr analysis and modeling applications with GIS have become more prevalent, especially in the environmental assessment arena. 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 non-point source pollutant applications. Only within the past decade have soil scientists begun to use 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 groundwater and vadose zone related NPS pollutant problems.

Coupling GIS to a Model

Currently, no GIS has the data representation flexibility for space and time, together with the algorithmic capability to be able to build process-based models internally; consequently, environmental models and GIS must be coupled. Coupling can range from loose to tight coupling. A loose coupling involves a data transfer from one system to another. The GIS is used to preprocess data or to make maps of input data or model results. A majority of the applications found in the literature represent this approach because it requires little software modification. Only the file formats and the corresponding input and output routines, usually of the model, must be adapted. In a 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. An example of a tight coupling of a hydrologic model is RAISON (Lam & Swayne, 1991), which brings together a GIS, hydrologic models, spreadsheet, and expert system. The tightest coupling is an embedded or integrated system where the GIS and the model rely upon a single data manager. The coupling of software components is within a single application with shared memory rather than sharing files and a common interface. Embedded systems require a substantial amount of time and money to develop, and are usually constraining when changes are needed.

Nyerges (1993) cites four steps in coupling a model to a GIS: (i) description of the data transformations required between the data representation constructs, (ii) specifying software to export and import between the constructs, (iii)
determining whether the software can run without intervention, and (iv) setting up the transfer as bidirectional.

Model

General Background

Mathematical models integrate existing knowledge into a logical framework of rules, equations, and relationships to quantify how a system behaves (Moore & Gallant, 1991). They range from simple empirical equations such as linear regression equations to sets of complex differential equations. Models incorporate descriptions of the key processes that determine a system’s behavior with varying degrees of sophistication; however, a “good model must not only produce accurate results, but must do so for the right reasons” (Klemes, 1986). Hillel (1986) points out four principles that should guide model development: parsimony, modesty, accuracy, and testability.

Theoretically, if all essential parameters and variables of the predominant transport processes are known for every point in a soil system, then a mechanistic model of solute transport can be applied with confidence. Practically speaking, this is unlikely and has spawned an interest in stochastic models of solute transport. Nevertheless, all initial attempts at modeling NPS pollutants with GIS have used one-dimensional deterministic models and assumed that the spatial heterogeneity of the transport parameters and variables could be characterized by delineating map units assumed to be spatially homogeneous. Of course, the level of homogeneity of a given map unit depends entirely upon the degree of accuracy of measurement or estimation, and the uncertainty associated with that accuracy. The use of deterministic transport models with GIS has been justified on practical grounds based upon availability, usability, widespread acceptance, and the assumption that a heterogeneous medium macroscopically behaves like a homogeneous medium with properly determined parameters and variables.

GIS-Based Models for NPS Pollution Estimation

Deterministic, GE-based, distributed-parameter models were initially applied to the assessment of NPS pollution of surface water resources. Poiani and Bedford (1995) recently presented a cursory review of GE-based NPS pollution models emphasizing surface applications. Numerous hydrologic-water quality models of runoff and soil erosion have been used with a GIS to determine surface sources of NPS pollutants from watersheds (Pelletier, 1985; Potter et al., 1986; Oslin et al., 1988; Sivertun et al., 1988; DeRoo et al., 1989, 1992; Rudra et al., 1991; Bhaskar et al., 1992; Drayton et al., 1992; Joao & Walsh, 1992; Tim et al., 1992; Walker et al., 1992; Wolfe, 1992; He et al., 1993; Heidtke & Auer, 1993; Levine et al., 1993; Mitchell et al., 1993; Warwick & Haness, 1994) agricultural areas (Hopkins & Clausen, 1985; Gilliland & Baxter-Potter, 1987; Hession & Shanholtz, 1988. 1991; Panuska & Moore, 1991; Hamlett et al., 1992; Lee & White, 1992; Geleta et al., 1994; Tim & Jolly, 1994) and urban areas (Smith & Brilly, 1992; Smith, 1993; Ventura & Kim, 1993). In addition, several groundwater models have been coupled to a GIS to simulate water flow and/or NPS pol-
lutants in aquifers (Kernodle & Philip, 1989; Baker & Panciera, 1990; Hinaman, 1993; Roaza et al., 1993; El-Kadi et al., 1994; Darling & Hubbard, 1994). Integrated surface and groundwater hydrologic models have been coupled to a GIS with the vadose zone either grossly simplified or completely ignored (Powers et al., 1989; Ross & Ross, 1989; Ross & Tara, 1993; Preti & Lubello, 1993). GIS also has been coupled to a simple functional model of recharge to map a regional assessment of relative potential recharge to the Floridan aquifer (Boniol et al., 1993).

