

Mapping atrazine leaching potential with integrated environmental databases and simulation models

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ABSTRACT: A methodology was developed to integrate a simulation model and environmental databases for mapping pesticide leaching potential at landscape scale. A deterministic, one-dimensional solute transport model was applied using soil, land use, and climate data compiled for the northeast region of the United States. Landscape units that combined soil and climate variables were modeled to produce estimates of atrazine leaching in agricultural lands. Model results were aggregated into class ranges indicating the proportion of a landscape unit susceptible to pesticide leaching. Significant results were, first, that pesticide leaching potential was related to the amount and distribution of rainfall and soil organic carbon, and second, that a functional deterministic simulation model and database were developed for use by environmental professionals to model and visualize soil behavior at regional scale. Implications of this study indicate that aggregated leaching indices should be mapped at scales no finer than 1:250,000 when using regional-scale databases; and uncertainty associated with spatial and temporal variability, model type, and environmental database quality limit interpretations of regional model simulations and resultant map products to landscape units similar in size to Major Land Resource Areas or individual states, whichever is larger.

Few pesticides have been observed under field conditions with sufficient detail to accurately assess their migration through unsaturated soils to groundwater. High costs of chemical analyses and field studies and restrictions on the use of hazardous substances make simulation modeling an attractive alternative for estimating fate and transport of pesticides over diverse landscapes. With the advent of large-scale environmental assessments using geographical information systems (GIS) and soil survey databases to estimate leaching, there is a need to accelerate the development of simplified, yet acceptably accurate pesticide leaching models. This simplification would minimize input

data requirements and, in the process, minimize and focus soil characterization programs and field observations beyond the information contained in existing environmental databases (Wagenet et al. 1991).

The use of computer simulation models as an aid in predicting the fate and transport of chemicals in soil has increased significantly over the past two decades (Ahuja et al.; Carsel et al. 1985; Carsel et al. 1988; Jury and Gruber; Loague et al.; Nicholls et al.; Nofziger and Hornsby; Wagenet and Hutson 1989). Most models that predict leaching of pesticides and nutrients are one-dimensional, mainly because chemical fluxes in agricultural systems occur predominantly in the vertical dimension. Multi-dimensional models are complex; they require increased execution time and parameter estimation is more difficult when two- or three-dimensional analysis is attempted. Relevant application of deterministic models to large land areas with considerable spatial heterogeneity has received little critical attention.

Several approaches relating static land characteristics, soil management histories, and GIS to land qualities such as leaching potential have been developed (Carsel et al. 1985; Carsel et al. 1988; Green et al.; Hamlett et al.; Thomasson and Jones). Advanced computer tools provide oppor-

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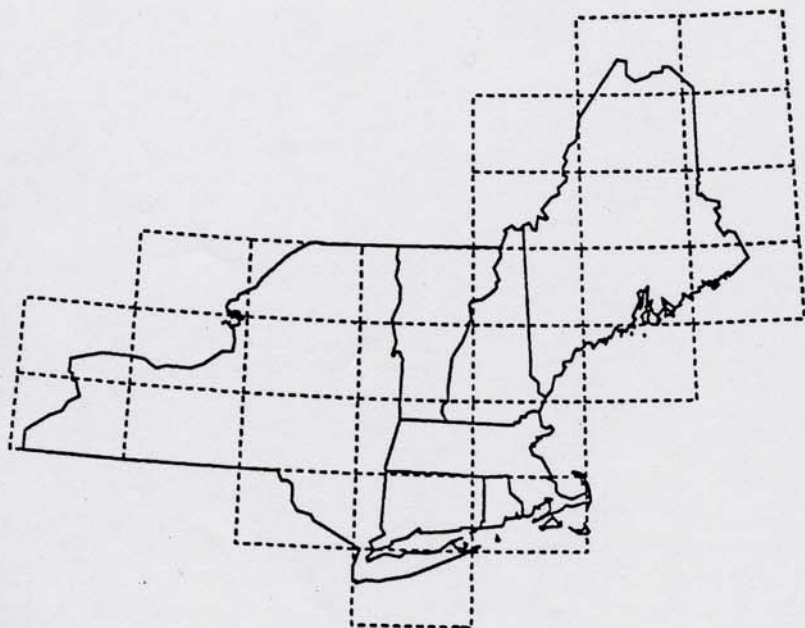


