

# PESTICIDE LEACHING ANALYTICAL MODEL AND GIS-BASED APPLICATION IN AGRICULTURAL WATERSHEDS

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**ABSTRACT:** Ground-water contamination by pesticides and other organic pollutants has been detected across agricultural areas and is on the increase. Because ground-water monitoring is too costly to define the geographic extent of contamination at such large scales, indirect methods are needed to predict transport and fate of pesticides in the subsurface and assess the potential for ground-water contamination that may result from applications of pesticides. In this paper, two analytical solutions that describe one-dimensional transport and fate of pesticides in the soil, were integrated with a geographic information system (GIS) to estimate spatial solute leaching distributions and to create ground-water vulnerability assessment maps. The GIS-based models use process-based equations that consider advection and complete mixing to simulate solute transport and to predict pesticide transport in both space and time. To demonstrate its capabilities, the modeling approach is applied to an agricultural watershed in the mid-Atlantic coastal plain using data from county soil survey and monitoring study in this region. The impact of processes, such as net infiltration, biochemical degradation, adsorption and advection on the spatial and temporal distribution of pollutant emissions to ground water are investigated. The applicability of GIS-based models for vulnerability assessment and determining the risk of ground-water contamination by pesticides is demonstrated in susceptible agricultural areas.

## INTRODUCTION

Fertilizers and pesticides are extensively used in the U.S. to increase agricultural production. These agrichemicals are significant sources of nonpoint pollution, and long-term exposure of land areas to these agrichemicals provides the potential for ground-water contamination. Across the country, pesticides and other organic pollutants have been detected in ground water underlying agricultural regions (*USEPA*, 1992). The possible deleterious effects of pesticides on humans and ecosystems have been documented (*Biradar and Rayburn*, 1995), and careful management of pesticides on agricultural areas in order to avoid ground-water contamination is desired by both farmers and the general public.

Ground water monitoring is too costly to adequately define the geographic extent of contamination at a large scale. Therefore, indirect methods are needed to assess the potential for ground-water contamination by pesticides over large areas. Agricultural practices that provide sources or enhance the potential for pesticide leaching to ground water need to be identified and their geographic extent defined. Examination of the spatial distribution of contaminant sources may help identify areas susceptible to pesticide contamination. Vulnerability assessments can provide essential screening tools to understand the relative mobility of pesticides and predict potential ground-water contamination.

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Ground-water vulnerability assessment methods can be classified into three general types: statistical methods, overlay and index methods, and process-based transport models (*Water Science and Technology Board*, 1993). In this paper, a process-based model that describes one-dimensional solute transport at subsurface is considered. Solute transport models have become a useful tool in understanding ground-water contamination caused by the migration of pesticides through soil into ground water. This method may be distinguished from the others in its potential to predict solute transport in both space and time. Several models that use process-based equations are capable of simulating the transport and transformation of pesticides in the subsurface. Models used to evaluate the ground-water contamination potential by pesticides range from one-dimensional to multi-dimensional models. Comprehensive transport models such as GLEAM (*Knisel et al.*, 1993), and PRZM-2 and 3 (*Carsel et al.*, 1997) are usually data intensive and require knowledge of soil, land use, environment, and pesticide parameters (*Rao et al.*, 1985). In most cases, such parameters are neither available nor likely to be obtained for a large number of soil-land-pesticide combinations. For these reasons, the modeling simulations are not always satisfactory to address potential ground-water contamination problems on a large scale.

In order to evaluate ground-water contamination potential on a large scale, several vadose zone solute transport models have been integrated with a geographic information system (GIS). A comprehensive review of GIS-based nonpoint source pollutant modeling in the vadose zone has been presented by *Corwin, et al.* (1997). *Wesseling and van Duersen* (1995) programmed dynamic mass transport models into a GIS. *Tim* (1996) coupled a one-dimensional advective dispersion-reaction equation with ArcInfo GIS to demonstrate the capabilities of embedding a vadose zone model into a GIS. *Lasserre et al.* (1999) linked an unsaturated zone transport model with IDRISI GIS to simulate nitrate fluxes into ground water. *Hantush et al.* (1999) coupled multi-phase mass fraction models with a GIS and applied the framework to the assessment of uncertainty of ground water vulnerability to some pesticides in agricultural watersheds in the mid-Atlantic coastal plains. The framework and the application to the Locust Grove study area demonstrated the existing uncertainty for predicted results when fixed input parameters are considered in fate and transport models. *Shukla et al.* (2000) coupled the attenuation factor (AF) model with a GIS on a county-scale to screen more than 70 pesticides. Based on the literature, the trend in coupling GIS and environmental models is leading toward more sophisticated process-based models.