Historically, three general categories of deterministic models have been coupled to GIS to estimate NPS pollution in the vadose zone: regression models, index models, and transient-state solute transport models. Regression models have generally used multiple linear regression techniques to relate various soil properties or conditions to groundwater vulnerability or to the accumulation of a solute in the soil root zone (Corwin et al., 1988, 1989; Corwin & Rhoades, 1988). Index models refer to those models generally used to assess potential groundwater pollution hazard with some calculated index generated from either a simple functional model of steady-state solute transport (Merchant et al., 1987; Khan & Liang, 1989; Evans & Myers, 1990; Halliday & Wolfe, 1991; Rundquist et al., 1991) or a steady-state mechanistic model (Wylie et al., 1994). Transient-state solute transport models include both stochastic and deterministic models capable of handling the movement of a pollutant in a dynamic flow system. The most recent progress has occurred in the coupling of transient-state solute transport models to GIS (Bleecker et al., 1990; Petach et al., 1991; Corwin et al., 1993a,b; Tiktak et al., 1996, this publication; Vaughan et al., 1996, this publication).

The first applications of GIS for assessing the impact of NPS pollutants in the vadose zone occurred in the late 1980’s. Corwin et al. (1988), Corwin and Rhoades (1988), and Corwin et al. (1989) delineated areas of salinity accumulation in the vadose zone by coupling a GIS of the Wellton-Mohawk Irrigation District to a phenomenological model of salinity development. GIS also has been used for assessing groundwater pollution potential by coupling to a weighted-index site assessment method such as DRASTIC or Seepage or others (Merchant et al., 1987; Evans & Myers, 1990; Regan, 1990; Halliday & Wolfe, 1991; Munnink & Geirnaert, 1991; Rundquist et al., 1991; Hendrix & Buckley, 1992; Richert et al., 1992; Zhang et al., 1993b; Hammen & Gerla, 1994; Kellogg et al., 1994; Smith et al., 1994); and to simple index-based models such as Rao et al.’s (1985) Attenuation Factor model (Khan & Liang, 1989), Shaffer et al.’s (1991) NLEAP model (Wylie et al., 1994; Shaffer et al., 1996, this publication), and Meeks and Dean’s (1990) Leaching Pesticide Index model (Pickus et al., 1993). All of these approaches, however, assume steady-state conditions. Furthermore, the DRASTIC index has been shown to be uncorrelated with the movement of pesticides into and through the soil, and neglects differences in adsorption, solubility and degradation of different pesticides under different climatic and soil management regimes (Banton & Villeneuve, 1989). Subsequently, Bleecker et al. (1990), Petach et al. (1991), Corwin et al. (1993a,b), and Scott et al. (1994) used transient-state solute transport models coupled to a GIS to assess the leaching potential of some common NPS agricultural chemicals under dynamic flow conditions; however, the work of Bleecker et al. (1990) and Petach et al. (1991) did
not use field measurements of input parameters and variables to calibrate their model LEACHM, nor did Scott et al. (1994) for Nofziger and Horsby’s (1986) CMLS piston-displacement model of pesticide transport. Rather, the input data were generalized from sources such as Soil Conservation Service soil survey maps. Hutson (1993), Hutson and Wagenet (1993), and Bleecker et al. (1995) have expanded upon the previous work of Petach et al. (1991).