Figure 1. Study area with 1:250,000 scale 1° x 2° quadrangle boundaries

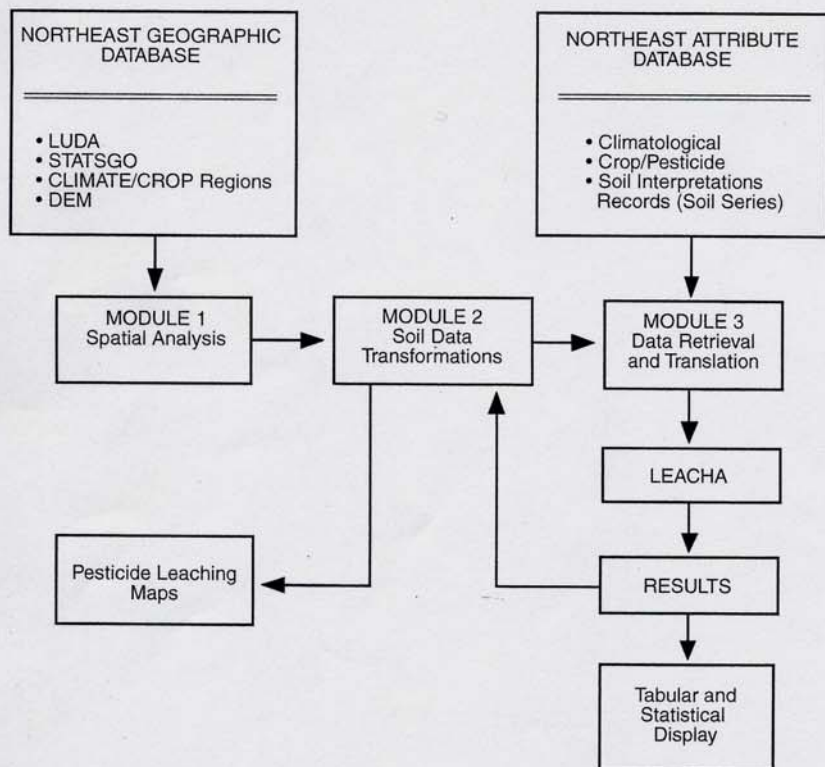


Figure 2. Structure and processing flow of environmental information for landscape-scale simulation modeling

tunities to combine knowledge of soil leaching processes with existing spatial information describing land use, climate,

and soils to predict groundwater contamination. It is also important to communicate the relationships between these

processes and their distribution over the landscape to the public using the integrative and display tools embodied in GIS.

This paper describes a methodology in which a dynamic simulation model was integrated with regional-scale environmental databases to map pesticide leaching potential in the northeastern United States. This study built upon previous work conducted at more detailed spatial scales by several investigators (Landre; Petach; Petach et al.). We briefly describe here the simulation modeling approach, spatial data requirements and sources, database development and linkages, and regional-scale mapping of atrazine leaching potential.

Methodology

Study area. The study area included all land areas within the states of Connecticut, Maine, Massachusetts, New Hampshire, New York, Rhode Island, and Vermont (Figure 1). All geographic data were accessed and compiled at 1:250,000 scale, and geo-referenced using the Universal Transverse Mercator grid and projection system. Digital input and output maps were catalogued and processed corresponding to USGS 1° x 2° topographic quadrangles, and can be reproduced based on administrative (state, county) or natural (watershed) units.

