ESTIMATION OF GROUNDWATER POLLUTION POTENTIAL BY PESTICIDES IN MID-ATLANTIC COASTAL PLAIN WATERSHEDS

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ABSTRACT: A simple GIS-based transport model to estimate the potential for groundwater pollution by pesticides has been developed within the ArcView GIS environment. The pesticide leaching analytical model, which is based on one-dimensional advective-dispersive-reactive (ADR) transport, has been directly integrated into the GIS with menu interface and display tools to estimate the spatial and temporal distribution of a potential pesticide's emission to groundwater. The ADR model was chosen because it requires readily available data as compared to other non-GIS models and it has the potential to handle multiple soil profile descriptions. The ADR model has been used to assist with pollution assessment such as the location and timing of pesticide spreading on watersheds, or choosing the most effective "Best Management Practices". By embedding ADR modeling capabilities into the GIS, one is able to evaluate the groundwater vulnerability to pesticide contamination on a large scale where variable source areas are responsible for a part or all of the groundwater contamination. To demonstrate the GIS-based contaminant transport model and its capabilities, the program was applied to Mid-Atlantic coastal plain agricultural watersheds, which are particularly vulnerable to agricultural pesticide pollution.

INTRODUCTION

The fate of pesticides in the environment has been of great concern for several decades because pesticides are a major source of nonpoint source (NPS) pollutants and a major contamination threat to groundwater and surface water. A comprehensive review of published information on the subsurface (groundwater and vadose zone), conducted as part of the USGS' National Water Quality Assessment (NAWQA), indicated that pesticides from every chemical class have been detected in ground waters of the United States (Barbash, 1995). Many of these compounds are commonly present at low concentrations in groundwater beneath agricultural land. Protecting groundwater resources is especially important in agricultural areas where most pesticides are used and where over 95 percent of the population relies upon groundwater for drinking water. Therefore, there is an increasing need for quantitative and objective assessment of environmental damage and water quality impacts resulting from pesticide pollution. It is particularly important to be able to identify the groundwater pollution potential due to pesticide leaching.

The description of pesticide pollution on a watershed scale is a complex environmental problem because of the physical and chemical heterogeneities of the subsurface. Pesticides are often spread over large areas, which makes it difficult to determine their fates and to evaluate if they pose a threat to soil and groundwater

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resources. Most aquifer contamination is discovered only after a water-supply well has been affected. To minimize the risk of groundwater contamination by pesticides and to avoid the need for costly remediation efforts, it is essential to be able to predict specific areas in a watershed that are at risk for pesticide leaching and to estimate the amount of leaching that is possible. These efforts are the first step in improving watershed management.

Because of the complexity of the processes involved, a recent trend in the regulation of pesticide use has involved an increased reliance on solute-transport models to predict the transport and fate of pesticides in the subsurface. Transport simulation models have become a useful tool in understanding and analyzing NPS pollution problems caused by the migration of pesticides through soil into groundwater. These models can be used for the preliminary screening of the areas susceptible to severe or high contamination as well as predicting the consequences of management alternatives. While groundwater contamination by pesticides may be predicted by several available leaching models, few models are currently available to predict the spatial pattern of variable source areas. Some of the limitations of models include the inability to handle and manage large amounts of model input data and to account for the spatial variability and heterogeneity that are important in NPS modeling processes. Moreover, improving model capability requires the management of increasing volumes of spatially referenced data.

For these reasons, simulating pesticide movement through the subsurface has been difficult. It has been recognized that the spatial-temporal variability in such factors as topography, soil, climate, land use, and land management influences the response of natural systems and limits the applicability of the models. GIS (Geographic Information Systems) technology has gained widespread acceptance as a data management and visualization tool for addressing spatially related environmental problems. Modeling the fate and movement of pesticides in the subsurface is a spatial problem well suited to the integration of a solute transport model with GIS. When GIS and transport models are merged, they provide an efficient means for handling the complex spatial heterogeneities of the surface and subsurface. The GIS-based model has simple data requirements and is defined within a spatial context as compared to more complex models that require routing information. The end products of a GIS-based model of NPS pollutant fate and transport in the subsurface are maps that show the spatial distribution of a solute within the unsaturated zone and solute loading to groundwater. In both cases, an improvement with respect to the classical non-GIS models has been accomplished (Zhang, 1998).