In this study, two solutions of a one-dimensional solute transport model were integrated with GIS for predicting the fate of pesticides in the subsurface. Pesticide transport mechanisms including advection and complete mixing were investigated for a case study with limited watershed field data. The purpose of this work was to develop a simple procedure which can be employed to estimate the relative behavior of pesticides on a large scale (e.g., watershed) and to evaluate the pesticide contamination potential. As compared to comprehensive transport models, a GIS-based transport model relies on georeferenced data which allows visualization of spatially distributed data on a true map scale. The modeling outputs give the spatial solute leaching distributions and the vulnerability assessment maps, which can be used to identify areas susceptible to potential ground-water contamination. To illustrate the modeling procedure, the ground-water vulnerability maps of three pesticides: atrazine, dicamba, and cyanazine, are presented for the case study. These results demonstrate the potential for GIS-based transport models to be used as pollution assessment screening tools for managing a large number of pesticides on an agricultural area.

## TRANSPORT AND FATE MODELS

Problems of solute transport involving first-order decay reactions frequently occur in soil and ground-water systems. When the volumetric moisture content and the pore-water velocity remain constant in time and space (steady-state flow), the governing solute transport equation in a one-dimensional system including linear equilibrium adsorption and first-order decay is given by Equation (1):

$$R \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial z^2} - \frac{v}{\theta} \frac{\partial C}{\partial z} - kRC \quad (1)$$

$$R = 1 + (K_d \rho_b + \kappa K_H / \theta) \quad (1a)$$

$$K_d = K_{oc} f_{oc} \quad (1b)$$

where  $C$  = the solute concentration in water ( $M/L^3$ );  $t$  = the time (T);  $z$  = the distance along the flow path (L);  $D$  = the dispersion coefficient ( $L^2/T$ );  $v$  = the Darcy velocity (L/T);  $\theta$  = the volumetric water content of the soil ( $L^3/L^3$ );  $k$  = the first-order decay coefficient in water (1/T);  $R$  = the soil retardation factor;  $K_H$  = the dimensionless Henry's constant;  $\kappa$  = volumetric air content,  $K_d$  = the linear distribution coefficient;  $K_{oc}$  = the organic carbon partition coefficient; and  $f_{oc}$  = the fraction of organic content of the soil by weight.

In general, analytical solutions offer substantial advantages over other solution methods for processing transport models. Two conceptual solutions which include advection and complete mixing are considered in this study. The solutions mentioned here do not represent all of the modeling options available for pesticide leaching simulation, but they may be worth of investigation. Approximation errors associated with complete mixing and advective solutions are relatively small for large Peclet number (*Hantush et al.*, 2000; and *Luckner and Schestakow*, 1991).

### Complete Mixing Solution

In this approach, the soil is considered to be composed of the crop-root zone and the vadose zone, each with uniform properties. The model simulates movement of the contaminant through both zones and complete mixing of the pesticide is assumed. The solution takes into account processes such as advection, adsorption, degradation, and volatilization from soil surface. Pesticide mass per unit area of soil is assumed to be instantaneously mobilized by infiltrating water into the root zone.

The solution of Equation (1) under the complete mixing condition has been given and described in detail by *Hantush and Marino* (1996). It is described separately for the root zone and vadose zone.