Simulation modeling approach. The modeling approach used in this study was based on LEACHP, the pesticide version of LEACHM, the Leaching Estimation And CHEMistry Model (Wagenet and Hutson 1989). LEACHP is a finite difference model designed to simulate the movement of water and pesticides through both layered and non-layered soils. The soil profile is divided into horizontal layers and the total simulation period is divided into small time increments. Fluxes and changes in the mass of water and chemicals are calculated at each time step for every layer. The Richards equation is used to describe water flow, and the convection-dispersion equation (CDE) is used for solute transport. Water contents and water fluxes calculated from the numerical solution of the Richards equation require knowledge of the relationship between water content, matric potential, and hydraulic conductivity. Functions describing this relationship can be estimated from soil survey data (Hutson and Cass). LEACHP simulations include the effects of sorption, degradation, volatilization, and growing plants. LEACHP has been used in a variety of applications, both for validation and as a predictive tool (Hutson et al.; Landre;

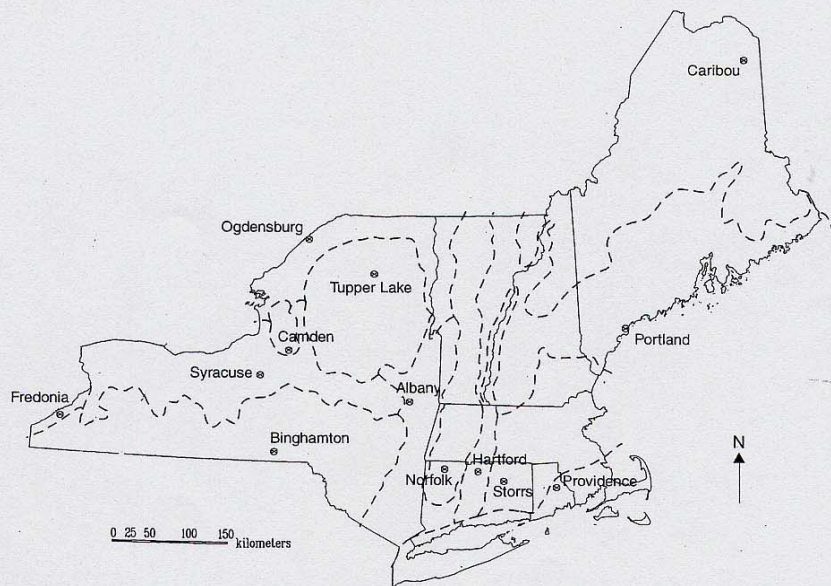


Figure 3. Climate regions and selected stations

Petach; Wagenet and Hutson 1986; Wagenet et al. 1989).

For this project, LEACHP was simplified by replacing the Richards equation and the convection-dispersion equation by a mobile-immobile capacity model (Addiscott; Addiscott and Wagenet; Nicholls et al.). This modified version of LEACHP is called LEACHA, and is most useful for regional-scale simulations when multiple model executions of large datasets are required. Comparisons between LEACHA and LEACHP in a pilot project showed good agreement, justifying the use of LEACHA for the multiple simulations required by this study (Hutson). The characteristics of the LEACHA model are described in detail by Hutson and Wagenet.

Data processing approach. The data processing flow for the study is shown in Figure 2. Spatial and tabular data were manipulated using two computing environments: (1) workstation ARC/INFO GIS software was used to manipulate and analyze the spatially-referenced environmental data; and (2) RBASE relational database management system was used to manipulate the tabular data in a PC environment.

Geographic and attribute databases

Agricultural land areas were determined using digital land-use/land-cover data published at 1:250,000 scale (U.S. Geological Survey). These land-use maps are a compilation of analyst interpretations

made from aerial photographs and satellite images using the land-use/land-cover classification scheme developed by the U.S. Geological Survey (Anderson et al.). The data were developed during the 1970s and represent land-use conditions for that period. The age of these data was not a significant concern in that the area of agricultural land in the region is not likely to have increased during the past 10-15 years. It is more likely that the current modeling effort overestimated the area of agricultural land and hence total pesticide leaching in the region.

