

# MODELING NON-POINT SOURCE POLLUTANTS IN THE VADOSE ZONE USING GIS

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## NON-POINT SOURCE POLLUTION: DEFINITION, SOURCES, SIGNIFICANCE, GLOBAL IMPACT, AND JUSTIFICATION FOR MODELING

Non-point source (NPS) pollutants are defined as “contaminants of [air, and] surface and subsurface soil and water resources that are diffuse in nature and cannot be traced to a point location” (1). Characteristically, NPS pollutants (1) are difficult or impossible to trace to a source; (2) enter the environment over an extensive area; (3) are related, at least in part, to certain uncontrollable meteorological events, and existing geographic and geomorphologic conditions; (4) have the potential for maintaining a relatively long active presence in the global ecosystem; and (5) may result in long-term, chronic effects on human health, and soil-aquatic degradation (2). The most common global NPS pollutants of soil and groundwater resources include biosolids and manure, persistent organic pollutants (POPs), nutrients (e.g., nitrates and phosphates), salinity, toxic heavy metals (e.g., Bi, Co, Sn, Te, Ag, Pt, Tl, Sb, Hg, As, Cd, Pb, Cr, Ni), trace elements (e.g., Se, B, Mo, Cu, Zn), and pathogens.

Often, NPS pollutants occur naturally, such as salts and trace elements in soils, or are the consequence of direct application by humans (e.g., pesticides and fertilizers), but regardless of their source, they are generally the direct consequence of human activities including agriculture, urban runoff, feedlots, hydromodification, and resource extraction (2). Specific sources of NPS pollutants include (1) excess fertilizers, herbicides, and insecticides from agricultural lands and residential areas; (2) oil, grease, and toxic chemicals from urban runoff and energy production; (3) sediment from improperly managed construction sites, crop and forest lands, and eroding stream banks; (4) naturally occurring salts and trace elements from irrigation practices; (5) acid drainage from abandoned mines; (6) pathogens (i.e., viruses and bacteria) and nutrients from livestock, and pet wastes; and (7) atmospheric deposition (2).

The significance of NPS pollutants as an environmental issue stems from their potential global impact and resultant chronic effects on human health. Because of their widespread use and often persistent and mobile nature, NPS pollutants have the capacity not only to injure the

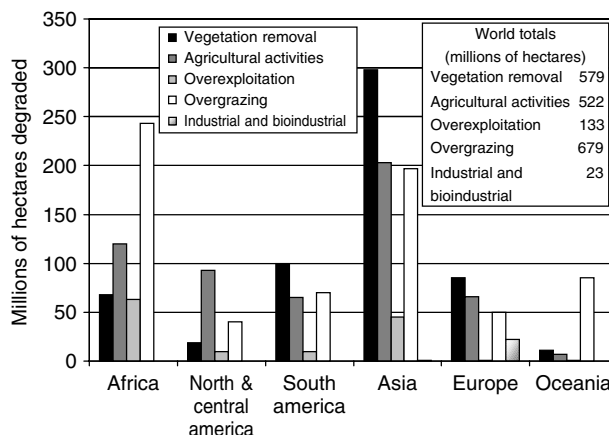


Figure 1. Human-induced soil degradation by region and by cause from 1945 to the late 1980s. Source: Ref. 7. With permission.

surrounding environment and ourselves, but also remote environments and their inhabitants (like the Arctic) and future generations of humans through the buildup of persistent toxic substances that mimic and disrupt human hormone systems (3). The impact of NPS pollutants on soil and water resources extends over millions of hectares of land and billions of liters of water. Throughout the world, 30% to 50% of Earth’s land is believed to be affected by NPS pollutant degradation from erosion, fertilizers, pesticides, organic manures, and sewage sludge (4). Worldwide, NPS pollutants are recognized as the major contributors to surface and groundwater contamination (5), with agriculture as the single greatest contributor of NPS pollutants (6). Agricultural activities result in the movement of NPS pollutants from the soil surface into rivers and streams via runoff and erosion, and into subsurface soil and groundwater via leaching through the vadose zone (i.e., the portion of the soil extending from the soil surface to the groundwater table). Figure 1 reflects the worldwide extent of human-induced degradation of soil by region and by cause over the period 1945 to the late 1980s.

