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ABSTRACT

Data from seven Management Systems Evaluation Areas (MSEA) were used to test the sensitivity of a leaching model, PRZM-2, to a variety of hydrologic settings common in the Midwest. Results of long-term simulations using regional and generalized input parameters produced ranks of leaching potential similar to those based on measurements. Atrazine leaching was simulated because the use of atrazine was prevalent in the MSEA studies and it frequently occurs in the region's groundwater. Short-term simulations used site-specific soil and chemical coefficients. Generalized simulations used data available from regional soil databases and standardized coefficients. Accurate short-term simulations were precluded by lack of antecedent atrazine concentrations in the soil profile and water, raising questions about simulations using data for less than five years. The ranks of simulated atrazine detections among the study sites were similar to the ranks of observed atrazine detection frequencies. Generalized simulations underestimated the occurrence of atrazine for the three sites where very small concentrations were observed. Simulations overestimated concentrations for the four sites with the greatest frequencies of atrazine detection. Simulations with generalized soils data produced concentrations that compared more favorably with observed detection frequencies than did simulations with site-specific soils data. This is encouraging for regional modeling efforts because soil parameters are among the most critical for operating PRZM-2 and many other leaching models.

ESTIMATING ATRAZINE LEACHING IN THE MIDWEST

Introduction

A variety of agricultural, environmental, and natural resource issues are associated with the occurrence of herbicides in groundwater. Agricultural and environmental nonpoint-source pollution may be effectively evaluated with information from regional assessments of groundwater quality in a variety of hydrogeologic settings.

Agricultural systems that use herbicides have been implemented relatively uniformly over large areas, such as the 12-state North Central Region (Figure 1). However, groundwater responses to these agricultural systems are not uniform because of the variability of the soils, underlying geologic materials, and the range of climatic conditions across the region. Several studies have provided information about the extent and variability of herbicide contamination of groundwater in the Midwest (Holden et al., 1992; Burkart and Kolpin, 1993; Hallberg, 1989). The collective knowledge gained from these and other studies, conducted at a variety of scales, clearly shows that certain combinations of pedologic, climatic, hydrologic, and agronomic factors give rise to conditions of greater groundwater vulnerability to contamination than others.

One approach to quantifying herbicide leaching has focused on aggregating the results of multiple simulations to a regional level for areas defined by political or agricultural boundaries (Bouzaher et al., 1993, 1995; Bleecker et al., 1995) rather than for areas that represent natural resources such as aquifers. Other approaches (Kellogg et al., 1994) have used groundwater vulnerability indices to define vulnerable areas by overlaying chemical use information with key soils characteristics.

This paper examines the potential for estimating regional herbicide leaching using both site-specific and regional data in a pesticide root zone leaching model (PRZM-2) (Mullins et al., 1993). The approach uses short-term simulations based on site-specific soil data and long-term simulations based on data from national soil databases available for points throughout the region. The use of a one-dimensional leaching model to estimate herbicide contamination below the root zone is part of a framework for regional estimation of the groundwater-quality response to herbicide use. An evaluation of the leaching model is a critical step in preparing regional estimates of groundwater responses to chemical use in the Midwest and other regions with similar intensive chemical applications.

Methods and Data Sources

Sites selected for this analysis are part of the Management Systems Evaluation Areas (MSEA) that represent several important groundwater settings in the region (Ward et al., 1994). The MSEA studies are a source of site-specific data that were used to test methods for estimating the relative potential for herbicide leaching (USDA, 1995). Sufficient data were available at seven of the ten MSEA sites to allow testing of the model with specific input data and at least summary information on groundwater concentrations of atrazine (2-chloro-N-ethyl-N'-[1-methylethel]-1,3,5-triazine-2,4-diamine) needed to evaluate simulation results.

Atrazine was selected for model evaluation because it is among the chemicals specifically being studied in the MSEA program. Also, atrazine was the most frequently observed herbicide in the MSEA studies and in surveys of the region's groundwater quality. This last consideration is important for regional analysis because it is necessary to have a sufficient number of detections of a chemical to evaluate the success in estimating its occurrence. If PRZM-2 can adequately simulate leaching of observed atrazine in research sites, then regional assessments of groundwater vulnerability can be improved by application of this model to consistent databases covering larger areas.

The use of previous versions of PRZM (Bouzaher et al., 1993) demonstrated the need to evaluate the effectiveness of the model by comparing simulations with specific observations of herbicide contamination in groundwater or soil water. The results of this study will ultimately be used to develop a metamodel similar to that described by Bouzaher et al. (1993). Metamodels, or regression models, will be developed for specific types of aquifers that have been classified and mapped to define potential vulnerability by hydrologic settings (Burkart and Feher, 1996).

PRZM-2 was selected primarily because it is well documented and many of the input variables are available in regional databases. These regional data can be geographically referenced with information included in the documentation or from existing literature. PRZM-2 has been applied or tested in a variety of conditions including a range of crop and chemical types in various soil and weather settings (e.g., Carsel et al., 1985, 1986; Jones et al., 1986; Loague et al., 1989; Mueller et al., 1992a; Penell et al., 1990; Sauer et al., 1990; Zacharias and Heatwole, 1994). The model is widely used, particularly by industry researchers conducting fate and transport studies required for chemical registration (Jones and Hanks, 1990; Travis, 1992). Finally, the model has been used by the U.S. Environmental Protection Agency (EPA) in several regulatory assessments (Jones and Hanks, 1990) and is currently one of two models (the other being GLEAMS) that are the focus of a more intensive validation effort between the EPA and other cooperators (BRC, 1994).