The experimentation and associated spatial data to test the results of these GIS-based NPS pollutants models have been essentially nonexistent. Corwin et al. (1989) provided a traditional nonspatial statistical analysis of measured and predicted results by separating a data set of measured soil root zone salinities into two subsets; using one data set for model development and calibration, and the other for model validation. The resultant statistical analysis showed a linear regression between measured and predicted values with a slope of 1.0 and y-intercept of zero, but an $R^2 = 0.80$. This is one of the few such evaluations. Typically most models used to simulate NPS pollutants have not been rigorously validated. For example, rating maps of soil nitrate leaching potential have been created using LEACHM-N and NLEAP by Khakural and Robert (1993). Both models were tested but only using data from a lysimeter study (Khakural & Robert, 1993). Rogowski (1993) compared simulated spatial distributions of recharge flux based on actual measurements of hydraulic properties to simulations based on soil survey data. Considerable discrepancies were found. Even though the comparison was not a validation of the recharge model, it did question the reliability of simulations based solely on soil survey data or solely on measured data. Nevertheless, actual data has the advantage that spatial correlations and cross correlations can be examined that can introduce a measure of confidence into the GIS-based predictions (Rogowski, 1993). The most significant studies to evaluate the potential reliability of using GIS-based NPS pollutant models with non-measured input data (i.e., input data estimated from pedo-transfer functions or obtained directly from soil survey data) have come from uncertainty studies conducted by Loague and colleagues (Loague et al., 1989; Loague & Green, 1990; Loague et al., 1990; Loague, 1991; Loague, 1994). Loague and colleagues ultimately showed that the “best use of the regional scale chemical leaching assessments based upon modeling approaches as simple as index methods is for guiding data collection strategies” (Loague, 1994).

The purpose for coupling a GIS to a solute transport model is to provide decision makers with a tool for attaining sustainable agriculture. Economic concerns are as crucial a component in sustainable agriculture as environmental impact. To account for economic concerns, Opaluch and Segerson (1991) have incorporated a microparameter distribution model for simulating economic responses to alternative agricultural management policies into a GIS. This enables the development of aggregate farm management policy while maintaining a focus on the site-specific aspect of groundwater contamination. The physical characteristics affecting pollution potential were summarized by a single statistic, a DRASTIC score; however, the relationship between pollution and such factors as soil characteristics and management practices could have been determined with a number of other models (e.g., LEACHM or others).
OVERCOMING THE INHERENT LIMITATIONS OF COUPLING GIS TO A DETERMINISTIC MODEL

The coupling of GIS to deterministic models for simulating NPS pollutants provides a means of storing, manipulating, and displaying complex data efficiently and cost-effectively beyond any previous approach. When GIS is coupled to a deterministic model, the mapping capabilities of GIS greatly enhance the time for data preparation and presentation; however, these GIS-related features do not enhance nor do they diminish the fundamental applicability of the model (Grayson et al., 1993). GIS does not by itself solve many of the problems related to the modeling of NPS pollutants including the temporal and three-dimensional measurement or estimation of essential transport-related parameters and variables; the uncertainty of these parameter or variable measurements and subsequent error propagation; the limitation of the current knowledge regarding basic transport processes and how to conceptually model them, most notably preferential flow; and the spatial scale dependence of solute transport processes. Each of these problems is related to the complex spatial heterogeneity of soil and each imposes a limitation on the modeling of NPS pollutants with GIS. Nevertheless, many uninformed users are so seduced by the ease of data manipulation and interpolation within the GIS that a notion is created that a GIS can be used to generate information (Vanderbroucke & Orshoven, 1991).

There are fundamental problems in the application of deterministic models, particularly physically-based mechanistic models, for practical predictions of NPS pollutants at various georeferenced scales. These problems result from limitations in the mathematical representations of complex transport processes in a heterogeneous media, the lack of cost-effective parameter measurement methods-instrumentation that are capable of establishing effective parameters at both local and field scales, and a recognition of the reliability of the simulated output. Beven (1989a) concluded that the development and application of deterministic hydrologic models must take account of the need for “...closer correspondence in scale between model predictions and measurements; closer correspondence between model equations and field processes; and the rigorous assessment of uncertainty in model predictions.” Decisions regarding the appropriate level of sophistication in the simulation model must consider the scale at which the model is being applied and the nature of the available environmental data at that scale. Quantitative comparisons between different types of models using standardized data is an important component of model selection. Measurement and monitoring methods need to be compatible with the spatial and temporal scales being modeled.