The world’s population has doubled since 1950 and is expected to range from 8 to 12 billion in 2050. Barring unexpected technological breakthroughs, sustainable agriculture is viewed as the most viable means of meeting the food demands of the projected world’s population. The concept of sustainable agriculture is predicated on a delicate balance of maximizing crop productivity and maintaining economic stability while minimizing the utilization of finite natural resources and the detrimental environmental impacts of associated NPS pollutants. Assessment of NPS pollutant impacts on soil-groundwater systems at local, regional, and global scales is a key component to achieving sustainable agriculture. Assessment provides the means (1) to establish the true extent of the NPS-pollution problem, (2) to evaluate mitigating management practices and regulatory policies, and (3) to predict future potential problems. The distinct

advantage of prediction is that it can alter the occurrence of detrimental conditions before they occur. The reasons for modeling NPS pollutants in the vadose zone are (1) to increase the understanding of cause-and-effect relationships of spatiotemporal processes occurring in soil systems and (2) to provide a cost-effective means of synthesizing the current level of knowledge into a useable form for making environmental policy decisions (8,9).

## MULTIDISCIPLINARY NATURE OF MODELING NPS POLLUTANTS IN THE VADOSE ZONE

Modeling NPS pollutants in the vadose zone is a complex environmental problem that requires a multidisciplinary, systems-based approach taken within a spatial context with an awareness of scale (10). The formidable barriers to modeling NPS pollutants are the consequence of the complexities of geographic scale and position; the complexities of the physical, chemical, and biological processes of solute transport in porous media; and the spatial complexities of the soil media's heterogeneity. The knowledge, information, and technology needed to address each of these issues crosses several subdisciplinary lines, including classic and spatial statistics, remote sensing, geographic information systems (GIS), surface and subsurface hydrology, soil science, and space science. Spatial statistics is useful in dealing with the uncertainty and variability of spatial information (11); remote sensing provides measurements of physical, chemical, and biological properties needed in environmental models (12); GIS is a means of organizing, manipulating, storing, and displaying spatial data (13); and water flow and solute transport models developed within soil science and hydrogeology are the tools for simulating future scenarios to assess potential temporal and spatial changes (2,14). Precise geographic location and areal extent are captured with the space science technology of the global positioning system (GPS).

## COMPONENTS OF A NPS POLLUTANT MODEL

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/variable must be simulated, measured, or estimated, which creates a tremendous volume of spatial information because of 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 essential components of modeling NPS pollutants consist of (1) a *model* of solute transport and/or accumulation, (2) input and parameter *data* for the model, and

(3) a *GIS* to handle the input, manipulation, and output of spatial data. Figure 2 shows the interaction among these three basic components based on flow of information.

