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Abstract

The ARS Root Zone Water Quality Model (RZWQM ver. 3.25) was used to simulate the effect of field measured macroporosity on atrazine transport to subsurface drain lines. Field data on atrazine concentrations in subsurface drain flow from corn fields, for modified no-till (mNT) and moldboard plow (MP) systems, were used to evaluate the performance of the RZWQM for the growing seasons of 1990, 1991 and 1992. The model was calibrated using field data from 1990 and data from 1991and 1992 were used to validate the model. Simulated subsurface drain flows and atrazine losses with and without macropore flow were compared with measured values. Although the preferential flow component slightly improved the predictions of peak subsurface drain flows for individual rain storms, it did not affect significantly the total annual flows. Simulated annual subsurface flows were within 11.6% of the observed values. Simulated atrazine concentrations in subsurface drain flows using mean values of macroporosity were in close agreement with the observed concentrations for 1990 (calibration year). Predicted total annual atrazine losses were also close to the observed values for 1990 (percentage difference = 17.6% for mNT and 34.8% for MP system). For 1991 and 1992 (evaluation years), with macropores, the simulated atrazine losses for mNT plots were within –9.9% of observed values and for MP plots were within +12.0% of observed values (combined for two years). The RZWQM predicted only trace amounts of atrazine in subsurface drain flows if macropores were not considered. The model showed sensitivity to lateral flow from macropores, Ksat of surface layer, and macroporosity in decreasing order in simulating atrazine losses to subsurface drain flows. Overall, the RZWQM showed good potential for simulating atrazine losses with subsurface drain water as affected by tillage practices.

Keywords

Preferential flow, Groundwater, Chemical transport, Tillage, Hydrology, RZWQM, Atrazine

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EVALUATION OF PREFERENTIAL FLOW COMPONENT OF RZWQM IN SIMULATING WATER AND ATRAZINE TRANSPORT TO SUBSURFACE DRAINS

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ABSTRACT. *The ARS Root Zone Water Quality Model (RZWQM ver. 3.25) was used to simulate the effect of field measured macroporosity on atrazine transport to subsurface drain lines. Field data on atrazine concentrations in subsurface drain flow from corn fields, for modified no-till (mNT) and moldboard plow (MP) systems, were used to evaluate the performance of the RZWQM for the growing seasons of 1990, 1991 and 1992. The model was calibrated using field data from 1990 and data from 1991and 1992 were used to validate the model. Simulated subsurface drain flows and atrazine losses with and without macropore flow were compared with measured values. Although the preferential flow component slightly improved the predictions of peak subsurface drain flows for individual rain storms, it did not affect significantly the total annual flows. Simulated annual subsurface flows were within 11.6% of the observed values. Simulated atrazine concentrations in subsurface drain flows using mean values of macroporosity were in close agreement with the observed concentrations for 1990 (calibration year). Predicted total annual atrazine losses were also close to the observed values for 1990 (percentage difference = 17.6% for mNT and 34.8% for MP system). For 1991 and 1992 (evaluation years), with macropores, the simulated atrazine losses for mNT plots were within –9.9% of observed values and for MP plots were within +12.0% of observed values (combined for two years). The RZWQM predicted only trace amounts of atrazine in subsurface drain flows if macropores were not considered. The model showed sensitivity to lateral flow from macropores, K_{sat} of surface layer, and macroporosity in decreasing order in simulating atrazine losses to subsurface drain flows. Overall, the RZWQM showed good potential for simulating atrazine losses with subsurface drain water as affected by tillage practices.*

Keywords. *Preferential flow, Groundwater, Chemical transport, Tillage, Hydrology, RZWQM, Atrazine.*

Atrazine (2-chloro-4-ethylamino-6-isopropylamino-1, 3, 5-trazine) is one of the most widely used herbicides in corn production in Iowa (Wintersteen and Hartzler, 1987). Surface-applied pesticides migrate to groundwater through the preferential flow mechanism (Thomas and Phillips, 1979; Bowman and Rice, 1986). Several researchers have established that macropores have a major influence on water and chemical movement in soils (Beven and Germann, 1982; Singh and Kanwar, 1991; Ahuja et al., 1993). The preferential transport of agrochemicals through macropores is of particular concern in no-till soil systems where agricultural chemicals are applied on the soil surface and macropores are not subjected to periodic disruption by tillage. This, combined with the fact that more pesticides may have to be used to control weed, insect, and disease problems for no-till systems compared to conventional tillage where cultivation and rotation are used to suppress these problems, increases the potential for chemical contamination of groundwater. Conventional tillage, consisting of moldboard plow-disc-harrow, under most conditions destroys macropore continuity at the surface, thus considerably reducing the entry of overland-flow solution into the macropores (Bouma et al., 1982).