Soil data were derived from the USDA-Natural Resources Conservation Service (NRCS) State Soil Geographic database (STATSGO), which provided attribute and geographic data used by LEACHA for each soil map unit in the study area. A STATSGO map unit can consist of more than 20 individual soil components defined as phases of soil series, each component being a defined fraction of the map unit area (Bliss and Reybold; Reybold and TeSelle; Soil Conservation Service 1991). Soil properties are recorded in the Soil Interpretations Record database for each soil series. Information in this relational database was used for the leaching simulations.

Climate data and definitions of climate regions were provided by the Northeast Regional Climate Center at Cornell University. Climate regions were defined by integrating boundaries of the Major Land Resource Areas (MLRA) (Soil Conservation Service 1981), state climate maps,

and station locations. One weather station was chosen to represent climate conditions within each region. The primary criterion for choice of station was that the station have a continuous record of daily precipitation and temperature for the period 1970 to 1989. The climate regions and weather stations selected are shown in Figure 3.

For all simulations, continuously-cropped corn was the agronomic practice of choice, and the soil was assumed to be fallow for the remainder of the year. Potential evapotranspiration was estimated using the Linacre equation. Crop growth patterns and chemical application rates and times were identical for all simulations, and typical of agronomic practices in the northeastern United States (Cornell Cooperative Extension).

Linking modules. All environmental data were processed, stored, and manipulated in the two graphic and attribute databases, and related by map unit identification codes (MUID). The GIS and relational database management system were used in three software linking modules.

The first module was a spatial model which defined landscape units having unique combinations of soil map units and climate conditions within agricultural lands. Land-use data were reclassified into a binary map indicating agricultural or non-agricultural land use. The STATSGO soil map was intersected with the binary land-use map to create a derivative map containing the distribution of soil map units by agricultural land use. This derivative map was then intersected with the climate regions map to sort agricultural soil map units by climate region resulting in the landscape unit of analysis.

The second module transformed STATSGO soil map units into new sets of individual soil components falling within the landscape units. These soil components related to the soil profile data used by the LEACHA simulations and formed the basis of the resultant maps. Soil map unit percent compositions were redefined to only include potential agricultural soils. Individual soil map unit components were excluded from the simulations based on excessive slope gradients (> 8%), muck soils, or non-soil conditions.

The third module retrieved data from the attribute database, and performed data translations required for input to the leaching simulation model. A data table listing all soil and climate combinations was then used by LEACHA to model solute transport. Mean values for clay content and bulk density (mid-points of

