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GIS based ArcPRZM-3 model for bentazon leaching towards groundwater

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Abstract

Groundwater contamination due to pesticide applications on agricultural lands is of great environmental concern. The mathematical models help to understand the mechanism of pesticide leaching in soils towards groundwater. We developed a user-friendly model called ArcPRZM-3 by integrating widely used Pesticide Root Zone Model version 3 (PRZM-3) using Visual Basic and Geographic Information System (GIS) based Avenue programming. ArcPRZM-3 could be used to simulate pesticide leaching towards groundwater with user-friendly input interfaces coupled with databases of crops, soils and pesticides. The outputs from ArcPRZM-3 could be visualized in user-friendly formats of tables, charts and maps. In this study we evaluated ArcPRZM-3 model by simulating bentazon leaching in soil towards groundwater. ArcPRZM-3 was applied to 37 sites in Woodruff County, Arkansas, USA to observe the daily average dissolved bentazon concentration for soybean, sorghum and rice at a depth of 1.8 m for a period of two years. Nineteen ranks of bentazon leaching potential were obtained using ArcPRZM-3 for all sites having different soil and crop combinations. ArcPRZM-3 simulation results for bentazon were compatible with the field monitored data in term of relative ranking and trend, although some uncertainties exist. This study indicated that macropore flow mechanism would be important in analyzing the effect of irrigation on groundwater contamination due to pesticides. Overall, ArcPRZM-3 could be used to simulate pesticide leaching towards groundwater more efficiently and effectively as compared to PRZM-3.

Key words: ArcPRZM-3; PRZM-3; GIS; pesticide leaching; groundwater contamination; bentazon

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Introduction

Pesticides play an important role in ensuring good crop yields in conventional agriculture (Whelan et al., 2007). As a result of agricultural practices, pesticides have been detected in many aquifers and surface waters (Capkin et al., 2006; Köhne et al., 2006). Contamination of groundwater by agrichemicals (pesticides and fertilizers) is now widely recognized as an extremely important environmental problem (Chang et al., 2008). Pesticides applied at or near the soil surface can leach to considerable depths (Loague et al., 1998). A more prudent approach to prevent groundwater contamination by pesticides must be based on understanding the relationships among chemical properties, soil properties, and the climatic and agronomic variables that induce leaching (Macur et al., 2000). Pesticide fate models account for a variety of processes including soil water flow, solute transport, heat transport, pesticide sorption, transformation and degradation, volatilization, crop uptake, and surface runoff. A particular modeling challenge is to predict pesticide transport at very low leaching levels important for pesticide registration (Köhne et al., 2006). The modeling of pesticide distribution in soil help to minimize health risks associated with soils contaminated by pesticides (Yang et al., 2009).

The Arkansas Delta region in USA has been very productive in agriculture contributing significantly to the economies of Arkansas, Mississippi and Louisiana states. Arkansas ranks first in USA in rice production, fourth in cotton, fifth in grain sorghum, and eighth in soybean (Arkansas Agricultural Statistics Service, 1994). Most of the agricultural lands of Arkansas are in the Delta region. More than four billion gallons of water were withdrawn from the alluvial aquifer per day in 1990 for irrigation, aquaculture, industry, and municipal water supplies (Holland, 1993). Groundwater is widely used for drinking, agriculture, industry, urban development, wetlands and recreation. Due to high crop productivity in this region, there is extensive use of pesticides including insecticides, herbicides, fungicides and defoliants. The wide use of pesticides contributes to the groundwater contamination. Heavy rainfall (about 50 inches per year), the extensive irrigation (approx. 3 million acres of cropland are irrigated annually), the spatial complex nature of soils and geological strata and diverse crop management activities are some of the factors that strengthen the hazardous effect of

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pesticides towards groundwater contamination. Our study area was Woodruff County which is located in Arkansas Delta region of USA and it was selected because of its importance for agricultural production.