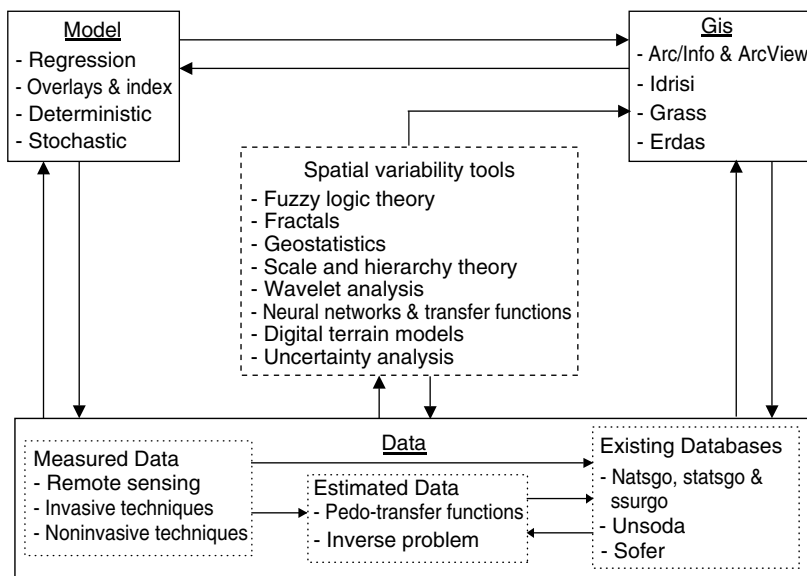
Because of the complex spatial heterogeneity of the vadose zone, a variety of sophisticated techniques are useful as tools to deal with the vicissitudes of soil (Fig. 2). Fuzzy logic theory provides a means of handling vague and imprecise data whether as a means to characterize map units or transitional boundaries between map units (16,17). Fractal geometry with its scale independence may offer a means of bridging a variety of gaps related to spatial variability from determining the predictability of complex spatial phenomena such as solute transport to relating difficult-to-measure soil hydraulic properties to other soil variables available from soil surveys (18). Geostatistics is useful in interpolating sparse spatial data and providing associated uncertainty (19). Hierarchical theory establishes an organizational hierarchy of pedogenetic modeling approaches and their appropriate scale of application (20,21). Wavelet analysis provides a means of determining spatial scales and the dominant processes at those scales (22,23). Neural networks and transfer functions provide a means of deriving complex hydraulic parameters from easily measured data (24). Digital terrain or digital elevation models (DEM) provide spatial geomorphologic information. Uncertainty analysis serves as a means of establishing the reliability of simulated model results based on model errors and data uncertainties (25).

## Data

The effectiveness of a model to simulate a practical application is highly dependent on how well model inputs and model parameters are identified. Basically, three sources of input and parameter data for NPS pollutant models exist (15): (1) measured data, (2) estimated data, and (3) existing data. Each source of data carries distinct advantages and limitations.

A review of current measurement techniques to determine flow-related properties of subsurface porous media and soil physical properties is provided by Dane and Molz (26) and Topp et al. (27), respectively. Although direct measurement of transport parameters and variables is the most reliable means of obtaining accurate information for modeling purposes, it is also the most labor intensive and costly. A quick and easy means of obtaining these measurements is crucial to the cost-effective modeling of NPS pollutants. Remote sensing and noninvasive measurement techniques have the greatest potential for meeting the thirst for measured spatial data.

Corwin (28) provided a cursory review of some instrumental techniques developed for the remote and noninvasive measurement of variables and parameters found in transport models for the vadose zone. The review covers geophysical resistivity methods, aerial photography, x-ray tomography, ground-penetrating radar, magnetic resonance imaging, microwaves, multispectral imagery, thermal infrared imagery, and advanced very-high-resolution radiometry (AVHRR). Barnes et al. (12) provided a more recent review of remote- and ground-based sensor technology for mapping soil properties.



**Figure 2.** Integrated components of a GIS-based NPS pollutant model system. Arrows show the flow of information. Modified from Ref. 15. With permission.

Even though considerable progress has been made over the past decade, the remote sensing instrumentation needed to measure *all* parameters and variables in even the simplest of transport models, for the vadose zone is not available or even on the drawing board. In most cases, remote sensing provides measurements of only the top few centimeters; consequently, it suffers from a lack of *depth information* needed in modeling the vadose zone. Noninvasive techniques such as electromagnetic induction (EMI) can provide information down to several meters in depth, but these techniques generally require measurements taken at or near the soil surface and their measurement volume is limited to tens of cubic meters or less. Nevertheless, geospatial measurements of apparent soil electrical conductivity ( $EC_a$ ) with EMI is currently the most widespread and reliable means of characterizing the spatial variability of a variety of physicochemical properties in the vadose zone including salinity, texture, water content, cation exchange capacity (CEC), organic matter (OM), and bulk density (29). Furthermore, in most cases, the parameters measured by remote sensing and noninvasive techniques are often not directly applicable to solute transport models. For instance, the use of EMI to measure soil salinity is not a direct measure of salinity in the soil solution, but rather it measures  $EC_a$ , which includes the conductivity of both the solid and liquid phases, thereby requiring ground-truth soil samples for calibration.