#### Root zone

The root zone extends from the ground surface down through the crop roots. Pesticide leaching occurs in this zone due to irrigation and rainfall. The analytical solution of the concentration with time below the root zone can be obtained by:

$$C_r(t) = [C_r(t_0) + C_0] \exp \left[ -\frac{1 + (T_r / \lambda)(\ln 2 + \mu)}{T_r} (t - t_0) \right] \quad (2)$$

$$\mu = \frac{(FS + \sigma / h)\lambda}{\ln(2)R_r\theta} \quad (2a)$$

$$T_r = \frac{hR_r\theta}{v^*} \quad (2b)$$

$$\sigma = D_g K_H / d \quad (2c)$$

$$C_0 = M_0 / \theta_r h R_r \quad (2d)$$

where  $h$  = the root zone depth (L);  $\theta_r$  = the moisture content;  $R_r$  = the retardation factor in the root zone;  $v^*$  = the net ground-water recharge (L/T);  $D_g$  = the soil-gas diffusion coefficient (L<sup>2</sup>/T);  $d$  = the air boundary layer thickness above the surface (L) and assumed to be equal to 5 cm;  $F$  = the transpiration stream concentration factor;  $S$  = the transpiration rate (1/T);  $\lambda$  = the half-life (T); and  $M_0$  = the total pollutant mass applied per unit area (M/L<sup>2</sup>).

#### Vadose zone

The vadose zone extends from the bottom of the root zone to the water table. Almost all the water that enters this zone percolates downward to the water table. An analytical solution of concentration with time to the water table from the vadose zone can be obtained by:

$$C_u(t) = \exp \left[ -\frac{1 + \ln 2(T_u / \lambda)}{T_u} (t - t_0) \right] C_u(t_0) + [C_r(t_0) + C_0] T_r \exp \left[ -\frac{1 + (T_r / \lambda)(\ln 2 + \mu)}{T_r} (t - t_0) \right] - \exp \left[ -\frac{1 + \ln 2(T_u / \lambda)}{T_u} (t - t_0) \right] \times \frac{T_r [1 + \ln 2(T_u / \lambda)] - T_u [1 + (T_r / \lambda)(\ln 2 + \mu)]}{T_r [1 + \ln 2(T_u / \lambda)] - T_u [1 + (T_r / \lambda)(\ln 2 + \mu)]} \quad (3)$$

$$T_u = \frac{HR_u\theta_u}{v^*} \quad (3a)$$

where  $H$  = the ground-water depth below the root zone (L);  $\theta_u$  = the moisture content; and  $R_u$  = the retardation factor in the vadose zone.

#### Advective-Reactive Solution below Root Zone

For solute transport in the subsurface, advection transport may be dominant. In this case, transport due to solute diffusion or dispersion may sometimes be neglected. When only advection is considered, the concentration in the liquid phase is provided by the equation (1) by

setting dispersion,  $D$ , to zero. The use of advective model allows for accounting for delayed breakthroughs, which are not accounted for by the complete mixing model. We consider the case of advection in the vadose zone. Given the following initial and boundary conditions:

$$C(z,0) = C_i \quad (4a)$$

$$C(0,t) = C_r(t) \quad (4b)$$

where  $C_i$  = the initial uniform concentration in the vadose [ $M/L^3$ ],  $C_r(t)$  = the concentration at the bottom of the root zone [ $M/L^3$ ] and is given by the above complete mixing model, and  $t$  = the time period [T]. With these boundary and initial conditions, a solution of Equation (1), in which only advection is addressed, is obtained using Laplace transformation:

$$C(z,t) = C_i e^{-kt}, \quad t < \frac{R(z-h)}{v/\theta} \quad (5a)$$

$$C(z,t) = C_i e^{-kt} + C_r \left[ t - \frac{R(z-h)}{v/\theta} \right] e^{-\frac{kR(z-h)}{v/\theta}}, \quad t \geq \frac{R(z-h)}{v/\theta} \quad (5b)$$

$$C_r \left[ t - \frac{R(z-h)}{v/\theta} \right] = [C_r(t_0) + C_0] e^{-\left[ \frac{1+(T_r/\lambda)(\ln 2 + \mu)}{T_r} \left( t - \frac{R(z-h)}{v/\theta} - t_0 \right) \right]} \quad (5c)$$

## GIS-BASED MODEL APPLICATION

The described transport model solutions were integrated with ArcView GIS to perform regional assessments of ground-water contamination potential by selected pesticides commonly used in the Delmarva Peninsula (*Koterba et al.*, 1993). GIS-based transport model simulations can be used to rank pesticides according to their relative leaching potential. With the model solutions programmed within GIS, an interactive and fully integrated contaminant transport modeling system is developed. To demonstrate its capabilities, the GIS based model was applied to a case study. Computation of the concentration for each soil type was performed for each pesticide and predictive spatial ground-water vulnerability maps were created. All the data layers required by the model were generated and organized within the GIS.