Several pesticides including metolachlor, bentazon, alachlor, atrazine, acifluorfen, fluometuron, and diazinon have been detected in wells in this region (Nichols et al., 1993; Senseman, 1994). For this study, benatzon was simulated using ArcPRZM-3 as it was the most commonly applied and detected pesticide in the study area. Bentazon is a general use pesticide (GUP) that is classified as toxicity class III – slightly toxic. It is a post-emergence herbicide used for selective control of broadleaf weeds and sedges in beans, rice, corn, sorghum, peanuts, mint, and others. It has low persistence in soils and its half-life is less than two weeks (Wauchope et al., 1992). It is subjected to breakdown by ultraviolet (UV) light from the sun and rapid degradation by soil bacteria and fungi (US National Library of Medicine, 1995). Bentazon does not bind to soil particles and it is highly soluble in water. These characteristics usually suggest a strong potential for groundwater contamination. Based on a national survey, the United States Environmental Protection Agency (US EPA) estimated that bentazon might be found in about 0.1% of the rural drinking water wells nationwide (US EPA, 1992). Bentazon has the potential to contaminate surface water because of both its mobility in runoff water from treated crops, and its pattern of use on rice, which involves either direct application to water or application to fields prior to flooding.

Mathematical models are cost effective methods which provide efficient ways to determine pesticide leaching towards groundwater as compared to field sampling studies. Moreover, modeling provides a useful tool in analyzing soil-plant-water interactions which makes it possible to determine the potential effect of a hazardous chemical on groundwater (Kaluli et al., 1996). Descriptions of models for simulating transport of pesticides can be found in several reviews and model comparison studies (Garratt et al., 2003; Šimůnek and Genuchten, 2008). Although many models for simulating pesticides have been developed, one of the most widely used in regulatory setting is the Pesticide Root Zone Model (PRZM). PRZM was developed for the US EPA by Carsel et al. (1985). It simulates the transport and transformation of pesticides after application through the crop root zone to the vadose zone. It is an appropriate tool to estimate pesticide concentration in both soil and groundwater (Carsel et al., 2003). This model has already been used in Fresno County in California to simulate 1,2-dibromo-3-chloropropane (DBCP) pesticide contamination in groundwater (Loague et al., 1998). This model has also been used to estimate the transport and fate of pesticides in potato cultures in the Nicolet River Basin, Canada (Pierre et al., 1996) and the fate and transport of ethoprophos and bentazon in a sandy humic soil (Trevisan et al., 2000). Moreover, PRZM-3 has the capability to simulate pesticide concentration in multiple zones. This allows the model to combine different root zone and vadose zone (i.e., unsaturated zone) characteristics into a single simulation, and the model has the ability to simulate as many as three chemicals simultaneously so that it gives the user the option to observe the concentrations of multiple chemicals without making additional runs (Chang et al., 2008).

Although PRZM-3 is an important pesticide simulation model but the specific format of input text file and very long output text files of PRZM-3 made it user-unfriendly and restricted its use to site specific studies only. We developed a user-friendly model called ArcPRZM-3 by integration of original PRZM-3 model using Visual Basic and Geographic Information System (GIS) based Avenue programming. GIS is extensively used in environmental pollution studies due to its strong capability of spatial analysis (Zhou et al., 2007). GIS was used to assess soil environmental quality in Zhejiang province of China (Cheng et al., 2007). The Visual Basic input interfaces and ArcView output results in the form of tables, charts and maps made ArcPRZM-3 a user-friendly model and it could be used for pesticide simulations for site specific studies as well as large spatial scale. The objectives of this study were: (1) to evaluate ArcPRZM-3 for bentazon simulations in groundwater contamination by comparing model predicted bentazon concentrations with the field monitoring data; (2) to develop bentazon leaching potential ranks for selected sites of the study area using ArcPRZM-3; and (3) to study the temporal effects and analyze the important factors affecting the bentazon leaching in soil towards groundwater.

1 Material and methods

1.1 Study area

The study area consists of thirty seven wells located in Woodruff County, Arkansas, USA (Fig. 1). The major crops in the study area are soybean, rice and sorghum. There are several hundred wells drilled in the area because groundwater is used for irrigating the crops and domestic water supply. Woodruff County has mild winters, hot summers and general abundant rainfall. The average temperature in winter is 31°F and it is 80°F in summer. The total annual rainfall is about 127 cm.

