FEATURE

The Challenge of Predicting Nonpoint Source Pollution

GIS can assess soil and groundwater contamination by pollutants, but uncertainties must be quantified.

KEITH LOAGUE, DENNIS L. CORWIN, AND TIMOTHY R. ELLSWORTH

Nonpoint source (NPS) pollutants threaten sustainable agriculture and are recognized as the single greatest threat to surface and subsurface drinking water resources. Ironically, agricultural activities are the leading cause of this pollution globally, particularly for NPS pollutants associated with the terrestrial and aquatic environments. The most common NPS pollutants include eroded sediments, fertilizers, pesticides, organic manures, salts, trace elements, and sewage sludge.

The alarming rate at which NPS pollutants are degrading soil and groundwater resources and increasing dependency on these resources for food and drinking water has heightened concerns about resource availability. Throughout the world, 30–50% of the Earth's land surface is believed to be affected by NPS pollutants (*1*). Evaluation of the effect of agricultural management practices on NPS pollution on local, regional, and global scales has become a key component of strategies for achieving sustainable agriculture and mitigating harmful environmental impacts. Decision makers want and need to know in advance the fate and behavior of agrochemicals applied to the soil surface and whether they pose a threat to soil and groundwater resources.

This is a challenging requirement. Assessment of NPS pollutants is a complex, multidisciplinary environmental problem that encompasses coupled physical and chemical processes that occur across disparate spatial and temporal scales. Moreover, NPS pollutants are spread over large areas in relatively low concentrations, and their detrimental environmental and health-related effects are chronic rather than acute. Nevertheless, they are of greater environmental concern than point source pollutants because they are ubiquitous and the task of cleanup is costly and nearly impossible to accomplish. Less expensive pollution prevention strategies are preferred that advantageously anticipate and prevent NPS pollution before it occurs and avoid the future need for costly remediation efforts.

This can be accomplished by forecasting the movement of NPS pollutants in soil to alter the potential occurrence of detrimental conditions, such as groundwater contamination, before serious impacts occur. To obtain this information, models of solute transport and accompanying input data are used to predict contaminant movement in soils, and a Geographic Information System (GIS) can be used as a tool for organizing, storing, manipulating, retrieving, and displaying spatially related information.

The assessment of NPS pollutants in soil and groundwater with GIS is an important environmen-

0013-936X/98/0932-130A$15.00/0

tal approach, from both a real-time event and a predictive perspective (*2–5*). GIS-based models of solute transport in soil are particularly well suited for modeling NPS pollutants. When GIS and environmental models are coupled, they provide an efficient means for handling the complex spatial and temporal heterogeneities of the Earth's surface and subsurface. GIS was introduced 10 years ago as a tool for assessing potential impacts of NPS pollutants on soil and groundwater (*2*), and coupling of GIS with environmental models has proliferated over the past decade. This trend continues to expand with the introduction of customized desktop GIS software, advances in computing technology, decreased software and technology costs, and growing demand for high-resolution spatial information.

Strategies for data acquisition

The spatial and temporal complexity of the Earth's near-surface makes the problem of modeling NPS pollutants in soil a data-intensive task. Collecting the necessary spatial information to satisfy the input data requirements for even the simplest solute transport model stands as one of the greatest challenges to modelers of the vadose zone (the zone from the soil surface to the water table). The time-dependent behavior of many solute transport parameters adds further complexity to the problems of measuring or estimating model input values.

Existing databases, such as those developed and maintained by the U.S. Department of Agriculture's Natural Resource Conservation Service (formerly the Soil Conservation Service), provide the easiest and cheapest means of obtaining soil data. Available databases differ in scale (county-level, state-level, and national soils databases) and detail of information. Specific databases are also available that contain data for basic soil properties, such as particle size distribution, bulk density, and organic matter, and associated unsaturated hydraulic properties, such as water retention, hydraulic conductivity, and soil water diffusivity. However, it is generally felt that most soil databases do not meet minimum data requirements for many of the presently used conceptual models of the vadose zone, nor do they provide useful statistical information about the uncertainty of the soil property data (*6*). This situation is due primarily to sparse spatial measurements, inaccurate measurement and estimation methods, and measurement of useless soil property data.