Hillel (1986) noted that, “Modelers often develop a vested interest in the success of their own creations and hence are in constant danger of losing their objectivity, like the mythic King Pygmalion who fell in love with his own Galatea.” This is nowhere more apparent than in the application of highly sophisticated, parameter-intensive, deterministic-numerical models to NPS pollutant problems where minimal data is available. Part of the problem lies in the notion that sophisticated numerical models are better because of their increased com-
plexity. In fact, model sophistication, and the intensity and accuracy of spatial data must be compatible with the intended application of the model that dictates the scale and accuracy requirements (Grayson et al., 1993). As pointed out in papers by Wagenet (1993), and Wagenet and Hutson (1995, 1996) concerning scale and hierarchical theory, most leaching models have been developed at one scale, but are applied at a different scale. Generally, models are up-scaled, i.e., developed at the laboratory column scale and applied at the pedon, field, farm, catchment, or regional scales. Conceptually, up-scaling of leaching models is allowed “as long as model assumptions are made to condense the lower scale dynamics into appropriate formulations of models that apply to higher hierarchical levels” (Wagenet & Hutson, 1996).

The following pragmatic set of guidelines is suggested to maximize the strengths and minimize the limitations of modeling NPS pollutants with deterministic models coupled to a GIS. First, to minimize scaling problems the model complexity and parametric data should be in agreement with the intended application. Two basic steps can assist in establishing this agreement:

Step 1: Based upon the intended application determine the appropriate scale (e.g., pedon, field, farm, catchment, regional, and global) and the required accuracy of the simulated output.

Step 2: Select or design a model that is appropriate for the determined scale so that all dominant transport processes are represented while those processes that are no longer of significance within the established spatial and temporal scales are ignored.

Second, to minimize the cost of expensive data collection perform a sensitivity analysis to determine the most and least sensitive parameters or variables. The most sensitive parameters or variables should be measured and the least sensitive can be estimated. Third, perform an uncertainty analysis using Monte Carlo simulations or First Order Uncertainty Analysis to determine the reliability of the simulated output. Maps of associated uncertainty will assist in avoiding the pitfall of false confidence created by the GIS visualizations. Finally, problems such as inadequate representation of the transport processes and possible discrepancies between measurement and model scale may mean that some calibration is required. This should be regarded as a selective improvement process for initial parameter estimates based upon discrepancies between observed and simulated outputs. Great emphasis should be placed on physical reasoning to guide this trial-and-error calibration. If calibration is necessary, then an estimation of uncertainty can be made using Generalized Likelihood Uncertainty Estimation (see Beven, 1989b; Binley & Beven, 1991).

CURRENT ADVANCES AND AREAS OF FUTURE STUDY

During the past half century the preponderance of solute transport models for the vadose zone have not incorporated spatial processes, but rather have consisted of one-dimensional, deterministic models. This situation can be traced to three principal reasons: (i) the computational complexity of spatial processes, (ii)
a broad range of scaling problems, and (iii) the relative paucity of statistical theory and methods for dealing with spatial data. Though currently less formidable, these three barriers still linger; however, impending advances will significantly diminish or even eliminate their influence. Traditionally, simulations of data-parallel contingent processes, such as contaminant transport, have been performed on computers based on the sequential operation of the von Neumann architecture. The characteristic behavior of spatial simulation with its multiple contingently-interacting scales and multiple temporally-nested processes will continue to present a significant computational problem until the impending use of parallel processors attenuates imposed constraints. In addition, GIS has emerged as a viable tool for dealing with spatially-related environmental problems. In fact, the current trend in GIS software is for the user to be able to customize the GIS to fit the desired application. The recent introduction of GIS software such as ArcView\textsuperscript{1} by ESRI\textsuperscript{1} demonstrates the desire of commercial GIS software vendors to provide the user with sufficient tools to develop their own application-oriented GIS software within a desktop computer environment. The introduction of this type of software will undoubtedly hasten the future development of tightly-coupled, GIS-based models. Concomitantly, a sound theoretical approach for rescaling is essential for simulation models to effectively exploit the potentially data-rich technologies of remote sensing and GIS. Currently, an active area of research concerns the scaling of data and processes to reflect varying degrees of spatial, temporal, and functional resolution (Rosswall et al., 1988; King, 1991). Finally, the development of statistical estimation and inference procedures dealing with spatial data has gained profound momentum (Ripley, 1988; Cressie, 1991; Journal, 1996, this publication).