The extreme spatiotemporal variability and the non-linearity of many soil processes make parameterization of landscape-scale models a daunting task. The inability of remote measurement techniques to meet the demand for spatial and temporal parameter and input data has resulted in the development of transport parameter estimation techniques that estimate parameters by fitting data or are based on the formulation of transfer functions. Inverse modeling is a powerful and practical means of estimating flow and transport parameters for landscape-scale

solute transport models using advanced optimization algorithms. Transfer functions relate readily-available and easy-to-measure soil properties to more complex transport variables/parameters needed for simulation.

Corwin et al. (15) provide a referenced list of the estimation methods for many common parameters in solute transport models of the vadose zone. The most common transfer function, the pedo-transfer function (PTF), uses particle-size distribution, bulk density, and soil organic-carbon content to yield soil-water retention or unsaturated hydraulic conductivity functions. Rawls et al. (30) provide a review of soil-water retention estimation methods. Reviews of methods of estimating soil hydraulic parameters for unsaturated soils have been written by van Genuchten et al. (31).

In most instances, limited resources do not permit the measurement or even estimation of needed input or parameter data. In these instances, the use of existing data is crucial. Existing soil databases for the United States include SSURGO (State Survey Geographical Database; <http://www.ncg.nrcs.usda.gov/ssurgo.html>), STATSGO (State Soil Geographical Database; <http://www.ncg.nrcs.usda.gov/statsgo.html>), and NATSGO (National Soil Geographical Database; <http://www.ncg.nrcs.usda.gov/natsgo.html>). SSURGO (map scale ranges from 1:12,000 to 1:63,360) is a county-level database, and it is the most detailed GIS database available from NRCS. STATSGO (map scale 1:250,000) is the state-level database designed for state, large watershed, and small river basin purposes. NATSGO (map scale 1:7,500,000) is the national soil database whose map units are defined by major land resource area (MLRA) and land resource region (LRR) boundaries.

The problem with the use of generalized rather than measured data has been associated uncertainties. Loague et al. (32) extensively reviewed the uncertainty associated with the use of an existing database for non-point source groundwater vulnerability and concluded that assessments based on this type of data are relegated to guiding

data collection strategies rather than their intended purpose of groundwater vulnerability assessment. Measured input data that captures natural variability both in space and time is essential for diminishing uncertainty in simulations.

## GIS

A GIS is defined by Goodchild (33) 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 that characterizes the full information content of the spatially variable data required by solute transport models. The advantages of GIS include (1) ease of data retrieval; (2) ability to discover and display information gained by testing interactions between phenomena; (3) ability to synthesize large amounts of data for spatial examination; (4) ability to make scale and projection changes, remove distortions, and perform coordinate rotation and translation; and (5) capability to discover and display spatial relationships through the application of empirical and statistical models (34). The principal benefit of coupling GIS to subsurface hydrologic models is to enable the models to deal with large volumes of spatial data that geographically anchor many environmental processes.

## Model

A review of GIS-based NPS pollutant modeling in the vadose zone has been presented by Corwin et al. (15). To date, most models of NPS pollutants in the vadose zone have used deterministic models of solute transport coupled to a GIS (15,28). However, a growing recognition exists that stochastic approaches may offer the most viable means of modeling an NPS pollution (35).

The use of deterministic transport models with GIS has been justified on practical grounds based on availability, usability, widespread acceptance, and the assumption that a heterogeneous medium macroscopically behaves like a homogeneous medium with properly determined parameters and variables. The philosophy of modeling NPS pollutants in the vadose zone with a one-dimensional deterministic model of solute transport is based on the representation of physical, chemical, and biological properties influencing transport in the vadose zone with a distributed parameter structure. The validity of the assumption that a heterogeneous medium macroscopically behaves like a homogeneous medium depends on whether spatial domains can be defined and characterized that behave as stream tubes or “representative element volumes” (REV).