The study area is an agricultural watershed drained by the Morgan Creek located in Kent County, Maryland (see, also, *Hantush et al.*, 1999). The soil coverage is shown in Fig. 1 and is predominantly loamy. Due to extensive agricultural activities at the site, the potential for ground-water contamination by pesticides exists. The GIS-based transport models are applied to this region to predict the spatial distribution of the pesticide leaching potential. Ground-water 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. The SCS curve number method was used to estimate surface runoff. Monthly evapotranspiration (ET) is estimated using the method described by *Thornthwaite and Mather* (1957). All of calculations are performed within a GIS.

For the case study, the pesticides listed in the Table 1 are chosen for assessing their relative contamination potential using GIS based models. These pesticides were selected based on assumptions of their potential use, which may differ from their actual use. A single application of

2.5 lb/acre is assumed to produce the predictive ground-water vulnerability GIS maps. Figures 2 displays the results for the three pesticides (atrazine, dicamba, and cyanazine) at a depth of 1.5 m, different time period after application. The spatial trend and magnitude of pesticide leaching concentration predicted by the GIS-based models indicated that the majority of regions with high pesticide concentrations are located in areas of high ground-water recharge for complete mixing model. Subsequent effect of dilution and decay cause the low concentration at the high recharge area.

Pesticides with relatively short half-life and low  $K_{oc}$  such as dicamba showed low leaching concentration levels in the vadose zone. So it is considered to have low mobility among the selected pesticides. Atrazine showed high leaching concentrations due to relatively large half-life and high  $K_{oc}$ . Cyanazine, which appears to be as mobile as atrazine, showed greater concentration as a consequence of its relatively large half-life and low  $K_{oc}$ .

The modeling results also indicate that advection plays a significant role in the pesticide leaching. As compared to the advection model, the complete mixing model may underestimate the leaching concentration at subsurface. For the complete mixing assumption, the solution tends to underestimate peak concentrations as shown in Fig. 2 because it ignores diffusion and does not explicitly treat advection. Pesticide movement through the vadose zone proceeds by both advection and dispersion. The vulnerability GIS maps show that the predicted concentration will decrease with the application time. These results provide an initial estimate of contaminant potential by these pesticides but the limited field data in this study preclude a detailed evaluation of the simulation results.

## **SUMMARY**

Ground-water vulnerability assessments are useful for pesticide management in order to prevent future ground-water contamination problems. This paper presents two GIS-based solute transport models that can be used to estimate the relative behavior of pesticides in the subsurface at a watershed scale. The assessment of the impact of contaminant sources on ground water on this scale is greatly enhanced by the use of georeferenced data in a GIS-based model, and the resulting vulnerability maps show the spatial distribution of a pesticide through the soil leaching to ground water. Relationships between the spatially distributed data and results can be established through the use of GIS.

This paper demonstrates that GIS-based transport models that incorporate the physical processes influencing ground-water vulnerability can be used to obtain estimates of solute leaching to ground water. The analytical solutions of solute transport used in the GIS-based models are based on many simplifying assumptions and their use may lead to serious errors if improperly applied. The complete mixing model may underestimate the pesticide contamination potential whereas the advective model appears to provide more accurate predictions for pesticide contamination potential.

The simulated results presented here are preliminary. Before simulated results are used for making regulatory and remediation decisions, assessments of past, current, and future pesticide use should be conducted. Future work in this area will concentrate on expanding both the soil and pesticide databases as well as increasing the range of the analysis to the soil series and parameters. The correlation between soil properties will also be considered. Additionally, future research on this subject will include the use of the analytical solutions in conjunction with additional program modifications to further enhance the model's applicability.

Table 1. Selected pesticide properties

No.	Pesticide	S (mg/L)	$K_{oc}$ (m <sup>3</sup> /kg)	$K_H$	$\lambda$ (day)	k (day <sup>-1</sup> )
1	Atrazine <sup>a</sup>	32	1.60E-01	2.50E-07	71	0.00976
2	Dicamba <sup>b</sup>	830	2.00E-03	8.90E-8	14	0.0495
3	Cyanazine <sup>a</sup>	750	1.68E-01	1.20E-04	108	0.00260

a. From Rao et al. 1985.

b. From Shukla et al., 1998.

c. S = solubility,  $K_{oc}$  = organic carbon partition coefficient,  $K_H$  = Henry's constant,  $\lambda$  = half-life, and k = decay rate coefficient.