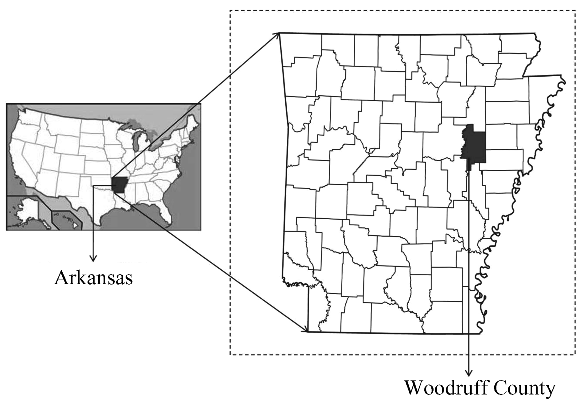

Fig. 1 Woodruff County in Arkansas State of USA.

1.2 ArcPRZM-3

We developed ArcPRZM-3 using Microsoft Visual Basic and ESRI Avenue programming by integration of Pesticide Root Zone Model version 3 (PRZM-3). PRZM-3 is a one-dimensional, dynamic, compartmental FORTRAN model developed by the US EPA (Carsel et al., 1998). This model simulates the chemical movement in unsaturated soil systems and it is widely used by chemical companies and environmental organizations in the USA. The PRZM-3 had limitations that included: (1) user-unfriendly format of text-based input file which required specific format for entering input values; (2) requirement of extensive input data for climate, crop, soil, chemical and site conditions; (3) user-unfriendly format of long output text files; (4) difficult output interpretation; and (5) restricted use to site specific studies. To overcome these limitations, we developed a user-friendly GIS based model called ArcPRZM-3. It had user-friendly input interfaces tied to crop, soil and chemical databases which could provide default input values to users. The input data, which were stored in a database, could be easily modified for updated simulations. ArcPRZM-3 could be used to run single simulation for a site-specific study or multiple simulations for a large area. The chemical and crop databases were built from the values given in the PRZM-3 manual. The soil database was built by obtaining the input parameters from the Soil Survey Geographic Database (SSURGO). The tools were developed in ArcView using Avenue programming that could allow the users to process the output text file results in the user-friendly formats of tables, charts and maps. ArcPRZM-3 was evaluated by simulating bentazon for 37 sites in our study.

1.3 ArcPRZM-3 input data

The ArcPRZM-3 has interfaces with databases for different input parameters including climate, crop, soil, irrigation and chemical. The climate input parameters included pan factor, snowmelt factor, soil evaporation moisture loss, daylight hours for each month in relation to latitude, daily precipitation, and temperature. The sources of data for the climate input parameters were PRZM-3 manual and meteorological files which were obtained from local Weather Station in Arkansas.

The crop input parameters included the number of cropping periods, crop emergence date, crop maturation date, crop harvest date, maximum interception storage, maximum active rooting depth, maximum areal crop coverage, maximum canopy height, surface condition after crop harvest, runoff curve numbers of antecedent moisture condition II-fallow, runoff curve numbers of antecedent moisture condition II-cropping, and runoff curve numbers of antecedent moisture condition II-residue. We selected crops in our study on which bentazon could be applied. These crops were soybean, rice and sorghum. The sources of data for crop input parameters were crop map developed by the Center for Advanced Spatial Technologies (CAST) located in University of Arkansas and PRZM-3 manual.

The soil input parameters included total depth of soil profile, total number of horizons, thickness of each horizon, thickness of the compartments in each horizon, soil bulk density, percentage of soil organic carbon, pesticide soil-water distribution coefficient, wilting point, initial water content of the soil, field capacity, soil water drainage rate, dispersion of pesticide. The data for soil input parameters was obtained from the PRZM-3 manual and SSURGO.

The irrigation input parameters included type of irrigation, leaching factor as a fraction of irrigation water depth, fraction of available water capacity and maximum sprinkler application rate. The data for irrigation inputs were obtained from PRZM-3 manual and a report on agriculture water management in the Mississippi Delta region of Arkansas (Scott et al., 1998).