GIS-based models used to estimate NPS pollution range from simple empirical models to complex physically based models (Corwin, et al. 1997). The pesticide leaching analytical model used in this paper is a simple one-dimensional advective-dispersive-reactive (ADR) transport model which estimates the potential leaching of pesticides occurring at any point in the watershed. It was developed with the objective of aiding management in identifying potential pollution source areas of watersheds. By integrating the ADR model into a GIS, a tool with menu interface is created for the prediction of pesticide leaching in the subsurface and making preliminary groundwater contamination assessments within a GIS environment. This approach also demonstrates the advantages of embedding subsurface transport modeling capabilities into GIS to evaluate the groundwater vulnerability to pesticide contamination on a large scale (e.g. watershed) where a variable source area is responsible for a part or all of the groundwater contamination.

In this study, the pesticide leaching analytical model was integrated within ArcView GIS and its associated databases to estimate the spatial and temporal distribution of pesticide leaching and potential vulnerability of the groundwater. The ADR model is based on an analytical solution of the advective-dispersive-reactive transport equation, which describes transport and fate of pesticides in the soil. The model has also been tested under field and laboratory conditions. This paper describes the model development within the ArcView environment and a field example application. The example is used to demonstrate the capabilities of the GIS-based pesticide leaching model.

PESTICIDE LEACHING ANALYTICAL MODEL

There are many pesticide leaching models available, ranging from simple to sophisticated numerical ones. The models can be classified as either deterministic or stochastic. Both deterministic and stochastic models can be further subdivided into lumped or distributed models, depending on the treatment of space. A lumped model represents the physical system as a spatially-homogeneous region which does not account for the spatial variation of input parameters within the area. On the other hand, a distributed model assumes that the physical system is made of discrete subareas, each characterized by a uniform set of properties and input parameters. The volume of information needed to temporally and spatially characterize the parameters and variables in even the simplest functional models of solute transport in the vadose zone is tremendous (Corwin, et al. 1997). Moreover, the most comprehensive models do not always provide better results than simpler ones (Hutson and Wagenet, 1991).

The pesticide leaching analytical model used in this work is described in detail by Ravi and Johnson (1992). The model is a one-dimensional advective-dispersive-reactive transport equation. The vertical transport of a pollutant dissolved in water through the soil can be described by the following principal governing equation:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} - \frac{\rho_b}{\theta}\frac{\partial S}{\partial t} - K_l C \qquad (1)$$

where C is the liquid-phase pollutant concentration (M/L^3); t is the time (T); x is the distance along the flow path (L); D is the dispersion coefficient (L^2/T); v is the interstitial or pore-water velocity (L/T); ρ_b is the bulk density (M/L^3); θ is the volumetric water content (L^3/L^3); S is the solid-phase concentration (M/M); and K_l is the first-order decay coefficient in liquid phase (1/T).

The term $\partial S/\partial t$ is the rate of loss of solute from liquid phase to solid phase due to sorption. Under the assumption of linear, instantaneous sorption, $\partial S/\partial t$ can be estimated by:

$$\frac{\partial S}{\partial t} = K_d\frac{\partial C}{\partial x} \qquad (2)$$

where K_d is the linear Freundlich sorption coefficient, $K_d = K_{oc} f_{oc}$; K_{oc} is the organic carbon partition coefficient; and f_{oc} is the fraction organic content of the soil.

Substituting (2) into (1), one obtains

$$R\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} - K_l C \tag{3}$$

where R is the retardation factor, $R = 1 + K_d \rho_b / \theta$.

Equation (3) describes advection and dispersion of a solute in the liquid phase. The model assumes that the pesticide mass per unit area of soil, M_a, is instantaneously mobilized by infiltrating water into the root zone. The initial concentration of pesticide at the surface can be written as:

$$C_0 = \frac{M_a}{R\theta h} \tag{4}$$

where M_a is the total pollutant mass applied (M/L^2), h is the root zone depth, and θ is the water content given by the following equation:

$$\begin{aligned} &\theta = \theta_s \left(\frac{r}{K_s}\right)^{\frac{1}{2b+3}}, && r \le K_s \\ &\theta = \theta_s, && r > K_s \end{aligned} \tag{5}$$

where r is the rate of infiltration, K_s is the saturated hydraulic conductivity, and θ_s is the saturated water content.