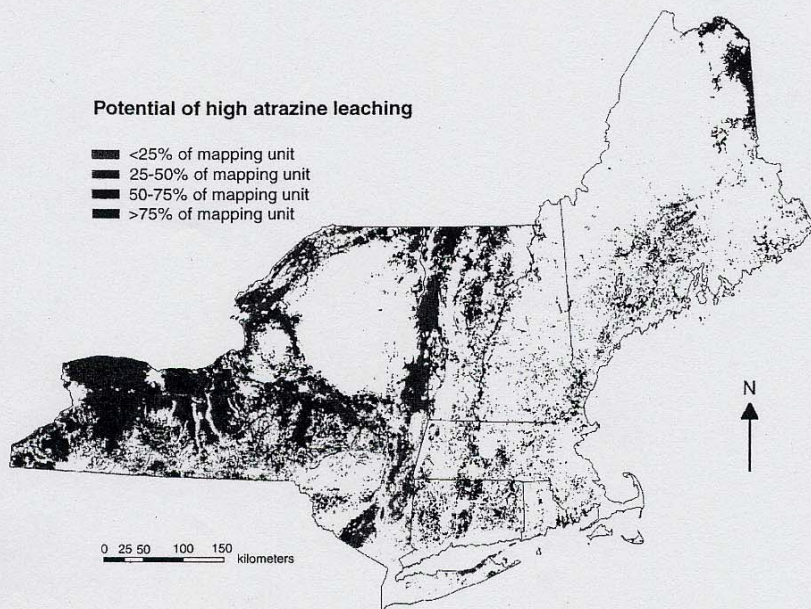


Figure 4. Map of atrazine leaching potential for northeast United States region

ranges) and the lowest (worst-case scenario) value for organic carbon were used. Water retention properties of the soils were estimated using regression equations developed by Rawls and Brakensiek, which relate water retention to particle size, bulk density, and organic matter data. The organic carbon content of the subsoils, which is not recorded in the attribute database, was set to 0.1%. Pesticide degradation rate constants, solubilities, and Koc (organic carbon partition coefficient) values were obtained from Wauchope et al. Pesticide Kd values were estimated in LEACHA as the product of Koc and the organic carbon fraction.

To produce maps of simulation model results, leaching categories were defined by the proportion of pesticide leached in relation to the amount applied on an annual time scale. High atrazine leaching for a soil component was defined arbitrarily as 25% or more of the atrazine applied (on May 25) leached from the bottom of the soil profile by the end of the simulation time period.

Model implementation. A sample set of 5-year simulations, using the same boundary conditions each year, was conducted to test the hypothesis that the pesticide mass balance components reach constant values after a few years. If an equilibrium can be achieved within a given time period, simulations could be run on each soil:climate combination, and the 'equilibrium' amount of chemical leached could be used as the representa-

tive leaching value for that soil. Results from the 5-year simulations indicated that equilibrium was reached within 3 years. Thus, all soils in the region were modeled using three repetitions of a single year's data.

A preliminary series of 20-year simulations was used to determine the most representative year of climate data for each region. A representative climate year was chosen for each station after simulating leaching in a sample soil for each year in the way described above. The distribution of the results of the 20 simulations was examined, and the year that corresponded most closely to the mean leaching for the long-term climate record was chosen as the representative year.

The 20-year simulations for each climate region demonstrated that the distribution of annual water drained exhibited great temporal variability within each climate region, and that leaching was related to rainfall and drainage flux. Despite the fluctuation in rainfall from year to year, a stable leaching pattern, characteristic of each soil modeled, was obtained (Hutson). This pattern varied in time, depending upon the rainfall regime of the particular year.

For mapping purposes, modeling results were related back to a landscape unit by using Module Two (soil data transformations). The amount of pesticide leached was tabulated for each individual soil component modeled. Each component was classified as either high (>25%)

or low (<25%) amount of pesticide leached in comparison to that applied. Each modeled component was weighted by the proportion of area the component occupied in the landscape unit. A legend of four classes was established for map generation to indicate the spatial proportion of landscape units (soil:climate combinations) having high leaching potential (<25%, 25-50%, 51-75%, >75%).

Characterization of map error and model uncertainty. Evaluation of map error and error propagation was performed at three levels: (1) assuming input soil, land use, and climate data were correct but checking map overlay operations to identify cartographic errors, documenting error tolerances for spatial map operations, and evaluating appropriateness of spatial distribution maps of input and output variables; (2) evaluating the nature of errors propagated through the processing modules; and (3) testing the sensitivity of grouping and ranking LEACHA results by visually inspecting the spatial distribution of leaching classes throughout the region based on different modeling parameters used.

Using geographic databases resident in the public domain contributes some uncertainty to landscape-scale modeling with respect to cartographic control and attribute data quality. Importing and integrating soil, land use, political units, and hydrography digital maps resulted in some spatial error and inconsistent characterization of landscape boundaries common to these maps (e.g., shorelines). STATSGO representations of these common boundary conditions were used because of their relatively higher spatial accuracy. Each digital map also had different minimum size delineation criteria. For this study the minimum size delineation was defined by the digital land-use data (4 ha [10 ac]) with minimum size tolerance of 2 ha (5 ac) for digital map overlay operations.