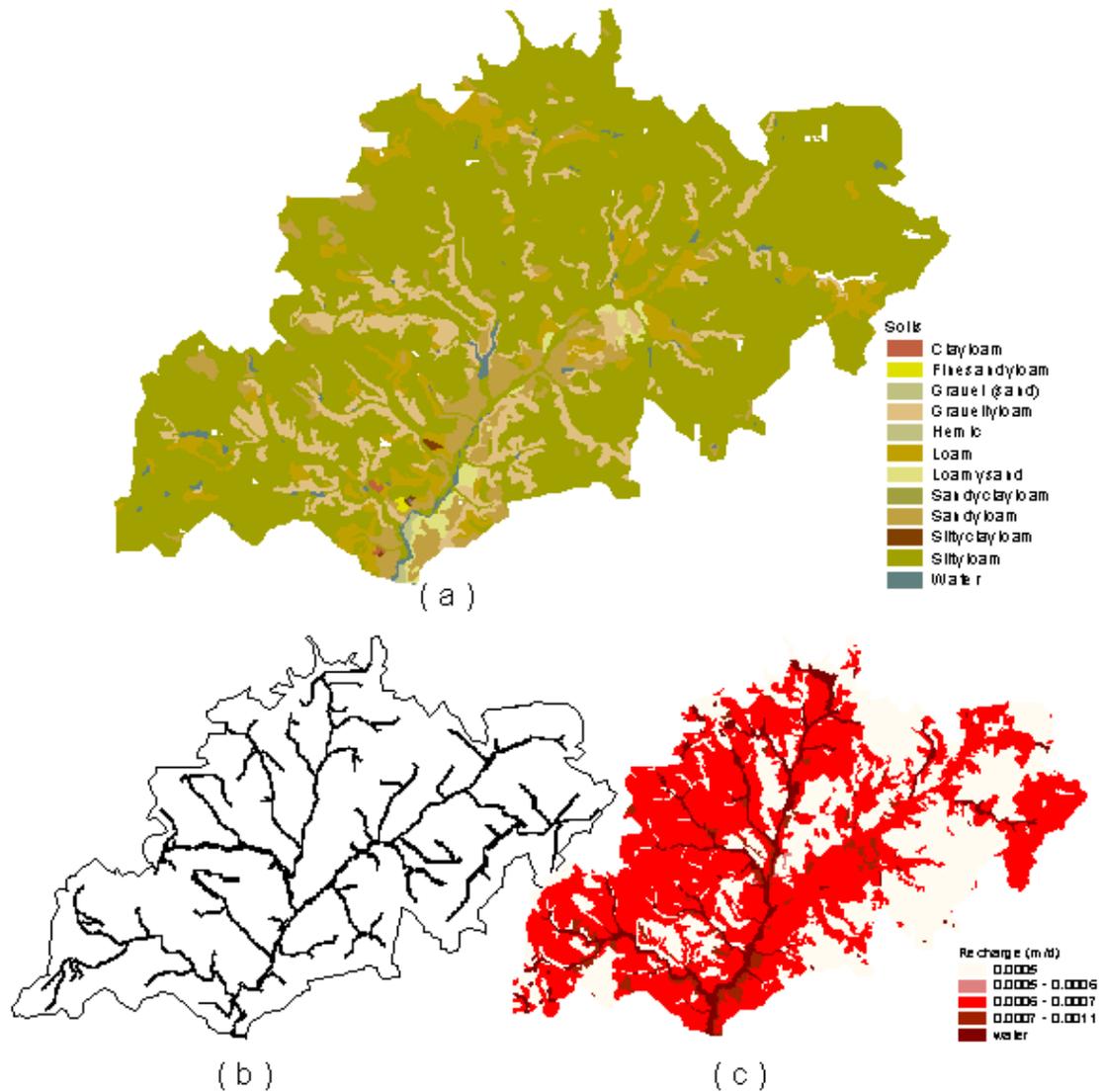


Figure 1. Soil distribution (a), watershed (b) and ground-water recharge (c) at Locust Grove site

