5

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

Dennis L. Corwin

USDA-ARS, U.S. Salinity Laboratory
Riverside, California

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

---

Application of GIS to the Modeling of Non-Point Source Pollutants in the Vadose Zone, SSSA Special Publication 48.

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, 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 useable form for making decisions in the environmental policy arena (Beven, 1989a; Grayson et al., 1992).

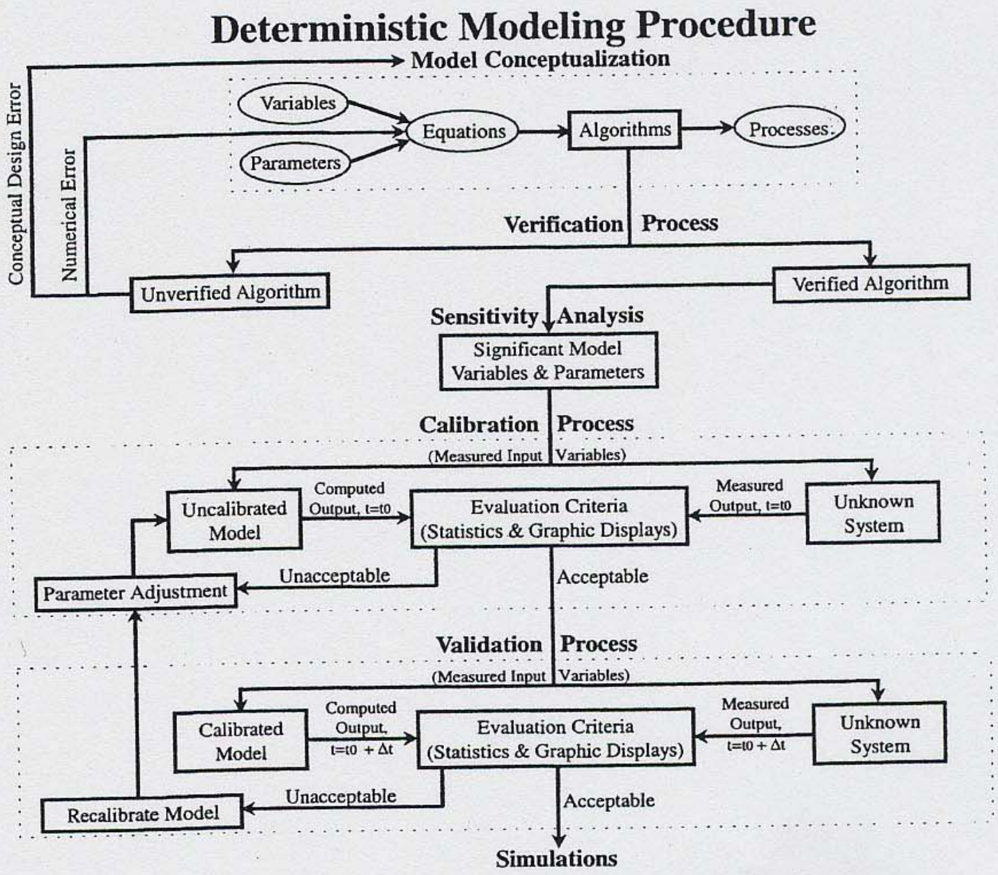

Fig. 5–1.Schematic of the deterministic modeling procedure (based on Donigan & Rao, 1986; Loague, 1993).

Table 5–1.Definition of modeling terms for environmental chemical fate models proposed in American Society for Testing and Materials' *Standard Practice for Evaluating Environmental Fate Models of Chemicals* (American Society for Testing and Materials, 1984) and by Bobba et al. (1995).

Algorithm:	A sequence of statements of computer code comprising the numerical technique representing an individual process of an environmental system.
Calibration:	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.
Model:	An assembly of concepts in the form of a mathematical expression comprised of variables, andparameters that portrays understanding of a natural phenomenon.
Parameter:	A constant with variable values.
Sensitivity:	The degree to which the model result is affected by changes in a selected input parameter or variable.
Uncertainty:	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).
Validation:	Comparison of model results with numerical data independently derived from experiments or observations of the environment.
Verification:	Examination of the algorithm to ascertain that it represents the conceptual model and that there are no inherent numerical problems.

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.

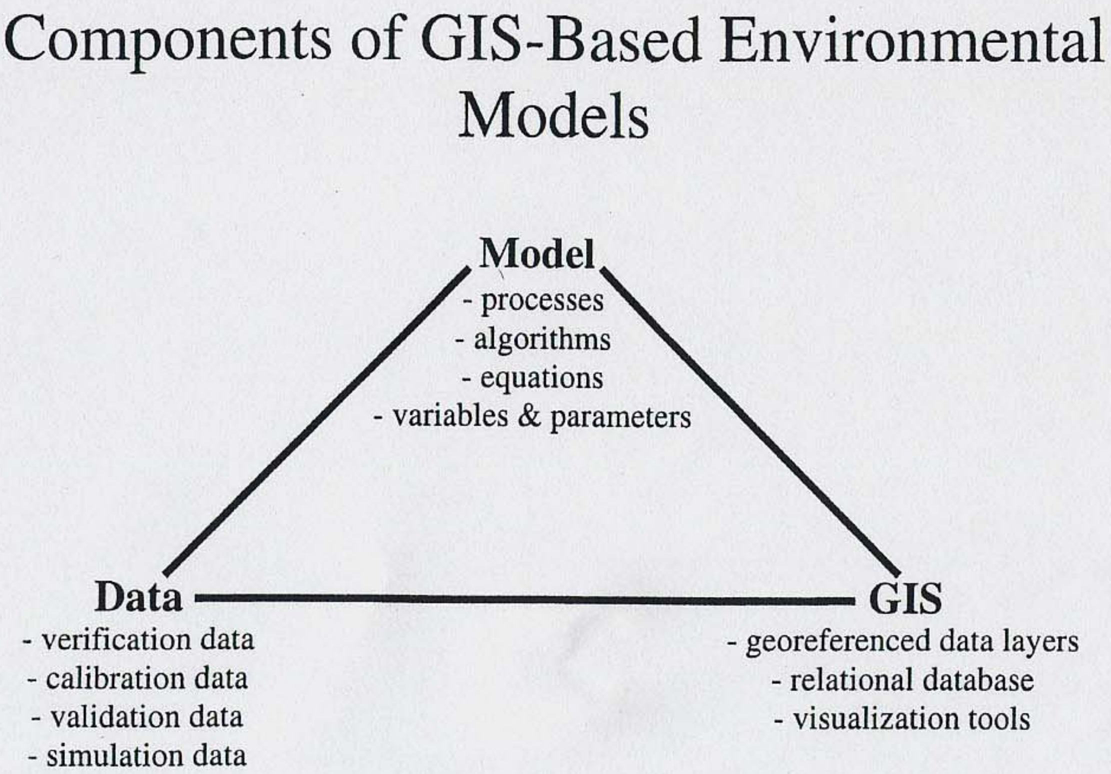

Fig. 5–2.Components and subcomponents of GIS-based environmental models (based on Burrough, 1996).

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 intensiveness 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 dispersivitiy, 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 determination 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 Wagenet & 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 al., 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