The amounts of water and chemical available for transport through macropores depend upon the amount of overland flow (rainfall excess), the amount of chemical available in the overland flow, and the flow capacity of the macropores (dependent upon their number, sizes, and continuity). As a result, transport of chemicals through macropores will depend upon the type of soil, surface conditions (tillage), rainfall intensities, and type of the chemical. Because of environmental concerns, groundwater pollution from agricultural operations is of vital interest. Understanding the magnitude and characteristics of preferential transport of chemicals under field conditions will guide us to develop better management practices to reduce groundwater pollution.

Monitoring subsurface drainage for water quality is useful because subsurface drains integrate the effects of spatial variability and preferential and matrix flows (Hallberg et al., 1986; Richard and Steenhuis, 1988; Sichani et al., 1991; Kladivko et al., 1991). The recent version of Root Zone Water Quality Model (RZWQM ver. 3.25) developed by USDA-ARS (1992) is capable of modeling the effects of various tillage and management practices on drainage water quality and quantity.

Ahuja et al. (1993) reported the results of a modeling study conducted to investigate the preferential movement

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of pesticides with RZWQM. However, there have been only a few studies conducted to evaluate the RZWQM with field data of preferential movement of pesticides to subsurface drainage. Therefore, this study was designed to evaluate the RZWQM for predicting preferential transport of atrazine to subsurface drain flows using field measured data on macroporosity. The objective of this study was to use the RZWQM (ver. 3.25) to simulate the effects of field-measured macroporosity, under two tillage systems, on subsurface drain flows and atrazine losses with drain water and compare the model predicted results with the field-observed data on pesticide concentrations in subsurface drain water. Field data on surface macroporosity for modified no-till (mNT) and moldboard plow (MP) tillage systems were collected in late summers of 1991 and 1992 and used for these model evaluations. Three years (1990-1992) of field data on subsurface drain flows and atrazine concentrations in subsurface drain water for mNT and MP systems were used to evaluate the RZWQM in predicting atrazine concentrations in subsurface drain flows.

Description of RZWQM Model

RZWQM is a physically based model that incorporates the important physical, chemical, biological, physiological, and management processes of an agricultural crop production system. Given the initial state of the system (i.e., soil water, temperature, nutrient, chemistry, and pesticide) along with daily climatic and management practices (i.e., planting, tillage, fertilizer, and pesticide applications), RZWQM predicts the growth of the plant and the movement of water, nutrients and chemicals, over, within, and below the root zone of a unit area. The model is one-dimensional with a normal time step of one day or less.

The hydrological processes in RZWQM consist of infiltration, macropore flow, redistribution, subsurface drainage, water uptake by roots, transpiration, and soil evaporation (DeCoursey, 1992). The excess rainfall which is the difference between rainfall and infiltration in each time step, is overland flow or runoff. The original formulation of the model was modified (Farhani, 1994) to incorporate the effects of residue on evaporation so the model now predicts potential evaporation from bare and residue-covered soil and crop transpiration on a daily basis. Data on the soil physical and hydraulic properties, rainfall, and evapotranspiration rates are required by the RZWQM (some of these can be estimated by the model). Soil physical properties required as inputs include the information about horizon delineation, bulk density, particle density, porosity and texture. Soil hydraulic properties including soil water content-suction, $\Theta(\Psi)$, and unsaturated hydraulic conductivity-matric suction relationships, $K(\Psi)$, are also required as input by the model. The hydraulic properties can either be specified for each horizon or can be estimated by the model based on texture, bulk density, and 33 kPa water content (Θ_{33kPa}). The RZWQM requires input information about depth to drain, drain spacing, and effective drain radius to calculate the drainage rate.

A detailed description of water flow and chemical transport processes is given in the technical documentation of RZWQM (USDA-ARS, 1992). A brief description of flow and transport processes related to macropore flow is given in the following sections.