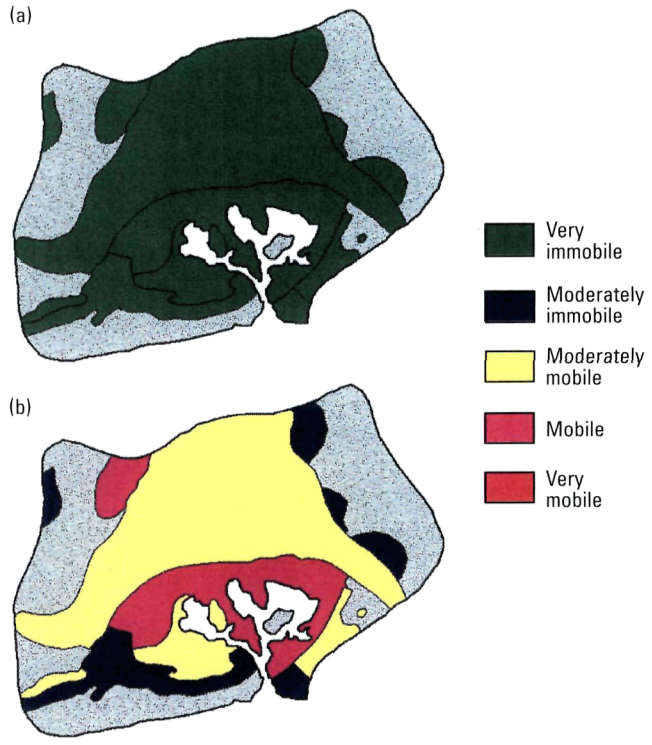
To meet model input requirements, directly measured data are the most reliable source. Remote sensing and noninvasive measurement techniques offer the greatest potential for cost-effectively meeting the data-intensive needs of GIS-based NPS pollution models (*2*). In modeling NPS pollutants, advancements are especially needed in the measurement of geo-referenced input and parameter data that are scale-relevant and have associated measures of uncertainty (*2*).

Estimation methods (transfer functions) of model parameters have been developed that estimate difficult-to-measure parameters from more easy-to-measure properties. The most common of these transfer functions is the pedotransfer function, which relates the more readily available properties of soil particle size distribution, bulk density, and organic carbon content to difficult-to-measure water retention or unsaturated hydraulic conductivity relations. Although transfer functions are a useful alternative when data are difficult to obtain or unavailable, they tend to be highly inaccurate.

FIGURE 1

Data uncertainties influence model outcomes

Leaching potential estimates are strongly influenced by the inclusion or omission of data uncertainties in the model simulation of groundwater vulnerability for the Pearl Harbor Basin, Oahu. This is evidenced by the difference in outcomes shown in (a), the leaching potential for Diuron based on the retardation factor (RF), and (b), the leaching potential for Diuron based on the estimates shown in (a) minus one standard deviation in the RF estimates. RF is an index of the retardation of a chemical leaching through soil because of sorption. The larger the RF value, the less mobile the chemical. Note that the index-based assessment did not yield any "very mobile" results.



Source: Reference 10. (Courtesy Soil Science of America)