Assuming the following initial and boundary conditions:.

$$C(x,0) = \begin{matrix} 0, & -\infty < x < -h \\ C_0, & -h \le x < 0 \\ 0, & 0 \le x < \infty \end{matrix} \tag{6}$$

$$\ell im \frac{\partial C}{\partial x} = 0, as|x| \longrightarrow \infty \tag{7}$$

the solution of (3) is obtained as follows:

$$C(x,t) = \frac{C_0}{2} e^{-k_l t}\left[erf\left(\frac{x + h - vt/R}{2\sqrt{Dt/R}}\right) - erf\left(\frac{x - vt/R}{2\sqrt{Dt/R}}\right)\right] \tag{8}$$

where erf(z) is the error function which is defined as $erf(z) = 2/\sqrt{\pi}\int_0^z e^{-y^2} dy$. It should be noted that the infinite boundary condition may cause prediction error at short time and low vadose zone depth

The model above simulates vertical solute transport over an area as if all parameters within the area are uniform. It does not consider the effects of spatial variability. Parameter values for the area as a whole are obtained by spatially-averaging individual values. The model provides a unique output result for the whole area, but it does not provide any information regarding the spatial behavior of the outputs. So the model above is a lumped parameter model. The problem with this lumped parameter model is that spatial variability can have significant impacts on area response.

MODEL INTEGRATION INTO GIS

An integrated GIS system is comprised of three components: the model, the GIS and the data. When working with vadose zone transport models, Tim (1996) and Corwin et al. (1997) refer to three potential levels of integrating GIS with NPS models. For the first level of integration, known as loose coupling integration, the GIS and the model are developed separately and are executed independently. The GIS serves only as a pre-processor of the input data for the model. The second level of integration, partial integration, is the result of establishing an interactive interface between the GIS and the model. In this level of integration, the GIS not only provides input data to the model, but also accepts modeling results from the model for further processing and/or presentation. The third level of integration is typically referred to as complete integration or "modeling within GIS" which was used in this paper. For this level of integration, the functionality of the model is implemented or programmed directly into the GIS. With the equations programmed within the GIS, an interactive and fully integrated contaminant transport modeling process can be performed within the same environment, so that data pre-processing and analytical functions are available under the same operating system. This level of integration is technically preferred by most modelers, but is often difficult to implement due to incompatibilities in the data structures of the model and the GIS, or due to proprietary rights of commercial GIS software limiting the introduction of additional processing routines. Fig. 1 shows a schematic illustration of the third level of integration for GIS and models.

The NPS model can be expanded to act as a distributed parameter modeling application through integration with the GIS. Distributed models break an area down into a number of smaller homogeneous subareas or elements with uniform soils, cropping, and topographic characteristics. Some distributed parameter models have a cellular or grid structure, which simplifies database creation. A grid is placed over the area of interest and then parameter values are obtained for each grid based on the predominate parameter in the grid, or by area weighting parameter values within the cell. In essence, averaging is done, but on a much smaller scale so that some spatial variability is still maintained. The area is then modeled by solving the equations describing the state of each individual element. The entire area response is obtained by integrating all the elemental responses. The distributed parameter model also gives information on what is happening within each element and can therefore be used to identify critical locations within the modeled region. Lumped models do not have this capability.

In order to run the model within ArcView, Avenue scripts were written to calculate each of the transport processes described above and produce modeling outputs at specified time steps. The GIS database in the project was created by extracting soil data for soil series occurring in the area. These data included soil classification, many chemical parameters, as well as soil-water parameters. Weather data input is read from interactive menus containing precipitation and potential evapotranspiration. Actual evapotranspiration is calculated for each land use using a table of crop factors. All other non-spatial data are entered from the menus within ArcView. Output maps display the pollutant concentration profile at any given time.