PRZM-2 is an enhanced version of PRZM (Carsel et al., 1985) that operates on a daily time step and simulates pesticide fate as a function of climate, farming practices, and soil, crop, and chemical characteristics. The analyses in this paper use the last day of each simulated month to represent monthly values. The model consists of two main components: hydrology and chemical transport. The U.S. Department of Agriculture Soil Conservation Service runoff curve–number method (Mockus 1969, 1972) is used to partition precipitation at the soil surface between infiltration and surface runoff. Generalized soil parameters such as field capacity and wilting point are used to route water vertically downward through the soil profile, and evapotranspiration is simulated from pan evaporation data or as a function of temperature. Simulated chemical transport and transformation processes include first-order decay, soil sorption, dispersion, advection, retardation, plant uptake, volatilization, and losses to leaching and surface runoff in both sediment and dissolved phases. Pesticide concentrations in the soil profile can be estimated for the dissolved, sorbed, and vapor phases.

Atrazine movement to a maximum depth of 2 m was simulated in soil profiles at all sites. Depth to saturation is known to vary considerably, and simulations using deeper water table conditions will likely produce smaller concentrations or smaller frequencies of atrazine detection. However, 2 m is a depth to which adequate data on soil variables are commonly available. Also, it is sufficiently shallow to represent a water table depth likely to produce maximum groundwater contamination, conditions that occur in many hydrogeologic settings early in the growing season when most herbicides are applied. It is expected that limiting simulations to 2 m depths will produce results that are not directly comparable to measurements of atrazine in the saturated zone. The assumption is made, however, that leaching to 2 m is an adequate indicator of the potential for leaching to the saturated zone. Obviously, data on hydrogeochemical variables for the deeper unsaturated zone would greatly improve the relevance of simulated results.

The model divides the soil profiles into several homogeneous layers. Each layer is further subdivided into compartments of equal thickness. These compartments are used in simulating vertical water movement and contaminant leaching and play a critical role in the solution of the numerical transport equations. The surface layer thickness was set at 1.0 cm with a single compartment that was also specified to be 1.0 cm. This thin layer was used at the surface to facilitate accuracy in simulating atrazine surface runoff and volatilization, although only predicted leaching losses will be discussed in this paper. Compartment sizes of 5.0 cm were used for the remaining soil layers, following recommendations given in Carsel et al. (1985) and Mullins et al. (1993).

Two types of simulations were used in this analysis: short-term site-specific and long-term generalized simulations. Short-term site-specific simulations were one to six years duration, the maximum periods for which weather and atrazine application data were available in the study sites selected. These simulations represent the most complete use of site-specific input data available at each MSEA. Long-term generalized simulations extended 30 years and used regional soils data obtained from the Map Unit Use File (MUUF) Interactive Soil Database (Baumer et al., 1994), standardized degradation rates and sorption coefficients, and uniform atrazine application rates. These simulations also used 30-year weather records created with a weather generator developed by Nicks and Lane (1989) that is embedded in the EPIC model (Williams, 1990, 1995). Long-term simulations using site-specific soil parameters were compared with simulations using MUUF soils as a measure of the model's sensitivity to soil input parameters. Generalized simulations represent prototypes that will be used to develop regional simulations from regionally consistent soil, weather, and management data.

Seven MSEA sites (Figure 1) were selected to represent the principal hydrogeologic settings in the Midwest. These projects provide specific observations of leaching response to similar agricultural systems in varying hydrologic settings. The hydrologic settings studied in this paper were selected to examine the sensitivity of the model to a variety of conditions in the Midwest and to determine the potential use of such a model in this range of conditions. The Walnut Creek watershed in Iowa represents Wisconsinan-age glacial till with extensive tile drainage. The Treynor watershed in Iowa represents deep loess deposits with moderate leaching potential. Three sites represent conditions associated with alluvial aquifers, a hydrologic setting that is among the most vulnerable in the region: the Scioto River site located on an alluvial aquifer in Ohio; the Arena site located in the Wisconsin River valley; and the Shelton site in Nebraska located in the Central Platte valley. Goodwater Creek watershed in Missouri was selected as representative of soil with very low downward water fluxes due to claypan soils developed on loess deposits. The Princeton site in central Minnesota represents glacial outwash deposits of sand and gravel in a setting hypothesized to have among the greatest potential for rapid recharge and potential herbicide leaching.

The site-specific data provided by MSEA researchers included weather, soil descriptions, crop and tillage system, atrazine application rates and dates, and concentrations of atrazine in water observed beneath each site. Daily weather data were available for four or more years at each MSEA. Irrigation schedules were provided for five years at the Princeton site and for six years at the Shelton site. These schedules were used to estimate long-term irrigation inputs as well. Annual data were provided for all seven sites covering planting, emergence, and harvest dates for continuous corn, atrazine application rates and dates, and other management inputs. Laboratory or field measurements of atrazine sorption coefficients (K_d) and degradation rates (half-lives) were provided for the Arena, Scioto River, Shelton, and Walnut Creek sites. Estimated K_d and half-lives were used for the Princeton, Goodwater Creek, and Treynor sites.

The hydrologic component of the model was calibrated prior to performing the simulations in this study (results not included). This calibration consisted of adjusting the standard runoff curve-numbers (as given by Mockus, 1969), within appropriate bounds, until a match was achieved between observed conditions and simulated annual average surface runoff volumes. This step assured partitioning of the precipitation between runoff and infiltration consistent with local observations.

The water media used for observed atrazine detections in the saturated zone varied among sites. Measurements taken in media ranging from tile-effluent to piezometer samples were used to represent drainage through the soil profile. Because the measured atrazine was derived from the saturated zone, these measurements are not directly comparable to what may be measured or simulated in the unsaturated zone at 2 m depth. Consistent data on atrazine detections are not yet available for soil or water at all MSEA sites. Consequently, the available data were summarized as frequency of detection at 0.2 $\mu g\ L^{-1}$. This provides a measure of relative leaching for comparison among the sites and with the simulations. Simulation results were soil solution concentrations of atrazine that also were summarized as detection frequencies for comparison to the observed detections.