Selection and capability of models

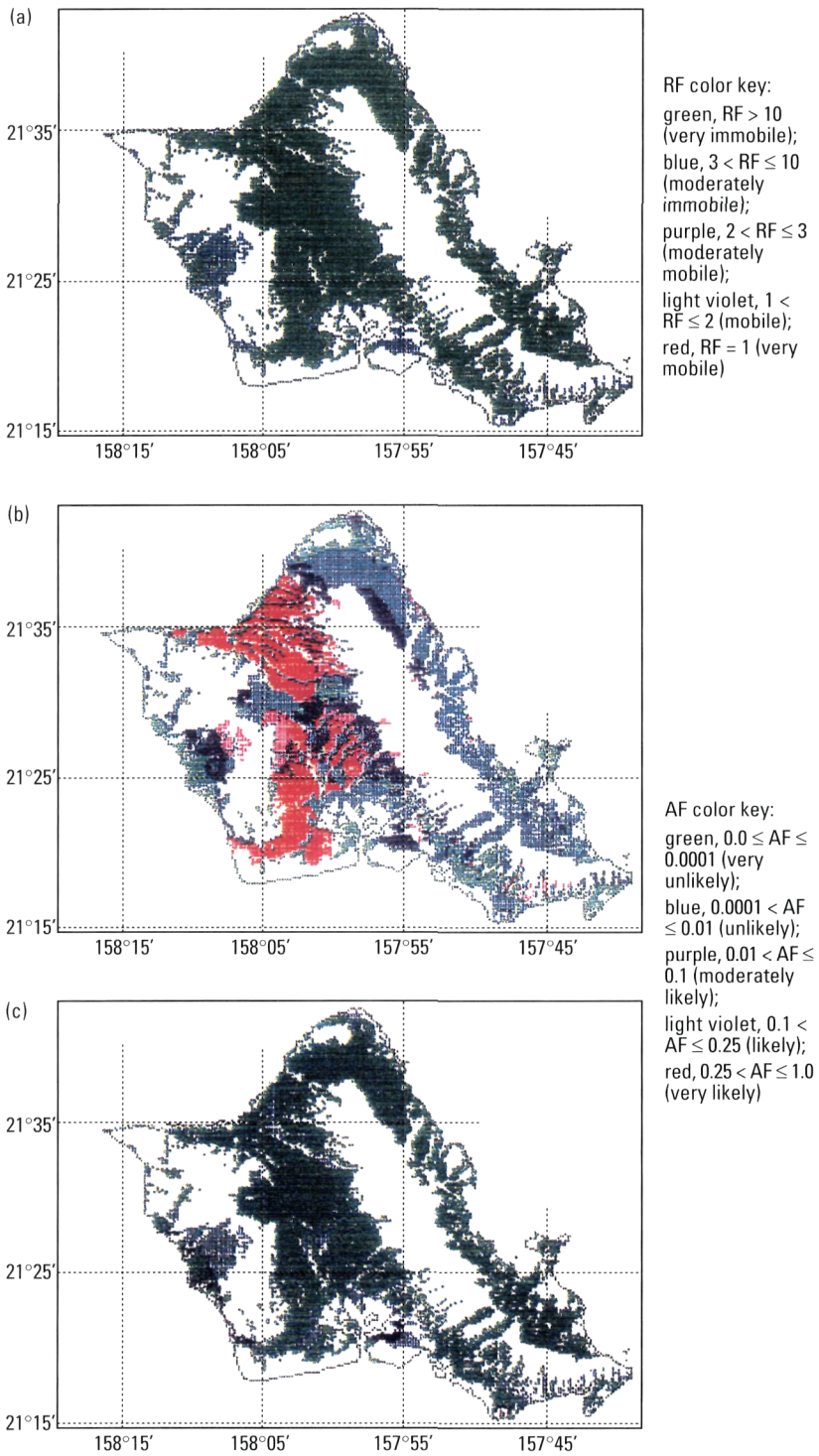
Mathematical models used in vulnerability assessments of NPS groundwater contamination can be classified into four major groups: stochastic-conceptual, stochastic-empirical, deterministic-conceptual, and deterministic-empirical (*7*). A model is stochastic if any variables in its mathematical expression are described by a probability distribution. A model is deterministic if all variables are viewed as free from random variations. Models are conceptual if their functional form is derived from consideration of physical processes; if not, they are empirical models.

A fundamental goal of mathematical modeling is to simulate real systems and provide information that can be used for decision making. GIS-based models used to estimate NPS pollution have ranged from

FIGURE 2

Modeling different chemicals gives mixed results

Groundwater vulnerability maps (a–c) of Oahu indicate why caution is needed when using models to predict contaminant impacts. The maps for EDB, (a) and (b), agree with field data. However, for Atrazine, (c), model results do not agree with field data. (a) Map for EDB based on the retardation factor (RF). (b) Map for EDB based on the attenuation factor (AF). (c) Groundwater vulnerability map for atrazine based on AF. RF is an index of the retardation of a chemical leaching through soil because of sorption. The larger the RF value, the less mobile the chemical. AF is an index of a chemical's mass emission from the vadose zone. The larger the AF value, the more likely it is that the chemical will leach. The large white areas are the locations where groundwater vulnerability assessments were not made.



RF color key:
green, RF > 10 (very immobile);
blue, 3 < RF ≤ 10 (moderately immobile);
purple, 2 < RF ≤ 3 (moderately mobile);
light violet, 1 < RF ≤ 2 (mobile);
red, RF = 1 (very mobile)

AF color key:
green, 0.0 ≤ AF ≤ 0.0001 (very unlikely);
blue, 0.0001 < AF ≤ 0.01 (unlikely);
purple, 0.01 < AF ≤ 0.1 (moderately likely);
light violet, 0.1 < AF ≤ 0.25 (likely);
red, 0.25 < AF ≤ 1.0 (very likely)

Source: Reference 13. (Courtesy *J. Environ. Qual.*)

simple empirical models, such as indices of contaminant movement, to complex physically-based models (*2*). Simple index models, such as the retardation factor (RF) and attenuation factor (AF), are used to screen and rank chemicals (*8*). RF is an index of the retardation of a chemical leaching through soil as a result of sorption. AF is an index of a chemical's mass emission from the vadose zone. Physically based models are designed to simulate chemical concentrations with depth and time (*9*).

Two factors primarily determine the selection of a NPS pollution model in any given situation: application and scale. For example, if a problem requires only an assessment of relative mobility for a list of selected chemicals, an index model can be used to screen and rank chemical contaminants. However, a conceptual model is needed if an estimate of concentration over a given region and time is required, for example, the peak arrival time of a chemical to a compliance surface such as the groundwater table. Scale determines the predominant processes that are influential and need to be accounted for in the solute transport model and has profound effects on the type of model used. Characterization of the principal processes determines what data must be collected. Qualitatively, as spatial scale increases, the complex local patterns of solute transport are attenuated and dominated by macroscale characteristics. For this reason, conceptual models that describe the physical mechanisms of water flow and solute transport are used more frequently at smaller scales, whereas simple empirical models are more often applied to larger scales.