APPLICATION TO MID-ATLANTIC COASTAL PLAIN WATERSHEDS

As an example application, the GIS-based pesticide leaching analytical model was used to assess the impact of pesticide leaching on groundwater quality within agricultural watersheds located in Kent County, Maryland. This example application is provided for preliminary assessment and is not intended to evaluate the water quality problems resulting from applied pesticides in this watershed region. To further this model as a highly effective pollution assessment tool would require improvements in the level of detail of source data.

The study area shown in Figure 2 is approximately 120 km^2. Agriculture dominates the landscape in the study area and most of the land there is used to grow corn and soybeans in an annual rotation with winter wheat. The soil in the study area is predominantly silt loam and to a lesser extent ranged from loam to sandy and gravely loams. The GIS database created for the pesticide leaching analytical model focused on the information required to implement the integrated GIS modeling. The primary data included the soil characteristics and other chemical parameters. The pesticides chosen in this study were Altrazine and Bromacil. Selected pesticide properties are listed in Table 1.

Groundwater recharge estimates are based on the monthly water balance between the infiltration water from precipitation and irrigation, and the outflow of water from surface runoff and evapotranspiration (Thornthwaite and Mather, 1957). The runoff volume, or rainfall excess, is estimated using the curve number approach developed by the Soil Conservation Services (SCS) (Haan et al., 1994). The SCS has classified more than 400 soils into four hydrologic soil groups according to their minimum infiltration rate obtained for bare soil after prolonged wetting. The hydrological soil groups are built into the GIS database in this study. Evapotranspiration is estimated using quasi-empirical methods which rely on energy balance and heat transfer concepts and empirical crop factors due to lack of real-time measurements.

The results presented in Figure 3 represent the preliminary groundwater vulnerability predictions to pesticides applied to soils that are suitable for agricultural lands. A single application of 2.5 lb/acre is assumed in the predicted groundwater vulnerability maps. The predicted results show that both Atrazine and Bromacil have degraded less than the Maximum Concentration Limit (MCL) before leaching into groundwater. Pesticides with short half-life and relatively high organic carbon partition coefficient as altrazine showed low concentration level. Compared to Atrazine, Bromacil is considered highly mobile since it has a relatively large half-life and low organic carbon partition coefficient. While a model like ADR can be used to identify problem areas in general, a more detailed examination may be necessary to determine the validity of the spatial groundwater vulnerability predictions and suggest conservation management practices which could lessen the problem. As more detailed data becomes available, comprehensive models are more suitable for these purposes.

CONCLUSIONS

In this study, an one-dimensional advective-dispersive-reactive transport model was programmed and embedded within the ArcView GIS environment to predict pesticide leaching potential. This approach provides a full range of model input/output data manipulation capabilities and an improved estimate for pesticide contamination in groundwater. This GIS-based transport model provides the descriptive framework to estimate a spatially variable pesticide leaching distribution in the subsurface that cannot be achieved by the original model. The GIS format allows data to retain its spatial relationships and keeps track of all modeling parameters and state variables. GIS also creates a user friendly environment and allows modification for simulating different scenarios.

The GIS-based ADR model can be used for pollution assessment such as the location and timing of pesticide spreading on watersheds, or choosing the most effective "Best Management Practices". The major advantage of a GIS-based transport model is that the procedure automates and facilitates spatial modeling assessment and considers the heterogeneities of land use and soil. However, like most simulation models, the ADR model used in this paper is mathematically and conceptually ideal. It therefore may not accurately simulate natural conditions since the approach is a simplified one and does not incorporate processes such as two dimensional convective-dispersive transport or adsorption reactions. In some cases the influence of these processes cannot be neglected and may therefore constitute a limitation to the practical use of the proposed model. Continued work on this topic will focus on developing an infiltration component and adding a plotting routine in ArcView.