Results and discussion

Landscape data. Summary statistics for land area, land use, soil map units and landscape units are shown in Table 1. The study area encompassed nearly 300,000 km² (115,830 mi²) with New York State representing more than 42% of the land area in the region. Agricultural area was defined by selecting only categories #21 (Cropland and Pasture), #22 (Orchards, Vineyards...), and #24 (Other Agricultural Land) of the land-use classification scheme (Anderson et al.). On average, the proportion of agricultural land was 15% throughout the study area, ranging from

Table 1. Summary statistics for land use, soil map units and soil:climate modeling units

State	Total Area (Km ²)*	Agricultural Area (%)	Total MUID (Count)	MUID Used (Count)	%	Soil:Climate
CT	12,912	14	31	30	97	221
MA	21,505	9	60	56	93	301
ME	85,801	6	69	65	94	233
NH	24,065	6	45	41	91	236
NY	127,152	35	175	142	81	1466
RI	3,122	7	18	15	83	96
VT	24,785	27	75	72	96	451
Total	299,342	$\bar{x} = 15$	473	421	$\bar{x} = 91$	3004 [†]

* Includes small water bodies within state boundaries, but excludes Great Lakes and coastal waters.

[†] Includes duplicate map units between states that were eliminated prior to model execution on 2270 soil:climate combinations.

Table 2. Summary statistics for STATSGO map polygons in study area

	CT	MA	ME	NH	NY	RI	VT	TOTAL
Count	720	454	1,082	376	3,278	168	286	6,364
Min. (ha)	76	16	67	22	1	29	76	1
Max. (ha)	83,600	139,000	477,000	107,000	624,000	31,900	101,000	624,000
Mean (ha)	1,770	4,860	7,520	6,250	4,150	1,650	8,460	4,700
% water	2	12	14	12	10	8	3	10

Table 3. Summary statistics components for all modeled map units

	CT	MA	ME	NH	NY	RI	VT	TOTAL
Count	235	344	550	271	1,074	138	481	3,093
Min. (%)	1	1	2	2	1	1	1	1
Max. (%)	39	57	42	57	77	26	63	77
Mean (%)	7.3	7.5	7.2	6.8	7.6	7.4	5.9	7.2
Std. Dev (%)	6.5	8.3	7.1	6.5	8.5	5.5	5.8	7.5

6% in Maine and New Hampshire to 35% in New York State. There were a combined total of 473 soil map units for the seven states in the study area in which 91% were used in the modeling effort. When soil map units were combined with climate regions within the agricultural land-use category, a total of 3,004 potential landscape units were generated for analysis. A total of 2,270 landscape units were used for modeling purposes after duplicate units were eliminated.

Summary statistics for STATSGO soil map unit polygons for the study area are shown in Table 2. The 421 soil map units used in the analysis (Table 1) were represented in the soil geographic database by a total of 6,364 polygons ranging in size from 1 to 624,000 ha (2.4–1,541,904 ac). The area of many polygons were below the specified minimum size delineation for STATSGO maps, and the polygons represented small geographic entities (e.g., islands) requiring some level of map delineation and attribute information. The average size polygon in the study area was 4,700 ha (11,613 ac), ranging from 1,650 ha (4,077 ac) average size delineation in Rhode Island to 7,250 hectare (17,914

ac) average size in Maine. The difference in average size delineation between states did not cause any significant problems with edge-matching of polygons between states because of high quality control in map production by the Natural Resources Conservation Service.

Summary statistics for selected individual components (S51D) used for modeling purposes for all state-level mapping units (MUID) are shown in Table 3. Frequency distributions of components for all state MUID's are skewed toward lower percentages which result from higher number of components occupying smaller proportions of map unit area. New Hampshire and Vermont have the lowest average percentage of MUID components among the seven states, indicating the map units in those states have fewer components, each occupying a higher proportion of land area in the map unit. Maine and New York have the highest percentage of MUID components in which each component occupies a lower proportion of map unit area. How these map units and their respective components are defined within each state significantly influences simulation modeling results at the

landscape scale by contributing disproportionate weight to critical soil properties that occupy small areas of the landscape.