Three categories of deterministic models have been coupled to GIS to simulate NPS pollution in the vadose zone: regression models, overlay and index models, and transient-state solute transport models (15). Regression

models have generally used multiple linear regression techniques to relate various causative factors to the presence of an NPS pollutant. These causative factors have included soil properties or conditions related to groundwater vulnerability or to the accumulation of a solute in the soil root zone. Overlay and index models refer to those models that compute an index of NPS pollutant mobility from a simple functional model of steady-state solute transport. Two types of overlay and index models have been developed: property-based and process-based. Property-based index models are established on a hydrogeologic setting (e.g., DRASTIC) or NPS pollutant properties (e.g., GUS). Process-based index models are founded on the characterization of transport processes (e.g., Rao’s attenuation factor model). Overlay and index models have been used largely to assess groundwater pollution vulnerability to pesticides and nitrates. Transient-state, process-based solute transport models include deterministic models capable of handling the movement of a pollutant in a dynamic flow system. Transient-state, process-based models describe some or all of the processes involved in solute transport in the vadose zone: water flow, solute transport, chemical reactions (adsorption-desorption, exchange, dissolution, precipitation, etc.), root growth, plant-water uptake, vapor phase flow, degradation, and dispersion/diffusion.

Jury (36) pointed out that the difficulty of constructing a three-dimensional model of chemical transport as a consequence of field variability has two significant implications: (1) Any hope of attempting to estimate a continuous spatial pattern of chemical transport must be abandoned; and (2) a possibility exists of extreme deviations from average movement so that significant concentrations of chemical may flow within relatively small fractions of the total cross-sectional area, which may be nearly impossible to detect from point measurements. The latter implication has fostered the development of stochastic solute transport models for the vadose zone as opposed to deterministic models.

Two distinct stochastic approaches are currently in use for dealing with the spatial variability encountered in modeling NPS pollutants in the vadose zone: geometric scaling and regionalized variables. Jury (36) indicates that geometric scaling uses specific “standardized variables to scale the differential equations describing transport and relates the standardized variables to some measurable or definable property of each local site of a heterogeneous field.” Once the variables are defined, the onerous task of characterizing the variability is reduced to determining the statistical and spatial distribution of these scaling parameters. In contrast, Jury (36) explains that the regionalized variable approach regards the “various parameters relevant to a field-wide description of transport as random variables characterized by a mean value and a randomly fluctuating stochastic component.”

In comparison with deterministic models, the coupling of a stochastic solute transport model to GIS is less explored. In a paper discussing the potential compatibility of stochastic transport models with GIS, Jury (35) suggested that stochastic-convective stream tube modeling seems the most compatible with GIS because it “utilizes

a relatively simple local process driven by parameters that might be associated with soil morphological features, and could be integrated up to a large scale by simple arithmetic averaging over the local sites." A stochastic stream tube model is made up of parallel, noninteracting one-dimensional soil columns whose properties are locally homogeneous, but vary from one soil column to the next. The collection of all stream tubes constitutes the field-, basin-, or regional-scale area being represented. This approach is in essence the same approach that has been undertaken in the past where deterministic piston-flow local transport models have been coupled to soil survey information; only now there is an associated stochastic component of information. Jury (35) warns that the challenge of this approach will be "to develop a reasonable local-scale model whose parameters can be related to identifiable local-scale features."

### CONSIDERATION OF SCALE WHEN MODELING NPS POLLUTANTS

Scale, as used in soil science and hydrology, refers to the "characteristic length in the spatial domain" and to the "characteristic time interval in the temporal domain" (37). So, even though space and time are continuous, only a discrete set of scales is of interest based on specific features that make them of particular use or interest (37). The existence of a hierarchy of scales has been postulated to relate to spatial or temporal features of systems of interest (see Fig. 3).

Temporal and spatial scales dictate the general type of model. The consideration of scale in model development requires observed information for the real system being

modeled at the spatial and temporal scales of interest, which is to say that microscopic-scale models developed in the laboratory are not appropriate for macroscopic-scale applications, and vice versa.