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Table 1. Selected pesticide properties

Pesticide	Solubility (Kg/m^3)	K_{oc} (m^3/kg)	K_H[1]	λ (days)[2]	MCL (ppb)[3]
Atrazine*	32×10^{-3}	0.16	2.5×10^{-7}	71	3
Bromacil*	82×10^{-2}	7.2×10^{-2}	3.7×10^{-8}	350	90

* Adapted from Hantush et al. (2000)

1. K_H is a Henry's constant , 2. λ is a half-life, and 3. MCL is a Maximum Concentration Limit.

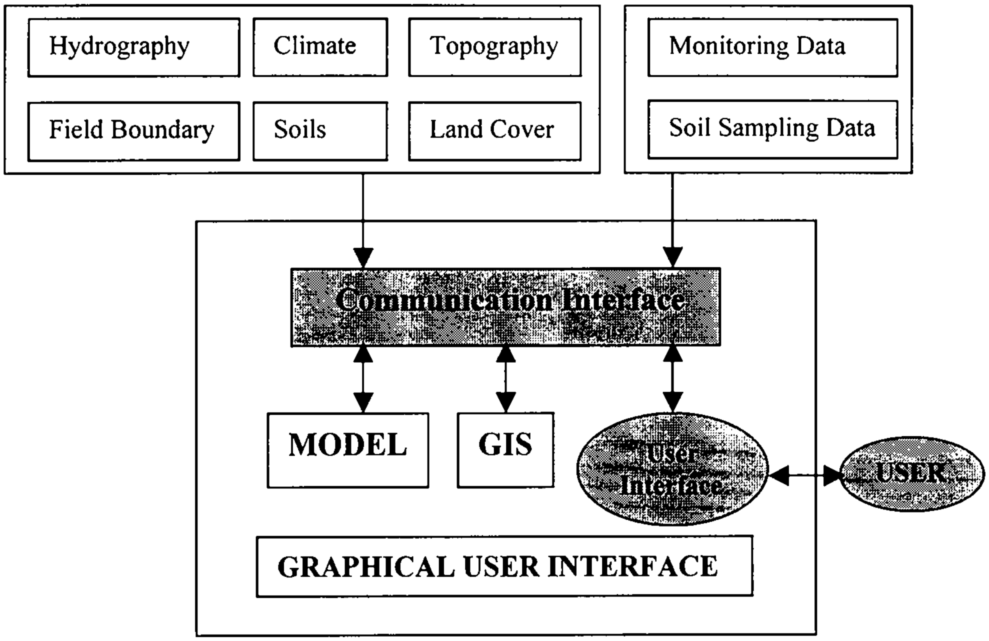

Fig 1. Schematic representation of GIS applications integrated with model (Tim, et al., 1996)