An example of pesticide leaching by soil components in a map unit is shown in Table 4. Component soils, with a limited selection set of soil variables, are shown with (1) annotations indicating status and rationale for component selection, (2) leaching model results, and (3) leaching class for digital mapping of model output. In this example, only 13 of the map unit components were selected for modeling and 34% were eliminated due to the exclusionary criteria (excessive slope gradient, muck, or non-soil conditions). These 13 components occupy 66% of the land area of the map unit.

In the example shown in Table 4, six map unit components were predicted to have high pesticide leaching, corresponding to 30% of the map unit area based on summing the proportional area these components occupy within the map unit. Thus, 45.5% (30/66) of the map unit can be considered as having a high pesticide leaching potential, and would be assigned leaching potential class "2" (25–50%) for map display purposes.

Regional simulations. Results from our regional-scale modeling methodology are mapped graphically in Figure 4. The four map classes of leaching potential are displayed in Figure 4. A visual inspection of this map illustrates some of the relationships between atrazine leaching, climate and parent material. Shifts in leaching potential are clear between certain defined climate region boundaries (e.g., Adirondack Mountain region) and STATSGO soil boundaries (e.g., southern New York). Most of the spatial distribution does not coincide with these mapped boundaries; statistical analysis of the results indicates that between 60–84% of leaching differences is explained by soil organic carbon content (Hutson). The other 16–40% is explained by climate region and parent material. Because these are not independent variables, a spatial interpretation offers clues to the interrelationships between the various elements through the Northeast region.

Integration of dynamic simulation models and environmental databases provides an opportunity to visualize the spatial distribution of landscape units that have the potential of leaching solutes to groundwater resources. Most commonly, modeling results are displayed using color-coded maps delimited by political or environmental boundary conditions. Maps allow decision makers to target selected landscape units for more detailed

Table 4. Example of STATSGO map unit NY084 composition and simulation modeling results in climate region 142

MUID	SSID	COMPNAME	#	COMPACT (%)	SLOPE (%)	ELIMINATED	LEACHED ATRAZINE (mg/m ²)	HIGH/LOW
NY084	NY0086	COLONIE	1	20	8-15			
NY084	NY0016	ELNORA	2	14	0-15	HIGH SLOPE	--	
NY084	NY0086	COLONIE	3	10	3-8		35.8	LOW
NY084	NY0016	ELNORA	4	9	3-8		54.0	HIGH
NY084	MI0038	OAKVILLE	5	7	8-15	HIGH SLOPE	35.8	LOW
NY084	MI0038	OAKVILLE	6	6	3-8		--	
NY084	M10038	OAKVILLE	7	5	0-3		69.5	HIGH
NY084	NY0086	COLONIE	8	5	0-3		69.5	HIGH
NY084	NY0195	CLAVERACK	9	5	3-8		54.0	HIGH
NY084	NY0195	CLAVERACK	10	3	0-3		36.1	LOW
NY084	NY0086	COLONIE	11	3	15-25	HIGH SLOPE	36.1	LOW
NY084	W10116	PLAINFIELD	12	2	0-3		--	
NY084	W10116	PLAINFIELD	13	2	3-8		76.0	HIGH
NY084	NY0195	COSAD	14	2	0-3		76.0	HIGH
NY084	DC0035	URBAN LAND	15	2	0-8	NON-SOIL	27.8	LOW
NY084	CT0070	ELMRIDGE	16	2	3-8		--	
NY084	CT0070	ELMRIDGE	17	1	0-3		37.4	LOW
NY084	W10116	PLAINFIELD	18	1	8-15	HIGHSLOPE	37.4	LOW
NY084	DC0029	PITS	19	1	0-3	NON-SOIL	--	

MUID = Map unit identification symbol; S51D = Soil interpretations record number; COMPNAME = Name of map unit component (soil series, taxonomic unit, or miscellaneous area); COMPACT = Percentage of the map unit occupied by component

Table 5. Proportional area by leaching potential class for each state in study area

Leaching potential class	CT	MA	ME	NH	NY	RI	VT	TOTAL
v. low (< 25%)	3	1	6	0	43	14	29	34
low (26-50%)	4	8	12	5	43	60	8	34
moderate (51-75%)	16	6	30	26	7	14	7	8
high (>75%)	77	85	52	69	7	12	56	24

and site specific studies. Knowing the regional distribution of landscape units serves to inform decision makers on both the scope and level of effort required to develop improved environmental protection strategies or to define more detailed scientifically-based field studies.