Short-term site-specific simulations were conducted to determine how closely the model simulated the observed concentrations of atrazine, using input parameters generated as part of the local research projects. Soil solution concentrations simulated at a common depth of 2 m were used in order to make consistent comparisons among sites. The depth of the available site-specific soil-layer data ranged from 1.3 m at Goodwater Creek to 2.0 m at Scioto River and Treynor. Data from the deepest layer were extended to 2.0 m for those sites with soil-profile depths of less than 2.0 m. Specific values of the input variables used in the short-term site-specific simulations at each site are listed in Table 1. Daily weather data collected at each site were used in these simulations; irrigation applications were added to daily precipitation totals in the Princeton and Shelton simulations.

Degradation of atrazine was estimated as a function of depth (see equation 1) for use in simulations for the Princeton, Goodwater Creek, and Treynor sites because no laboratory or field values of sorption or degradation were available for the materials in those sites. Generally, atrazine half-lives in the subsurface (down to 2) increase between two and ten times that of the surface soil (upper 25 cm). The variation in half-life at depth is attributed to variability in the activity of soil microbial populations that, in turn, are influenced by the availability of organic substrates, porosity, and properties of the chemical itself (Moorman, 1994). Equation 1 was derived from recent studies of degradation measured in surface and subsurface soils under optimal moisture and temperature conditions. The equation describes a least-squares fit to half-life determinations from many published studies. These studies include determinations for atrazine (Kruger et al., 1993; Stolpe and Shea, 1995; Jayachandran and Moorman, written communication); for alachlor [2-chloro-(2,6-diethylphenyl)-*N*-(methyoxymethyl)acetanalide] (Pothuluri et al., 1990; Stolpe and Shea, 1995; Yen et al., 1994); for fluometuron [*N,N*-dimethyl-*N'*-[3-(trifluoromethyl)phenyl]urea] (Mueller et al., 1992b); for metribuzin [4-amino-6-(1,1-dimethylethyl)-3-(methylthio)-1,2,4-triazin-5(*4H*)-one] (Kempson-Jones and Hance, 1979; Moorman and Harper, 1989); and for chlorsulfuron [2-chloro-*N*-[[(4-methoxy-6-methyl-1,3,5-triazin-2-yl)amino]carbonyl]benzenesulfonamide] (Walker et al., 1989). Pesticides that are degraded abiotically, such as aldicarb [2-Methyl-2-(methylthio)propanal *O*-((methylamino)carbonyl)oxime], were not included because they may not respond in a similar manner to soil depth. The application of this function to depths greater than 2 m may not be appropriate because the relationship between depth and half-life may not be linear below 2 m.

$$HL_d = [0.0284 * \text{DEPTH} + 1] * HL_s \tag{1}$$

where:

DEPTH = soil depth (cm),

HL_d = half-life at depths of up to 2 m (d),

HL_s = half-life of surface soil (d), and

0.0284 is the slope of the regression line relating depth to half-life.

A surface half-life for atrazine of 60 days was used for the Princeton, Goodwater Creek, and Treynor short-term simulations. Values for half-life were calculated for each soil layer depth and used in subsequent simulations where generalized inputs were needed.

Results and Discussion

Short-Term Site-Specific Simulations

One important result from the short-term simulations is the general trend of increasing concentrations throughout the simulated periods at all sites. A plot of the simulated concentrations at the last day of each month for the Goodwater Creek site (Figure 2) shows this typical trend of increasing concentrations and the Treynor, Walnut Creek, and Shelton sites where very small concentrations of atrazine were simulated. Following application of atrazine each year, the simulated annual maximum concentrations at 2 m increased substantially for the first three years.

Simulated concentrations showed seasonal variations with peak concentrations following the annual application date and declining concentrations during the remainder of the year. Each atrazine application provided an additional source that moved the atrazine front deeper as the sorption and degradation capacity of the soil was exceeded. Annual increases in the maximum concentration at 2 m were less after the initial years, but the profile had not reached a balance after six years among dissolved, transformed, and sorbed atrazine. Simulated concentrations at several depths showed a front of larger concentrations that moved into progressively deeper compartments following each application period. In general, even extremely small concentrations (10^{-7} μg L^{-1}) were not simulated at 2 m depths until at least the second simulated year.

A different short-term pattern of atrazine concentrations was simulated for the Princeton and Arena sites, where relatively large concentrations were simulated at the end of the first year (Figure 3). For both of these sites, the simulated annual maximum concentration at 2 m increased each year for the first three years, as for the sites described above. However, the relatively rapid water flux and small K_ds at these sites did not retard the transport of atrazine as greatly as at the other sites. For these sites with rapid flux, atrazine transport may respond more readily to precipitation events, annual precipitation patterns, or irrigation schedules.

These examples illustrate a general problem encountered when simulating short-term responses using limited information on antecedent concentrations of atrazine in the soil column and water. Without consistent data on concentrations of atrazine throughout the soil profile and in groundwater at each site before the simulated period, the lag in response to atrazine inputs at the surface makes it difficult to conduct accurate simulations. The short-term simulation results raise a question about the utility of data sets with less than five years of data. Ideally, short-term data sets would be more useful if they included historical crop information and chemical use rates as well as preliminary measures of both water and soil atrazine concentrations to represent antecedent conditions. These types of data sets are rare, however, and are not available even in an extensive, multiagency program such as MSEA.

Short-term simulation results did not approximate the measured concentrations of atrazine in groundwater at any of the sites, as expected. Short-term simulations for all seven sites were compared using summary box plots of concentrations at 2 m for the last day of each month during the simulation periods (Figure 4). Simulations for the Princeton and Arena sites produced the largest atrazine concentrations of all the simulated sites. Groundwater measurements at these sites had among the greatest frequencies of atrazine detection (Table 2) but few of these concentrations exceeded 1.0 µg L^{-1}.