Decision making and uncertainty

Uncertainty has significant practical implications, either affirming or negating the use of predictive outputs for guidance and action in a decision-making process. Regulatory decisions, based on NPS vulnerability assessments with less uncertainty, are easier to make. The end-products of a GIS-based model of NPS pollutant transport in the vadose zone are maps that show the spatial distribution of a solute within the unsaturated zone and solute loading to groundwater. Errors in a NPS pollution assessment result in analysis uncertainty and affect model reliability (a model's ability to predict

vulnerability). Associated uncertainty is often unavoidable and sometimes even undetectable in environmental modeling.

Quantification of uncertainty establishes the extent to which simulated results are reliable predictions of observed truth (actual conditions) (*10*). Uncertainty can be due to model errors produced from simplification of process complexities described by the model. Uncertainty can also result from data error—errors in input data or lack of information. Without a doubt, the current generation of potentially useful, deterministically derived, GIS-driven groundwater vulnerability maps are undercut both by model and data errors. A map generated from a GIS-based model has no real utility without a corresponding map of associated uncertainties. This is shown in Figure 1 (*10*), in which leaching potential estimates are changed by accounting for data uncertainty.

To further emphasize that GIS-based modeling of NPS must be performed with caution, consider the groundwater vulnerability maps of Khan and coworkers shown in Figure 2. These are among the first ever generated to assess the potential for pesticide leaching at a regional scale and illustrate an important issue in the characterization of NPS pollution vulnerability using GIS technology (*11*). Khan and coworkers used RF and AF indices to estimate groundwater vulnerability for the Pearl Harbor Basin on the Hawaiian island of Oahu. Inspection of the 1,2-dibromoethane (EDB) maps (Figures 2a and 2b) shows that the chemical is characterized as highly sorbed (RF classified as very immobile or immobile) but leachable in some locations (AF classified from very unlikely to very likely). As EDB is in groundwater in the Pearl Harbor Basin, one might consider the AF map for EDB to be a test of model performance and assume the approach is valid and appropriate for making estimates of leaching potential for other chemicals. However, the AF map for atrazine (2-chloro-4-ethylamino-6-isopropylamino-S-triazine) shows (Figure 2c) that this chemical is at best only moderately likely to leach to groundwater, when in fact atrazine has already been detected in groundwater in Hawaii (*12*). Characterizing the uncertainties associated with the pioneering NPS groundwater vulnerability assessments for Hawaii was the focus of a 10-year effort, recently reviewed by Loague and coworkers (*13*). The magnitude of the uncertainty in the RF and AF estimates for Hawaii was found to be similar to the estimated RF and AF values, clearly showing the importance of accounting for uncertainty in NPS groundwater vulnerability assessments.

Although software advances have fostered growth in model development and deployment, caution must be taken in the application of GIS-based models of NPS pollution. NPS pollution models typically rely on soil, climate, and chemical data that, because they are sparsely measured, are usually estimated. Both models and data contain varying degrees of associated uncertainty. Historically, GIS-based models of NPS pollutants have not been accompanied with the associated measures of uncertainty that are needed to assess the reliability of simulated results. Without inclusion of associated uncertainties, the primary application of GIS-based models can be used only for identifying data and model shortfalls (*14*).

Researchers are working to resolve these modeling and data-driven limitations, but no environmental protection decision yet made concerning agricultural chemical use has depended solely on a GIS-based regional-scale groundwater vulnerability assessment. Although GIS-based models of nonpoint source pollution have great potential, they must still be used with caution. Measures of uncertainty of modeling outcomes must be provided that establish the reliability of simulated results. The sophisticated visualizations created from GIS should never disguise the legitimacy of the rendered results, nor should simulated results ever supplant field observation.

Acknowledgments

The authors wish to thank the American Geophysical Union, the Soil Science Society of America, Stanford University's Center for Earth Science Information Research, NASA, and NSF.

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Keith Loague is associate professor of hydrogeology in the Department of Geological and Environmental Sciences at Stanford University and co-director of the Stanford/USGS Center for Earth Science Information Research. Dennis L. Corwin is a soil and environmental scientist at the USDA-ARS, U.S. Salinity Laboratory, in Riverside, Calif. Timothy R. Ellsworth is associate professor of soil physics in the Department of Natural Resources and Environmental Science at the University of Illinois–Urbana.