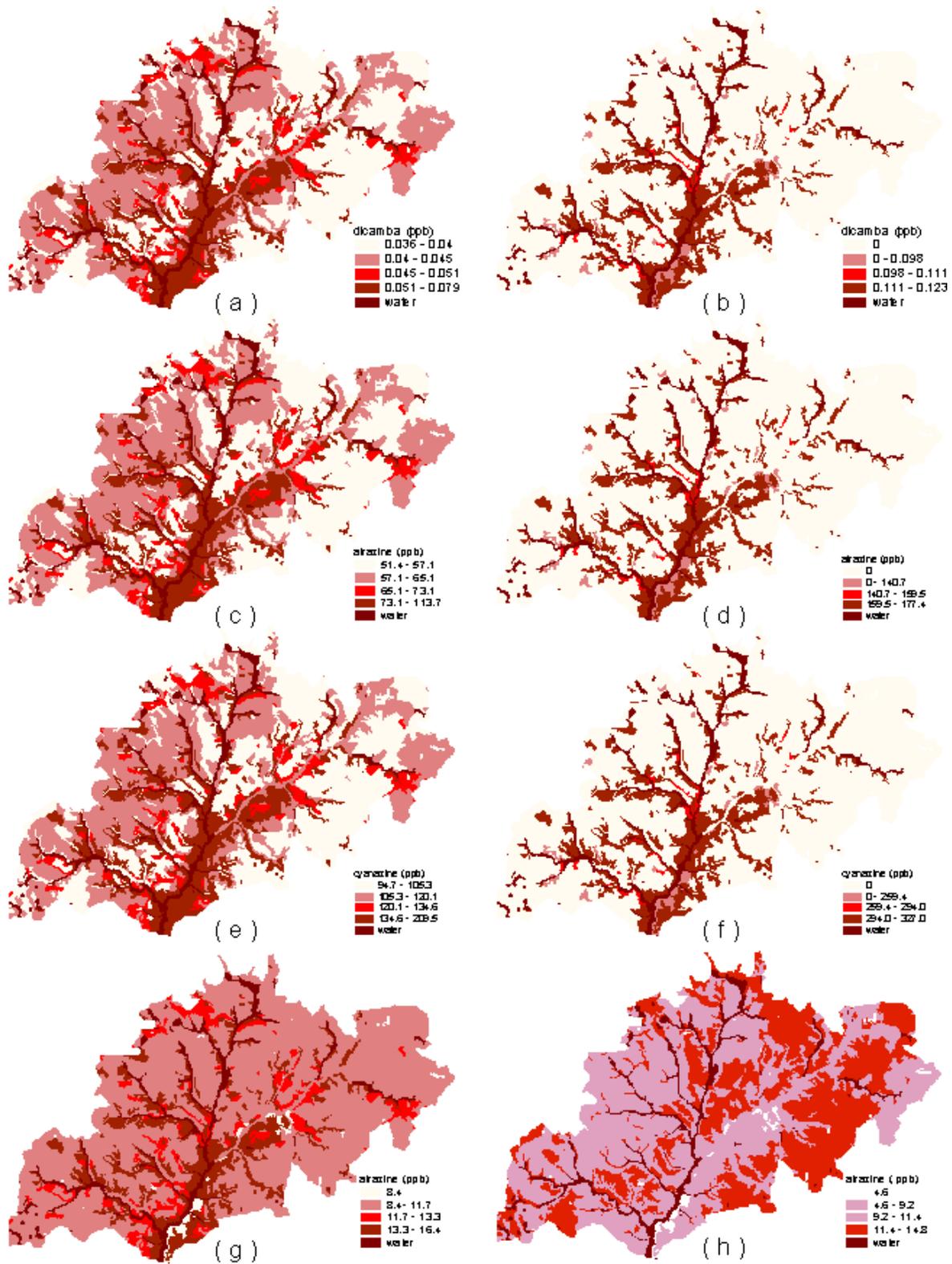


Figure 2. Predicted pesticide concentration: (a) dicamba (6 mnh), (c) atrazine (6 mnh), (e) cyanazine (6 mnh) and (g) atrazine (1 yr.) from complete mixing model; (b) dicamba (6 mnh), (d) atrazine (6 mnhs), (f) cyanazine (6 mnhs) and (h) atrazine (1 yr.) from advective model.

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