Simulation results were ranked using the 75th percentile of concentrations because many sites produced no atrazine in excess of 0.2 µg L^{-1}. Using this variable to rank simulated leaching potential took advantage of information at exceptionally small concentrations that could be simulated but not detected. Goodwater Creek and Walnut Creek had among the smallest frequencies of detection, and simulations reflected these relatively small detection frequencies. Simulations of the Scioto River site showed no atrazine leaching, a result that correlates well with field measurements. But simulated atrazine detections (0 %) at the Shelton site were well below the frequency of atrazine detection at the site.

Short-term simulations of leached atrazine concentrations at the Shelton site (Figure 4) are less than those simulated at all other sites except Scioto. These results contradict the reported concentrations of 2.0 to 6.0 µg L^{-1} in groundwater in this area (Fausey et al., 1995; R. Spaulding, personal communication). The half-life and K_d were obtained from experiments using soil collected from the site (Stolpe and Shea, 1995). The soil had a long history of atrazine use, and subsequent research revealed a large population of atrazine-degrading microorganisms in the surface soil, which is consistent with the short atrazine half-life (Jayachandran et al., 1998). The small half-life used in the simulations substantially reduced the fraction of atrazine that was leached. The site is irrigated, however, and this practice introduces sufficient water to support macropore flow, which would effectively bypass the surface soil and transport atrazine deep into the profile where longer half-lives and lower K_ds would favor further leaching. PRZM-2 does not include a mechanism for simulating macropore flow.

Short-term simulations resulted in no atrazine leaching to 2 m depth at the Scioto River site, which is in agreement with the absence of atrazine detection in groundwater at this site and low concentrations in the soil profile (Workman et al., 1995). These results are somewhat unexpected because soil texture and drainage properties suggest that the atrazine leaching would be similar to that of the Shelton site. Several factors may be responsible for the lack of atrazine leaching. A K_d value of 8.2 was used in the surface 30 cm and a half-life of 53 days. These values were determined in soil collected from the rotated-corn system at that site (Blume, 1995). The K_d value exceeds the sorption of atrazine predicted from the organic C content of the soil and a K_{oc} value of 100. Recent reports suggest that the aquifer microorganisms at the site degrade atrazine at rates greater than that predicted by the depth-degradation function (equation 1), although half-life estimates were not computed. The sediments used in these studies were collected under a field with a long history of continuous corn and atrazine use, which has apparently resulted in enhanced atrazine degradation similar to that observed at the Shelton site (Radosevich et al., 1996; Ostrofsky et al., 1997). Although the site-specific model results agree with field observations at the site, estimates of degradation rates from site-specific studies can be difficult to extrapolate for regional analyses.

Long-Term Generalized Simulations

Long-term generalized simulations were conducted to determine the model's performance using data from national soil databases and generalized values for K_d and half-life. Soil-layer data for long-term simulations (Table 3) were obtained from the MUUF soil database (Baumer et al., 1994). The MUUF database contains an interface that enables the user to access the Natural Resources Conservation Service (NRCS) Map Unit Interpretation Record (MUIR) data records (previously known as SOILS5) by state and county and to output the data in one of several possible formats. Estimation of properties that are not included in the MUIR, such as field capacity and wilting point, are incorporated in this data translation step. For this study, the pertinent soil data were output in the format required for the Erosion-Productivity Impact

Calculator (EPIC) model (Williams 1990, 1995) and then further processed into the desired PRZM-2 formats, because an option was not available for direct output in PRZM-2 format. It was assumed that the bottom layer again extended to a depth of 2 m for sites where the total MUUF soil layer depth was less than 2 m.

A uniform atrazine application rate of 1.0 kg ha^{-1} was used in each simulation. Atrazine half-lives were calculated using equation (1) with a surface half-life of 60 days (Wauchope et al., 1992). Values for K_d were calculated as the product of soil organic carbon content and a K_{oc} of 100. Irrigation inputs for the Princeton and Shelton simulations were based on the irrigation schedules used in the short-term simulations. Rainfall totals for the 30 years were ranked; irrigation schedules for the year with the smallest application in the short-term record were added to the years with the most rainfall and vice versa.

Long-term simulations from all seven sites were compared using summary box plots of concentrations at 2 m for the last day of each month during the simulation periods (Figure 5). Concentrations in all sites were generally larger in the long-term simulations (Figure 5) than in the short-term ones (Figure 4). Median and quartile values were larger in all cases, particularly at sites such as Goodwater Creek, Scioto River, Shelton, and Walnut Creek. The larger concentrations were due, in part, to the fact that the long-term simulations included sufficient time (more than five years) for concentrations in the simulated soil column to establish a balance among annual atrazine application, flux, sorption, and degradation. Values for K_d calculated as above for the long-term simulations, were generally less than those used in the short-term simulations, and the half-lives were generally larger. The result was an increase in the atrazine residual available for water transport in long-term simulations. However, these differences were substantial only in simulations of the Shelton and Scioto River sites.

Results of the long-term simulations compare more favorably with the total frequency of detection observed at each site (Table 2) than did the short-term simulations. The ranking of leaching potential based on simulated results also compares favorably with the ranking of measured results. In the three sites with the least leaching potential (Table 2), the long-term simulations generally resulted in an underestimation of the concentrations of atrazine (Figure 5). Those three sites—Goodwater Creek, Scioto River, and Walnut Creek—had fewer than 10 percent atrazine detections and no simulated detections exceeding 0.2 μg L^{-1}. Simulations of the Scioto site resulted in median and 75th percentile concentrations slightly larger than those of Goodwater Creek. The median and 75th percentile concentrations for Walnut Creek were larger than both of the other two, and this site had the largest frequency of simulated atrazine occurrence among these three sites.