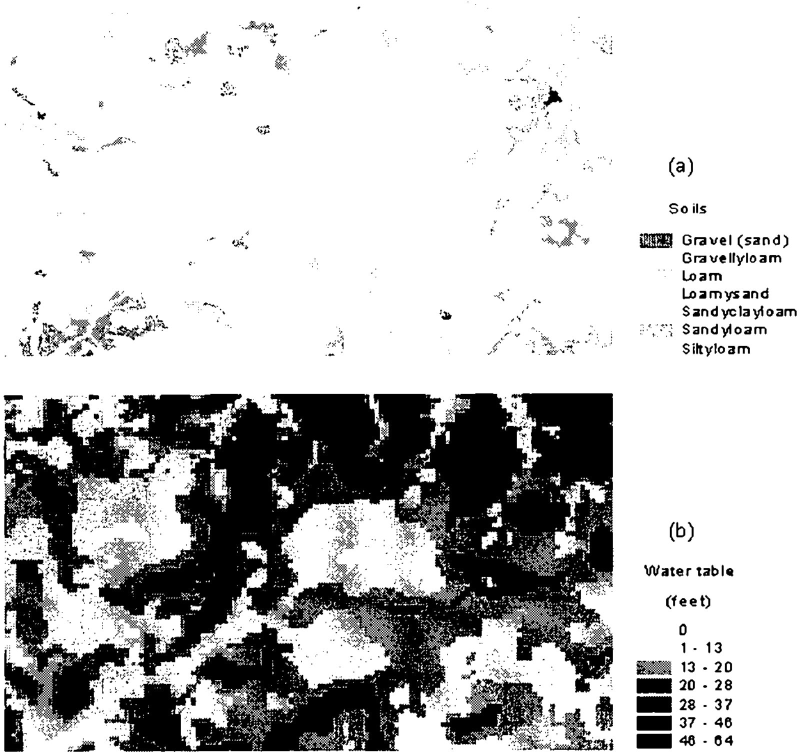

Fig. 2. Study area (a) soil characteristics and (b) groundwater table

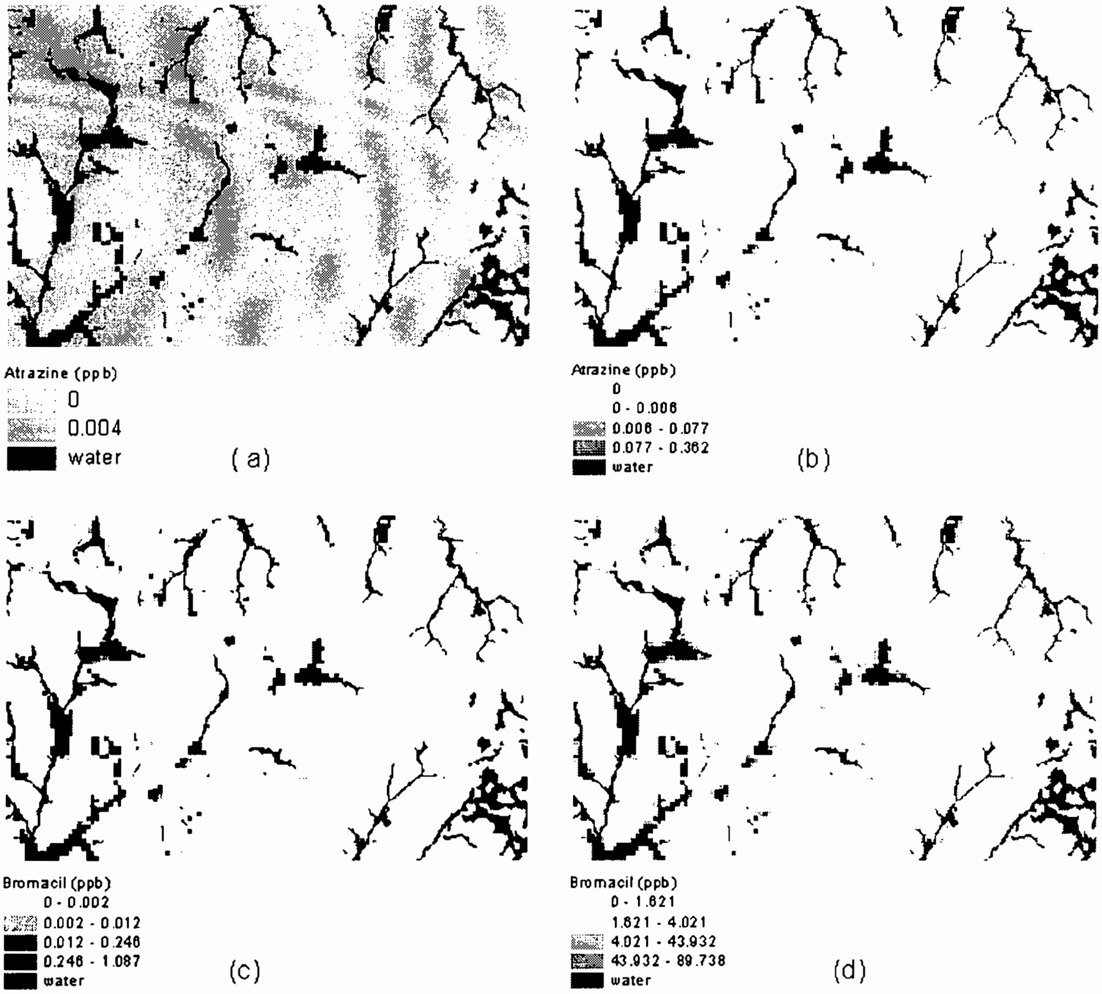

Fig. 3. Simulated contaminant concentration in groundwater (a) atrazine (3 months), (b) atrazine (6 months), (c) bromacil (3 months), and (d) bromacil (6 months).

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16. ABSTRACT

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