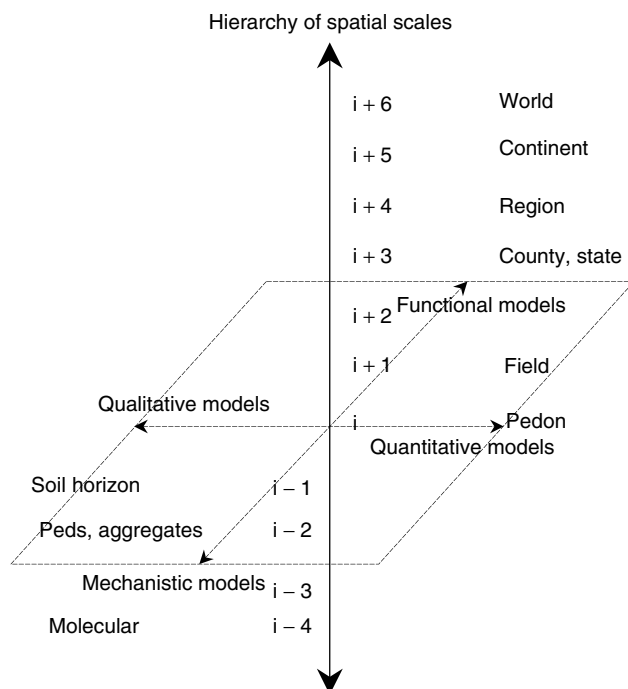
Models of solute transport in the vadose zone exist at all scales. A hierarchical depiction of the scales from molecular to global showing the relationship between scale and model type is depicted in Fig. 3. An important consideration in model conceptualization is for the model to account for the predominant processes occurring at the spatial and temporal scales of interest, which complies with the guideline of parsimony. Qualitatively speaking, as spatial scale increases, the complex local patterns of solute transport are attenuated and dominated by macroscale characteristics. For this reason, mechanistic models are used more frequently at the (i) to (i - 4) scales, whereas functional models are more often applied to scales ranging from (i + 1) to (i + 6). The stochastic application of deterministic models is found at the (i + 1) scale, and stochastic models generally are used at (i + 1) and (i + 2) scales. Statistical models are applied most often at the larger scales, (i + 3) to (i + 6).

The relevance of temporal domain is also a consideration not to be overlooked. Larger spatial scales appear more constant because the rapid dynamics of the lower scales are disregarded (20). For this reason, time steps of functional models can expand over days, such as the time between irrigation or precipitation events, whereas the time steps of mechanistic models characteristically extend over minutes.

The integration of solute transport models of the vadose zone into a GIS provides the ability to dynamically describe NPS pollutant transport at a range of spatial scales allowing the user to rapidly scale "up" and "down." However, this integration introduces incompatibilities between the model and data and raises basic questions regarding (1) the compatibility of the model with input and validation data, and (2) the relevance of the model to the applied spatial scale. Wagenet and Hutson (38) addressed the issue of scale dependency and proposed three scale-related factors to consider when applying GIS-based solute transport models to the simulation of NPS pollutants in soils: (1) the type of model (i.e., functional or mechanistic) must consider the scale of application, and the nature of the available data at that scale; (2) sampling and measurement of input and validation data must be spatially consistent with the model; and (3) measurement and monitoring methods must be relevant at the temporal domain being modeled.

### FUTURE DIRECTION

Beven (39) asserts that the real constraint on predictability by landscape-scale environmental models is not the detail of the model structure, but rather the ability to spatially and temporally characterize the variability of model inputs and parameters. Among the various techniques for characterizing the spatial variability of model inputs (e.g., electromagnetic induction, ground penetrating radar, time domain reflectometry, remote imagery, etc.), electromagnetic induction will be the most



**Figure 3.** Organizational hierarchy of spatial scales pertinent to NPS pollutant models. Source: Ref. 21. With permission.

useful in the short term (29), whereas greater future potential exists for hyperspectral imagery, which is in its infancy for soil and plant science applications.

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