The sites with simulated concentrations exceeding 0.2 μg L^{-1} (Princeton, Arena, Shelton, and Treynor) were also sites with more than 25 percent observed detections of atrazine. The ranking from largest to smallest observed frequencies among these four sites (Table 2) is similar, but not identical, to the ranking of the simulated concentrations (Figure 5). The Shelton site simulations do not rank as high among the four, but the Princeton, Arena, and Treynor sites have the same rank between the observed and simulated results. With the exception of Shelton, simulations generally overestimated the concentrations and frequency of observed atrazine detections. The Shelton simulated concentrations were all less than the majority of observed concentrations that exceeded 1.0 μg L^{-1}.

Three MSEA sites are underlain by alluvial aquifers: Arena, Scioto River, and Shelton. Simulation results of these sites provide some useful results for regional simulations. There is a large range of simulated concentrations from those of the Scioto River site to the Arena site, with Shelton in between. Alluvial aquifers have been considered among the most vulnerable to herbicide contamination, although herbicides of any kind were detected in only 28 percent of alluvial and other unconsolidated aquifers in the Midwest (Kolpin et al., 1994). The diversity of responses from the generalized simulations may represent the diversity of soil and hydrologic conditions in the region-wide sampling by these researchers.

The sensitivity of the model to soil variables was tested. Soil variables are among the most critical parameters that control simulations of herbicide leaching, but also are most readily and consistently available for large regions such as the Midwest. Long-term simulations using the MUFF files of soil parameters (Table 3) were compared with simulations where only the soil parameters were replaced with locally derived soil parameters (Table 1). The results are illustrated (Figure 6) using two sites to represent quite different simulated and measured atrazine detection frequency—Arena and Goodwater Creek. The results show sufficient similarity in the outcomes of the two sets of simulations to allow the credible use of regional soils data to simulate leaching with PRZM-2 in a variety of Midwest soil and hydrologic conditions.

Conclusions

Neither short-term simulations using site-specific input data nor long-term simulations with generalized inputs resulted in concentrations of atrazine equal to those observed. However, the long-term generalized simulations produced results that compared more favorably with observed detection frequencies than did the short-term site-specific simulations.

More accurate results of short-term site-specific simulations could not be achieved without measures of antecedent atrazine concentrations in the soil profile and water. This raises questions about the utility of data sets of less than five years for modeling long-term leaching.

Simulations using site-specific, measured values of some input variables, particularly half-life and K_d, produced results that were less consistent with measured atrazine occurrence than simulations with more generalized values for these variables. This may result from the use of values derived from either field or laboratory tests, but not both at any site. Laboratory determinations, in particular, may not represent adequately the response to all processes affecting sorption or degradation of atrazine.

In general, it was found that data available from MSEA projects were more anecdotal than representative of general conditions. These data also lacked the consistency necessary to make the specific comparisons among sites or with simulations.

Ranks of simulated atrazine leaching potential using PRZM-2 and generalized input data for the seven sites studied were similar to ranks of the observed frequency of atrazine detection at those sites. This is justification for the application of PRZM-2 to the estimation of leaching potential in the Midwest region.

Generalized, long-term simulations tended to underestimate the frequency of atrazine detection at sites where very small frequencies were observed. In contrast, simulations generally overestimated detection frequencies in three of the four sites with the largest frequencies of atrazine detection.

Long-term simulations using soils data available in a national database produce estimates of atrazine leaching that are not substantially different from those using site-specific soils data.

This is encouraging for regional modeling efforts because soil parameters are among the most critical for operating PRZM-2 and many other leaching models.