The chemical input parameters included the number of pesticide applications, pesticide application date, the number of days after the target date that the model checks for ideal moisture conditions, target application rate for pesticide, the depth of pesticide incorporation, application efficiency of pesticide application, spray drift fraction, plant uptake efficiency factor, Henry's constant, vapor phase diffusion coefficient, enthalpy of vaporization, solution phase degradation rate constant, absorbed phase degradation rate constant. The data for chemical inputs were obtained from PRZM-3 manual, United States Department of Agriculture (USDA) and FIFRA Exposure Model Validation Task Force (FEMVTF) reports.

1.4 ArcPRZM-3 based bentazon simulation scenarios

Nineteen unique bentazon simulation scenarios were developed for 37 monitoring wells and each simulation scenario consisted of a unique soil-crop combination. The bentazon simulation scenarios with corresponding soil-crop combination and well ids are presented in Table 1. The purpose of developing these simulation scenarios was to test the leaching potential of ArcPRZM-3 by comparing simulations for the monitoring wells where bentazon was

Table 1 ArcPRZM-3 based bentazon simulation scenarios with soil-crop combinations and corresponding wells

Simulation scenario id	Soil-crop combination	Well id
1	Bosket loam-soybean	7-10-16-28-32
2	Askew fine sandy loam-soybean	9
3	Yancopin silty clay loam-soybean	25-21-22-44
4	Grenada silt loam-soybean	26-20
5	Dundee silt loam-soybean	34-15-42
6	Bulltown loamy fine sand-sorghum	1-2-3-8-12
7	Askew fine sandy loam-sorghum	4
8	Bulltown loamy fine sand-rice	6
9	Wiville fine sandy loam -sorghum	13-33-38
10	Wiville fine sandy loam-soybean	11-41
11	Bosket loam-sorghum	18-31
12	Calloway silt loam-soybean	19
13	Amagon-rice	23
14	Bulltown loamy fine sand-soybean	24
15	Taylorbay silt loam -soybean	35
16	Wiville fine sandy loam-rice	36
17	Kobel sicl-rice	43
18	Kobel sicl-soybean	45
19	Dubs sil-sorghum	47

detected and the simulations for monitoring wells where it was not detected. We simulated bentazon for nineteen representative wells (7, 9, 25, 26, 34, 1, 4, 6, 13, 11, 18, 19, 23, 24, 35, 36, 43, 45, and 47). Each representative well represented the particular simulation scenario group of specific soil-crop combination as presented in Table 1. The different soil profiles in bentazon simulation scenarios had different thicknesses, but to make a relative comparison for all these sites, it was decided to simulate bentazon leaching using ArcPRZM-3 at depth of 1.8 m. It was expected that limiting simulations to a depth of 1.8 m would produce results that would be used to make a relative comparison for bentazon leaching potential for all sites. The daily average dissolved bentazon concentration (mg/L) was selected as the ArcPRZM-3 output.

1.5 Box plot

The box plots were used to compare the daily average dissolved bentazon concentrations for the nineteen representative wells in the study area. A box plot is presented in Fig. 2. It provides a visual summary of many important aspects of a distribution. It stretches from the lower hinge which is defined as the 25th percentile to the upper hinge that is the 75th percentile and therefore contains the middle half of the scores in the distribution. The median of the 50th percentile is shown as a line across the box. The ArcPRZM-3 model simulations were compared based on the 75th percentile of summary box plots. The use of this variable to rank simulated leaching potential took advantage of information at exceptionally small concentrations that could be simulated but not detected (Burkart et al., 1999).

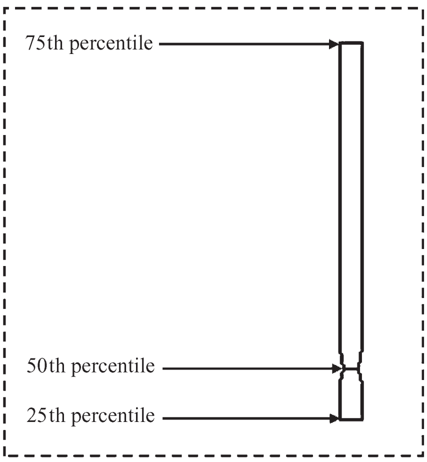

Fig. 2 Description of a summary box plot.