Water and Chemical Transport through Macropores

RZWQM (ver. 3.25) is capable of simulating the preferential transport of water and chemicals through macropores. Macropores are assumed to be cylindrical in the top soil horizon and planar cracks in the bottom horizons. Continuous macropores are idealized to be vertical and well dispersed within the soil matrix continuum. The continuity extends to the water table or any specified depth. However, a certain number of dead-end macropores are assumed to branch horizontally off the continuous pores in each soil horizon. Average volume fraction of macroporosity and size (radius of cylindrical pores and width of cracks) is assumed to be known. Number of pores or total length of cracks per unit area of soil is calculated from this information. Poiseulle's law is used to calculate the maximum flow capacity (K_{mac}) of these pores assuming unit hydraulic gradient (gravity flow). K_{mac} for cylindrical pores:

$$K_{mac} = N\,\rho\,g\,\pi\,g\,r_p^4/8\,\eta \quad \text{or}$$

$$K_{mac} = P_{mac}\,\rho\,g\,r_p^2/8\,\eta\ (\mathrm{ms^{-1}}) \qquad (1)$$

For planar cracks:

$$K_{mac} = L\,\rho\,g\,d^3/12\,\eta \quad \text{or}$$

$$K_{mac} = P_{mac}\,\rho\,g\,d^2/12\,\eta\ (\mathrm{ms^{-1}}) \qquad (2)$$

where

ρ = density of water (g cm^{-3})
g = gravitational constant (m s^{-2})
r_p = radius of cylindrical holes (cm)
d = width of planar cracks (cm)
η = dynamic viscosity of water (g cm^{-1}s^{-1})
N = number of pores per unit area
L = total length of cracks per unit area (cm)
P_{mac} = macroporosity as a fraction of soil volume

After ponding begins, water and solutes available at the soil surface are allowed to flow into macropores to the limit of their flow capacity. For each time step, the flow is routed downward through the continuous macropores sequentially in 1-cm depth increments. The macropore flow in each depth increment is allowed to flow into the dead-end macropores, and be absorbed by the soil matrix by radial or lateral infiltration from both continuous and dead-end parts of the macropores. The dead-end macropores can also store the solution. The time dependent lateral absorption of the solution occurs only in the soil matrix below the transient wetting front generated by the continuing vertical infiltration into the soil matrix. This absorption is computed by radial or lateral Green-Ampt type equations. Maximum absorption is achieved when the soil water content in the depth increment reaches 90% of porosity. The above routing continues until the available solution within a given time step is exhausted or the lowest depth of interest is reached. Below the lowest depth, the solution is allowed to drain away freely. Record of the cumulative absorption and changing soil water content is maintained for each depth increment.

The transient radial infiltration rate from a cylindrical macropore is calculated based on the Green-Ampt approach as:

$$V_r = 2 \pi K_s H_c / \ln (r_{wf}/r_p) \quad (3)$$

where K_s and H_c are the saturated hydraulic conductivity and capillary drive terms for the soil matrix, r_{wf} is the wetted radius at any given time, and r_p is the macropore radius. The wetted radius, r_{wf}, is calculated from the quantity of water that has infiltrated. Equation 3 is not applicable for the very first time step when $r_{wf} = r_p \times V_r$ is then calculated by linearized Green-Ampt lateral absorption as:

$$V_r = 2 \pi r_p [2 K_s H_c (\Theta_s - \Theta_i)/(\Delta t_1/2)^{1/2}] \quad (4)$$

where $(\Theta_s - \Theta_i)$ is the initial soil moisture deficit in the depth increment, and Δt_1 is the first time step.

For planar cracks, the equation for lateral infiltration rate per unit length of crack is:

$$V_l = [2 K_s H_c (\Theta_s - \Theta_i)/t]^{1/2} \quad (5)$$

where all terms are the same as defined previously, and t is the cumulative time for lateral flow. Both equations 4 and 5 are constrained by an upper limit of lateral flow, which depends upon the initial deficit and average distance between holes or cracks. For holes, the average soil volume per hole is assumed to be an equivalent cylinder, whose radius is the maximum radial distance of flow. The distance between cracks was derived as $(1 - Ld)/L$.

Chemicals in macropore flow are absorbed with water by the soil matrix in each depth increment. However, before water and solutes flow into the dead-end macropores or are absorbed into the soil matrix, the reactive chemicals in the macropore flow equilibrate to the wall of the 0.1-mm diameter pore, resulting in either a net adsorption to the wall or desorption from the wall. The wall is assumed to consist of only 0.1 mm of soil. After absorption into the soil matrix, the chemicals are uniformly mixed and equilibrated with the soil and water in the mesopores within the depth increment.