Three areas of intensified research are needed to enhance the capability of modeling NPS pollutants in the vadose zone: (i) more cost-effective and efficient methods and instruments for measuring transport parameter or variable data at an increased resolution, (ii) a knowledge of the uncertainties associated with the visualized results generated from transport models coupled to a GIS, and (iii) further research into those mechanisms involved in solute transport in the vadose zone that are not clearly understood (e.g., preferential flow).

Reliable and cost-effective approaches for measuring the spatial distribution of transport parameters and variables have not kept pace with developments in solute transport modeling or GIS applications to NPS pollutants. 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. Because of this lag, the thirst for data essential to model NPS pollutants has driven researchers to develop transfer functions which utilize basic soil properties to derive sophisticated transport parameters. This has resulted in a low level of success due to the extreme uncertainty associated with the estimated transport data. The need for direct measures of transport parameters and variables with remote instrumentation cannot be

\textsuperscript{1}Trade names and company names are included for the benefit of the reader and do not imply any endorsement or preferential treatment of the product by the author or the USDA-ARS.
stressed enough. The greatest progress needs to be made in the area of instrumentation.

Currently, GIS applications for the modeling of NPS pollutants have burgeoned to a point where generated maps of groundwater pollution vulnerability and of solute accumulation in the vadose zone may be creating a false sense of confidence in the information for nontechnical decision makers. The nontechnical decision makers who rely upon the display maps of NPS pollution are visually seduced into accepting as absolute the boundary lines between innocuous and toxic zones of contamination. This can lead to misguided decisions that may unfairly discriminate against manufacturers of an acceptable product or practitioners of an acceptable resource management strategy, while potentially overlooking those products and individuals responsible for environmental degradation (Loague, 1994). As suggested by Loague (1994), associated maps of uncertainties need to accompany pollution hazard assessment maps to reduce the risk associated with decisions based upon models.

Even though the fate and movement of solutes in the vadose zone have been intensively studied since the 1950s there are still gaps in our understanding of basic processes involved in solute transport within the vadose zone. In particular, the inability to model preferential flow poses a significant challenge to soil physicists. It is well known that preferential flow can be responsible for the rapid movement of usually small volumes of pollutants which are potentially high in concentration. This can occur for both point or non-point sources. Preferential flow can result in nearly a direct movement of the pollutant at its original concentration, though at a much reduced volume, from the soil surface to the groundwater. It is this rapid movement of low volumes of a pollutant at high concentration that poses the greatest threat to groundwater systems.

SUMMARY

Because of the spatial heterogeneity of the earth’s surface and subsurface soil, and the complexity of the processes involved in solute transport within the vadose zone, a multidisciplinary approach is required to simulate the environmental impacts of NPS pollutants upon soil and water resources from a local to a global scale. The knowledge and information required to assess the impact of NPS pollutants upon soil and water resources crosses several subdiscipline lines including spatial statistics, remote sensing, GIS, hydrology, and soil science; therefore, integrated methodologies are required.

The development of GIS-based deterministic models is a significant step in the integrated environmental assessment of NPS pollutants; however, the proliferation of GIS-based deterministic models for simulating NPS pollutants in surface and subsurface soil and water systems is cause for both optimism and caution. Developing technologies, like GIS and remote sensing, are catalysts for innovative approaches to heretofore unsolvable problems. If nothing else, new technologies spawn innovation by inspiring unconventional applications of the newly developed technology. GIS can serve as the catalyst to bring transport modeling, data acquisition and spatial statistics into a self-contained package to address NPS pollution problems. On a more pessimistic note, GIS can create the
illusion of legitimacy by making the package more appealing than the contents warrant. In addition, GIS reduces variation by providing lines of delineation between properties that are fuzzy in reality. Caution must be taken not to fall into the trap of allowing GIS to create black-and-white pictures of the impact of NPS pollutants upon the environment. Concomitantly, models, though intrinsic to the scientific method, should not supplant observation, but rather complement observation. Even though the misinterpretation and misuse of models may be an expected consequence of differences in the nature of the ventures of science and professional practice as pointed out by Philip (1991), the application of environmental models should augment and not replace actual observation regardless of the user.

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