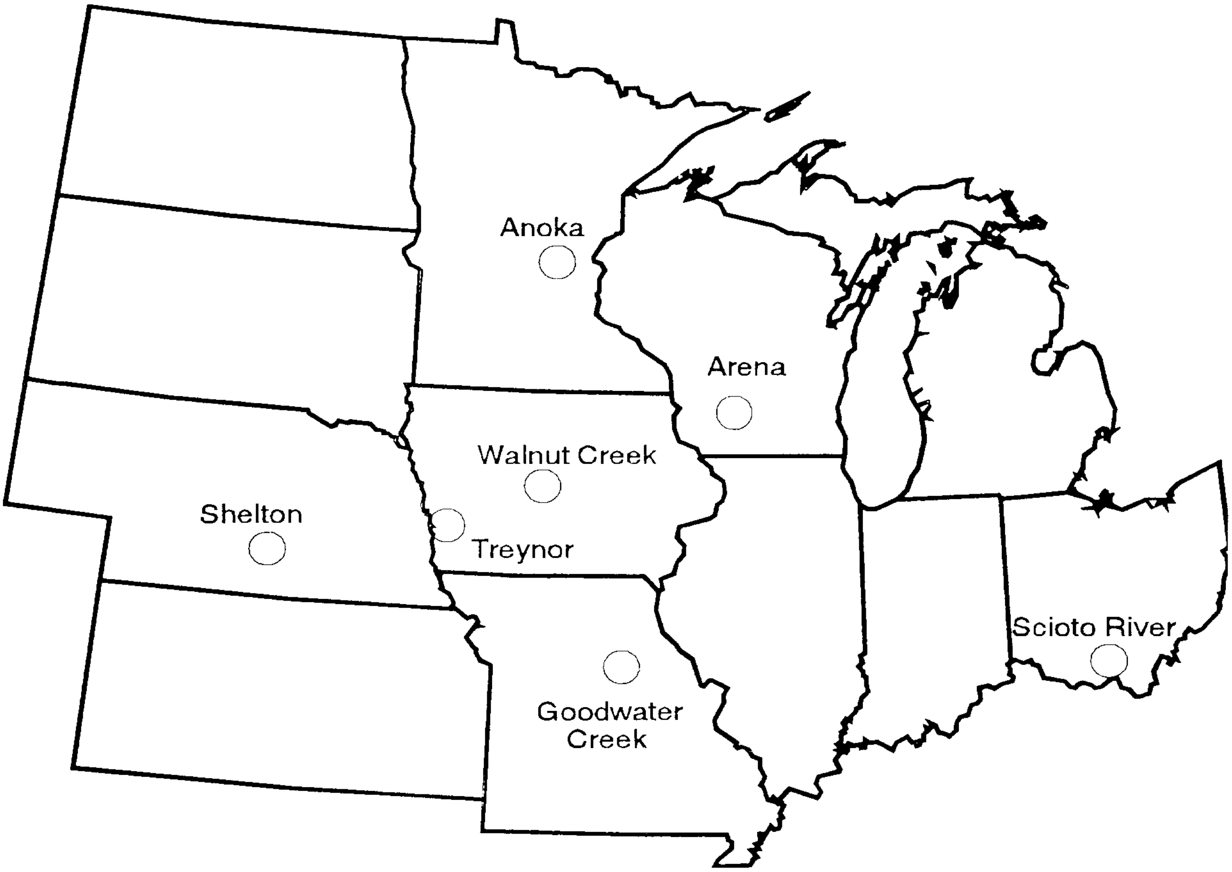

Figure 1. Midwest corn and soybean producing region showing location of Management Systems Evaluation Areas used in simulations

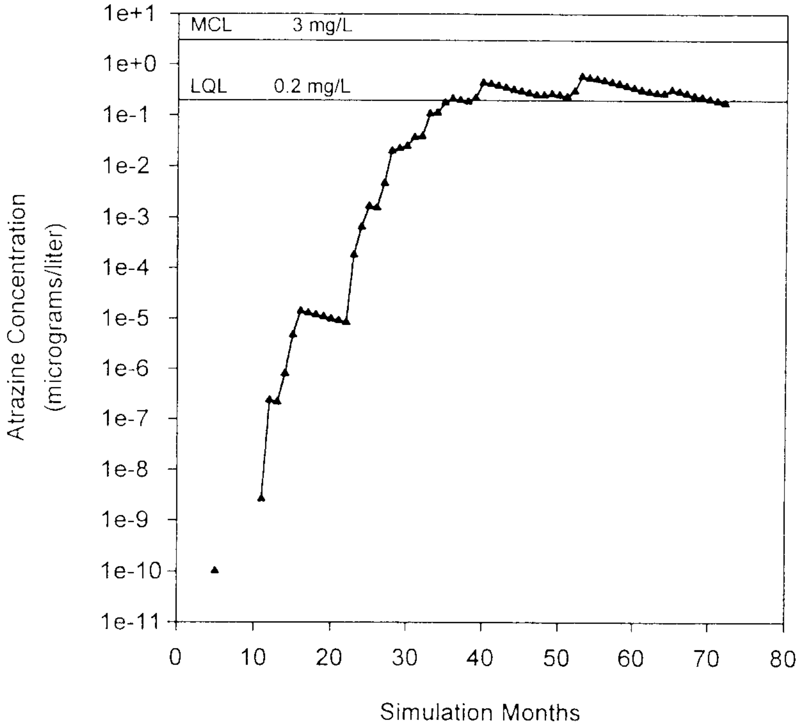

Figure 2. Short-term simulated dissolved atrazine concentration in water at 2m depth for the Goodwater Creek, Missouri site. (MCL is 3.0 $\mu g\, L^{-1}$, the maximum contaminant level, and LQL is 2.0 $\mu g\, L^{-1}$, the quantitation limit commonly reported in MSEA studies)

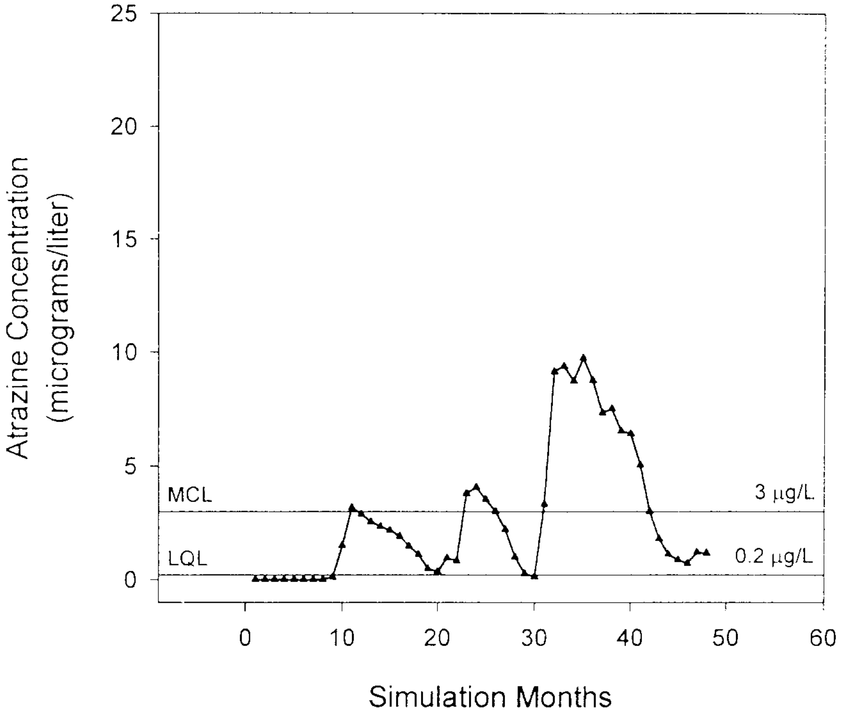

Figure 3. Short-term simulated dissolved atrazine concentration in water at 2 m depth for the Arena, Wisconsin site. (MCL is 3.0 µ*g* L^{-1}, the maximum contaminant level, and LQL is 0.2 µ*g* L^{-1}, the quantitation limit commonly reported in MSEA studies)