2 Results and discussion

2.1 ArcPRZM-3 predicted bentazon concentrations and temporal effects

The summary box plots for ArcPRZM-3 predicted dissolved bentazon concentrations at 1.8 m for 37 wells were obtained for a period of two years. The bentazon simulation results were compared using the 75th percentile of the simulated average concentrations. The wells, which showed higher 75th percentile, have higher potential of bentazon leaching as compared to those wells that have lower 75th percentile of average concentration. The ranks of leaching potential for bentazon using ArcPRZM-3 predicted bentazon concentrations for all thirty seven wells are presented in Table 2. The ranks for wells ranged from 1 representing the greatest leaching potential to 19 representing the least leaching potential. The wells 9, 26, 34, and 25, where bentazon was detected, showed model predicted leaching potential ranks of 1, 2, 3, and 4 respectively. In these four cases, ArcPRZM-3 simulations showed an agreement with the monitored bentazon data in the wells. The rank 2 was given to two wells 26 and 20 because both of them had the same soil-crop combination (Grenada silt loam-soybean). The wells 15 and 42 were given rank 3 as well 34 because all these three wells had the same soil-crop combination of Dundee silt loam-soybean. The wells 21, 22, and 44 were given rank 4 as well 25 because these four had the same soil-crop combination of Yancopin silty clay loam-soybean. Well 7, where bentazon was also detected, however, showed a rank of 9 for ArcPRZM-3 simulations.

From Table 2, we found that ten wells (20, 15, 42, 21, 22, 44 10, 16, 28, 32) where bentazon was not detected, were in the same rank of leaching potential as those where bentazon was detected. The reason for not detecting bentazon in these wells might be related to the time of bentazon monitoring in the wells. To understand the temporal effects, we plotted the model predicted dissolved bentazon concentration against the detected dissolved bentazon concentrations for well 26 in Fig. 3. From this analysis, we found that higher detected bentazon concentrations corresponded to higher model predicted bentazon concentrations and lower values corresponded to lower model predicted values. The detected bentazon in Fig. 3 indicated a similar trend of bentazon concentrations as the trend of predicted bentazon concentrations. From this

Table 2 ArcPRZM-3 predicted bentazon leaching potential rank

Simulation scenario id	Well id	Bentazon leaching potential rank
2	9*	1
4	26*-20	2
5	34*-15-42	3
3	25*-21-22-44	4
18	45	5
12	19	6
14	24	7
15	35	8
1	7*-10-16-28-32	9
8	6	10
13	23	11
10	11-41	12
16	36	13
6	1-2-3-8-12	14
17	43	15
11	18-31	16
9	13-33-38	17
19	47	18
7	4	19

* Wells where bentazon was detected during physical monitoring.

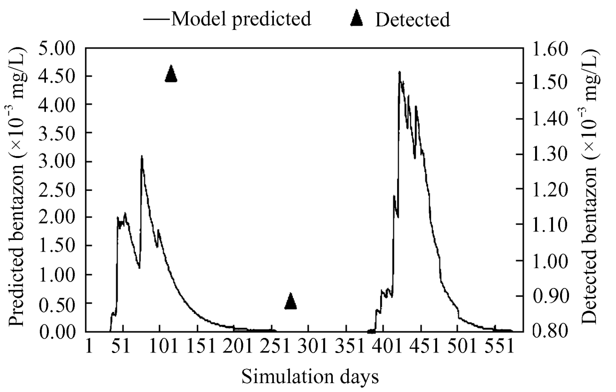

Fig. 3 Temporal distribution of ArcPRZM-3 predicted and field detected dissolved bentazon concentration in well 26.

observation, we figure that these wells (20, 15, 42, 21, 22, 44 10, 16, 28, 32) might have been monitored at a time when bentazon was not in a detectable concentration. The temporal variability of soil hydraulic properties had long been recognized. The rate of infiltration and the permeability of soils, for example, may fluctuate significantly from time to time because of changes in soil moisture, cropping practices, and biological activities in soils (Lin et al., 1996).