Use of GIS has the advantage that it is easy to produce a series of maps demonstrating the effect that each modeling criterion had on a final leaching assessment. However, as is the case with much computer-generated data, GIS-generated maps may be viewed by users as having greater reliability than is warranted. Depending upon the criteria chosen, leaching hazard maps could appear very different, thus it is important to define and understand exactly what a particular map displays.

The spatial frequency distributions of map unit leaching potential by class and by state are summarized in Table 5. Five of seven states in the study area have the highest proportion of modeled land units in the highest leaching potential class due to the combination of climatic conditions and soil properties for the landscape units in those states. For the entire region, how-

ever, 68% of the modeled landscape units fell in the two lower leaching potential classes as a direct result of the high proportion of land units in New York State occurring in these lower two leaching potential classes.

Improving simulation model results at regional scale will require enhanced knowledge and documentation of precipitation patterns, intensity, and variability that could not be derived from the climate database used in this study. More refined definition of climate regions taking into account a denser network of climate stations and interpolation of climate variables for major landscape units not characterized by such stations would significantly improve the precision of leaching estimates generated by model simulations using regional-scale environmental data.

The type and management of land-use practices contribute to soil organic matter content that significantly influences the amount of pesticide leached in soils under a variety of landscape conditions. Organic carbon values used in most regional scale modeling studies are derived from organic matter estimates published in soil survey

databases. These estimates are generalized for a wide spectrum of soils, and do not necessarily reflect organic matter conditions for the landscape unit being modeled. Given the importance of this soil property in mitigating pesticide transport, improved methods are required for determining organic matter contents at landscape scale (Yost et al.). Improvements in the way field soils are characterized and compiled in soil survey databases for simulation modeling purposes has received considerable attention in the soil science literature (Wagenet et al. 1991).

Recommendations

The approach used in this study is applicable at variable spatial and temporal scales, provided the relevant environmental data and knowledge are used at the appropriate scale. Modeling results can be sensitive to the nature and quality of input variables at a given scale. Estimates of solute transport at farm- or field-scale require environmental data that reflect the complexity and variability of detailed soil survey data and microclimatic conditions. Detailed environmental data will not be available for regional scale estimates of solute transport, and interpretation of model output will be limited to the resolution and quality of environmental data used.

Decisions regarding the type of dynamic simulation model to employ for regional-scale estimates of solute transport must consider the scale at which the modeling is being applied and the nature of available environmental data at that scale.

Quantitative comparison tests between model types using a standard set of environmental data is an important component of model selection for each environmental study at any scale. The relative importance of soil or climate parameters in predicting solute transport could be more a function of the computational algorithms or adsorption isotherms used in the model than of the numeric value of the parameter. The biases of each model reflect the scientific training and experience of the model builder, and the application of a particular model to issues such as pesticide leaching to groundwater must take this into consideration.

This study has served to clarify a set of issues related to simulation modeling of pesticide leaching at landscape scale. Additional water quality research issues and research questions that need to be addressed include the following: (1) are definitions of pesticide hazard levels adequate for regional-scale environmental protection strategies, (2) should these levels be defined in terms of mass, concentration, or flux, (3) how do we account for the influence of lower boundary conditions, (4) is predicted leaching from profiles having slowly-permeable subsoils as severe as leaching from freely-draining profiles, and (5) should we consider proximity to aquifers in our regional-scale leaching assessments? These and related questions need to be addressed by the soil and water conservation community through the integration of resource inventory data and simulation models using information technologies relevant to the environmental processes being investigated.

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