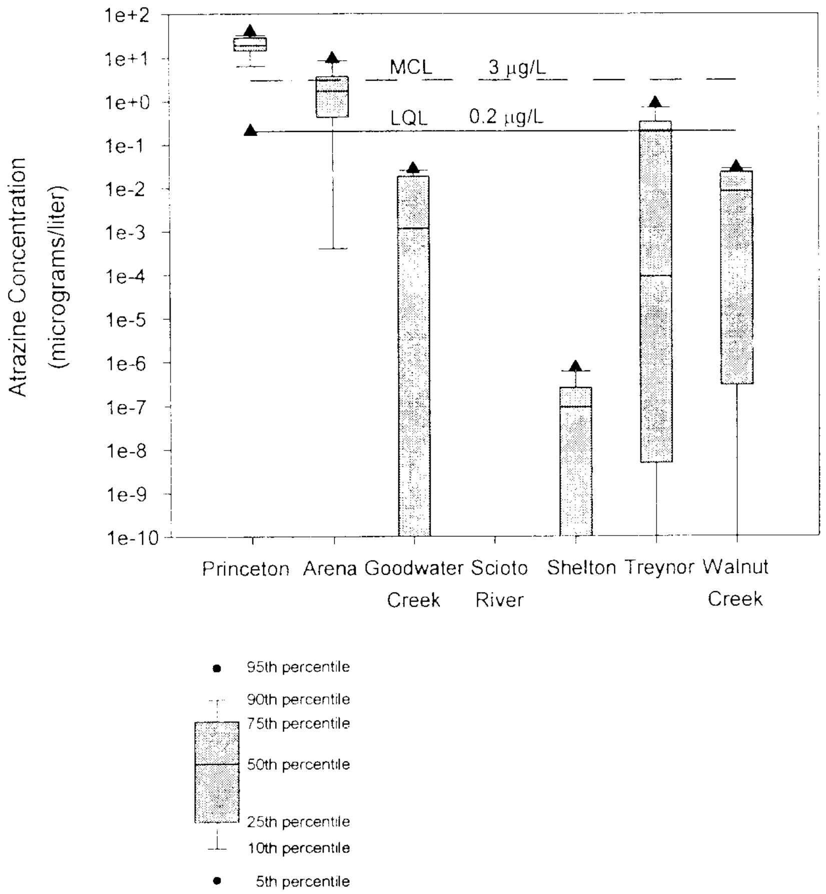

Figure 4. Summary box plots from the short-term simulated concentrations of the last day of each month at 2 m depth for the seven study sites. An example box plot is also shown.

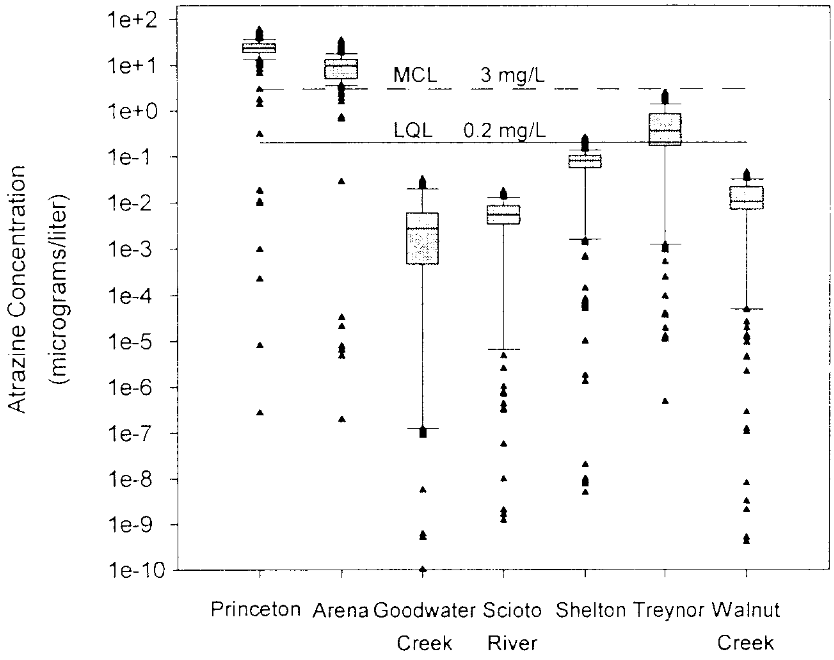

Figure 5. Summary box plots from the long-term simulated concentrations of the last day of each month at 2 m depth for the seven study sites

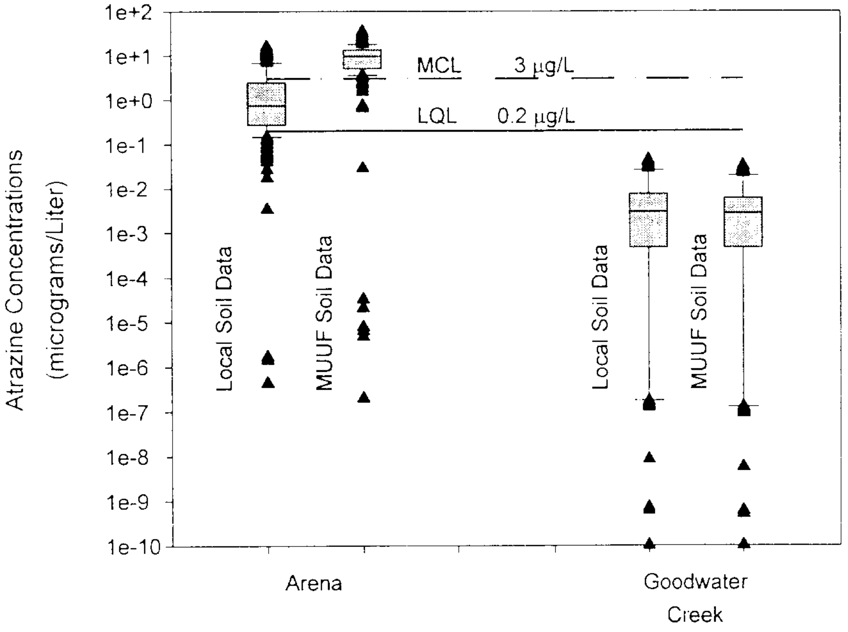

Figure 6. Summary box plots of simulated atrazine concentrations using MUUF and locally derived soils data

Table 1. Values for input variables used in short-term, site-specific simulations.