2.2 Effect of precipitation and irrigation on bentazon leaching

From ArcPRZM-3 simulations, we found the trend of higher dissolved bentazon concentrations in the second year as compared to the first year. To understand this behavior of bentazon leaching, a comparison between ArcPRZM-3 predicted dissolved bentazon concentration and precipitation data was made for well 26 in Fig. 4. In this comparison, it was observed that the pattern of bentazon leaching was driven by precipitation. Figure 4 shows higher dissolved bentazon concentrations at higher precipitation values whereas low bentazon concentrations are found at lower precipitation values. We also found that after the application of bentazon each year, the simulated bentazon concentrations increased substantially for both years. The simulated concentrations showed seasonal variations with peak concentrations following the pesticide application date and declining concentrations during the remaining year.

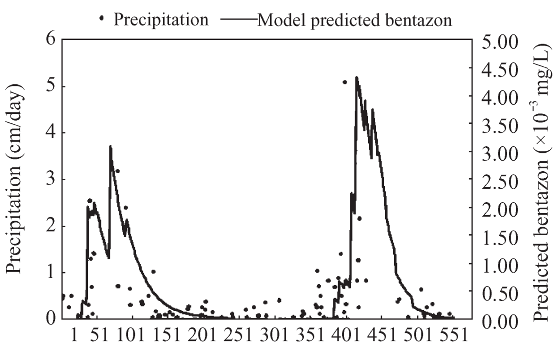

Fig. 4 Effect of precipitation on ArcPRZM-3 predicted dissolved bentazon concentration for well 26.

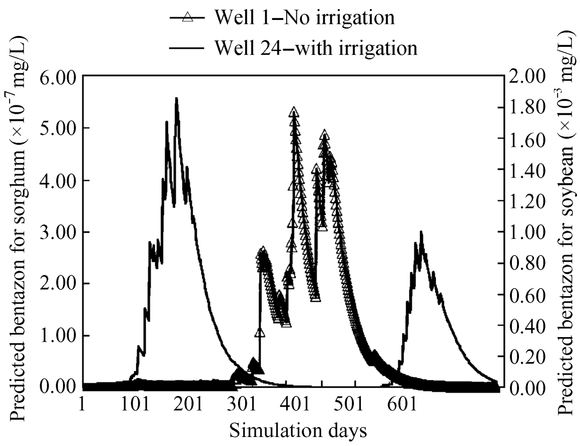

Fig. 5 Effect of irrigation on ArcPRZM-3 predicted dissolved bentazon concentration for well 1 and well 24. The irrigation was not applied to sorghum in case of well 1 and it was applied to soybean in case of well 24.

We also analyzed the effect of irrigation on bentazon leaching by making a comparison of ArcPRZM-3 simulated dissolved bentazon concentration at 1.8 m for well 1 and 24 (Fig. 5). The type of soil was the same, i.e., Bulltown loamy fine sand. Two different crops used in well 24 and well 1 were soybean and sorghum, respectively. The irrigation was applied to soybean but not to sorghum. From the results of Fig. 5, we found that the irrigation process might introduce sufficient water to transport bentazon into the soil leading to a higher likelihood of bentazon leaching for well 24 as compared to well 1. The bentazon leaching without irrigation was much lower (about three times lower).

3 Conclusions

Thirty seven sites in Woodruff County of Arkansas Delta were selected to observe daily average dissolved bentazon concentration for soybean, sorghum and rice at 1.8 m for a period of two years using ArcPRZM-3. The study sites were the locations for thirty seven wells, which were monitored physically for detection of pesticide residues. The simulation results were ranked using the 75th percentile of summary box plots for the simulated average dissolved bentazon concentrations. The simulation results were compared with monitoring well data of the county. We found that wells with bentazon detection (well id 9, 26, 25, and 34), showed the highest leaching as compared to all other wells. Some of the wells, where bentazon was not detected, were in high leaching potential classes and the possible reason might be the well monitoring time that could affect the pesticide detection level in the groundwater. However, the detected and predicted concentrations for bentazon showed a similar trend of relative leaching. The evaluation results of ArcPRZM-3 demonstrated that it could be used to simulate pesticides leaching potential more efficiently and effectively as compared to PRZM-3.

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