MSEA Site	Depth (cm)	Half-life (days)	K_d	Bulk density (g/cm^3)	Organic carbon (%)	Field capacity	Wilting point	Soil Type	Atrazine Application Rate (kg/ha)
Princeton, MN	0-25	60	0.5	1.45	0.50	0.10	0.06	Zimmerman (sand)	1.67
	25-200	*	0.1-0.5	1.41-1.45	0.10-0.50	0.05-0.10	0.03-0.06		
Arena, WI	0-65	37	0.15-0.56	1.48-1.59	0.15-0.56	0.08-0.11	0.04-0.11	Sparta (sand)	0.84
	65-200	116	0.01-0.08	1.48-1.50	0.01-0.08	0.46-0.51	0.03		
Goodwater Creek, MO	0-25	60	1.39-2.09	1.25-1.32	0.87-1.27	0.30-0.33	0.15-0.26	Mexico (silt loam)	2.24
	25-200	*	0.22-1.58	1.25-1.40	0.14-0.99	0.30-0.35	0.16-0.27		
Scioto River, OH	0-30	53	8.2	1.19	1.58	0.40	0.16	Huntington (silt loam)	1.40
	30-200	53	3.3	1.19-1.43	0.09-1.37	0.35-0.41	0.15-0.18		
Shelton, NE	0-20	17	3.82	1.27	1.22	0.36	0.14	Hord (silt loam)	2.07
	20-45	60	1.74	1.27-1.47	0.29-1.22	0.34-0.36	0.17		
	45-120	183	0.68	1.47	0.29	0.32-0.34	0.14-0.17		
	120-200	118	0.59	1.47	0.29	0.32	0.14		
Treynor, IA	0-25	60	0.75	1.34-1.44	0.75-1.4	0.25-0.27	0.12-0.13	Ida (silty clay loam)	1.40-3.40
	25-200	*	0.52-0.55	1.26-1.39	0.19-0.75	0.26-0.30	0.10-0.13		
Walnut Creek, IA	0-30	58	2.7-3.0	1.41-1.44	2.7-3.0	0.25-0.26	0.13-0.14	Clarion (loam)	0.39-0.56
	30-115	250	0.4	1.50-1.51	0.2-1.4	0.26-0.28	0.12-0.14		
	115-200	1730	0.31	1.51	0.1	0.28	0.13		

*Half-life increased as linear function of depth.
Values were varied with depth in intervals where a range of values is shown.
Ranges of atrazine application rates represent reported variations in annual application.

Table 2. Comparison of atrazine detection frequency in groundwater beneath simulated Management Systems Evaluation Areas.

	Measured Detections		**Long-term Simulations**		**Short-term Simulations**	
Site	Detection Frequency (%)	Rank of leaching potential	Detection Frequency (%)	Rank of leaching potential	Detection Frequency (%)	Rank of leaching potential
			Sites with most leaching potential			
Shelton	98	1	3	4	0	6
Princeton	68	2	96	1	100	1
Arena	41	3	96	2	98	2
Treynor	29	4	69	3	27	3
			Sites with least leaching potential			
Walnut Creek	9	5	0	5	0	4
Goodwater Creek	6	6	0	7	0	5
Scioto	7	7	0	6	0	7

Note: Frequency of occurrence is expressed as percent of samples exceeding 0.2 $\mu g\ L^{-1}$. Ranks for sites are from 1 representing the greatest leaching potential to 7 representing the least leaching potential based on the frequency of measured detection or the 75 percentile for simulated concentrations.

(Measured frequencies provided by Sharon Clay, Robert Dowdy, Geoffrey Delin, Norm Fausey, Jerry Hatfield, Robert Lerch, Roy Spalding, and Thomas Steinheimer, oral and written communications.)

Table 3. Values for input variables used in long-term, generalized simulations.

MSEA Site	Depth (cm)	Half-life (days)	K_d	Bulk density (g/cm^3)	Organic carbon (%)	Field capacity	Wilting point	Soil Type
Princeton, MN	0-26	60	0.44	1.68	0.44	0.08-0.09	0.04-0.05	Zimmerman
	26-200	*	0.15	1.77	0.15	0.09	0.05	(sand)
Arena, WI	0-26	60	0.32-0.73	1.65-1.69	0.32-0.73	0.08	0.04	Sparta
	26-200	*	0.15-0.32	1.69-1.81	0.15-0.32	0.05-0.08	0.03-0.04	(sand)
Goodwater Creek, MO	0-26	60	0.44-1.74	1.25-1.31	0.44-1.74	0.32-0.48	0.13-0.28	Mexico
	26-200	*	0.15-0.44	1.25-1.40	0.15-0.44	0.42-0.45	0.26-0.36	(silt loam)
Scioto River, OH	0-26	60	2.62	1.19	2.62	0.40	0.16	Huntington
	26-200	*	0.29-2.62	1.19-1.48	0.29-2.62	0.35-0.41	0.15-0.18	(silt loam)
Shelton, NE	0-26	60	1.74	1.27	1.74	0.35	0.13	Hord
	26-200	*	0.29-1.74	1.27-1.47	0.29-1.74	0.35-0.38	0.13-0.16	(silt loam)
Treynor, IA	0-26	60	0.15-1.45	1.30-1.51	0.15-1.45	0.34-0.35	0.13	Ida
	26-200	*	0.15	1.51	0.15	0.34	0.13	(silty clay loam)
Walnut Creek, IA	0-26	60	2.33	1.30	2.33	0.31	0.13	Clarion
	26-200	*	0.15-2.33	1.30-1.59	0.15-2.33	0.24-0.31	0.10-0.16	(loam)

*Half-life increased as linear function of depth.

Values were varied with depth in intervals where a range of values is shown.

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