Methods and Materials

Field Experiment Site and Observed Data

Field data for this study were collected at Iowa State University's Northeast Research Center (NERC) near Nashua, Iowa (Kanwar et al., 1993). The experimental site is located on Kenyon, Readlyn and Floyd soils with 3 to 4% organic matter. The study site consists of 36 plots of 0.4 ha each. Each plot is drained by a single subsurface drain line installed at 1.2-m depth. The drains are spaced at 28.5 m apart. Data on subsurface drainage outflows, and NO_3-N and pesticide concentrations in drain water are available for this site. A detailed discussion on the automatic subsurface drain monitoring system is provided by Kanwar et al. (1993). For pesticide analysis, subsurface drain water samples were collected three times a week for first 60 days after pesticide application. Samples were then composited for weekly analysis. Additional samples were collected for every major rainfall (> 2.54 cm) event, which occurred within 60 days of pesticide application. For the remainder of the year, sampling frequency was based on flow but never exceeded more than once a week. However, any unusual rainstorm was sampled in addition to regular sampling. The data on subsurface drain flows and atrazine concentrations in subsurface drain flows, collected from three mNT and three MP plots for the years 1990 through 1992, were used in this study to evaluate the RZWQM model. These data sets were collected under continuous corn production practice.

Field Observed Surface Macroporosity

Infiltration experiments, using tension infiltrometers, were conducted in the summers of 1991 and 1992. Infiltration measurements were made at 0, 30, 60, and 90 mm tensions at three locations in each of the mNT and MP plots. A detailed description of the infiltrometer studies is given by Logsdon and Jaynes (1993). Infiltration data at different tensions are very useful in determining the average volume fraction of macroporosity which is used as an input to calculate the flow and solute transport through macropores. Infiltration data from both years (1991, 1992) were used for calculating macroporosity. Because the infiltration measurements at different tensions were made under approximately steady-state conditions, macropore conductivity (K_{mac}) used in equation 1 was assumed to be the difference between the ponded infiltration rate (I_0) and the infiltration rate at 30-mm tension (I_{30}). Based on this assumption, the macroporosity for the soil at the experimental site was determined by applying Poiseulle's equation using the assumptions of laminar flow and cylindrical macropores as described by Watson and Luxmoore (1986). After calculating K_{mac}, the macroporosity as a fraction of soil volume is determined using equation 1 for a given size of macropores. Analysis of the field data indicated a large variability in the macroporosity. Hence minimum, arithmetic mean, and maximum values of field macroporosity were calculated under both tillage systems. Macroporosity of the MP system was higher than that of mNT system (table 1). This is not unreasonable as the infiltration tests were done in the summer well after the MP tillage and after row cultivation in both the MP and the mNT fields. The field observed surface macroporosity (average volume fraction of macroporosity) for both tillage systems were used as input to the RZWQM for simulations for all three years.

Table 1. Surface macroporosity under two tillage systems*

	Minimum			Mean			Maximum		
Treatment	Pore Diameter† (mm)	No. of Pores ($/m^2$)‡	Macro Porosity (%)	Pore Diameter† (mm)	No. of Pores ($/m^2$)‡	Macro Porosity (%)	Pore Diameter† (mm)	No. of Pores ($/m^2$)‡	Macro Porosity (%)
Modified No Tillage	> 1	3	0.00024	> 1	114	0.009	> 1	269	0.021
Moldboard Plow	> 1	12	0.00094	> 1	163	0.013	> 1	289	0.023

* Logsdon and Jaynes (1993).

† The number of macropores and percentage porosity are calculated by assuming that pores are of the minimum radius of the tension range (30 mm) and therefore represent maximum values.

‡ Calculated using Poiseulle's equation.

Model Input Parameters

Climatic Data. Most of the weather data needed for model simulations were available for the study site. The model requires daily input values of air temperature (minimum and maximum), wind speed, short wave radiation, and relative humidity. When wind speed data are missing, the model assumes a calm wind speed of 4.2 km/h. Surface albedo for dry and wet soil, crop residue cover amount, and sunshine fraction were also needed for model simulations. The albedos are modified as environmental conditions change. Surface albedos were taken from Jury et al. (1991). Breakpoint rainfall data are needed as input by the RZWQM. For this purpose, hourly rainfall data for 1990, 1991, and 1992 from the Nashua weather station were used to calculate the breakpoint rainfall data. For each rainfall event, cumulative rainfall was plotted as a function of time. Breakpoints were recorded wherever there was a substantial change in the slope (representing a change in rainfall intensity). Therefore, the time increments for the rainfall data were equal to or more than one hour. Although a smaller increment of rainfall (less than an hour) would give better breakpoint estimation, unfortunately such data were not available for the study site. Total rainfall amounts for 1990, 1991, and 1992 (DOY 70-334) were 1130, 972, and 727 mm, respectively. The long-term average rainfall at the study site is approximately 750 mm.

Soil Properties Data. A 2.52-m deep soil profile was considered for model simulations. The soil profile was divided into seven or nine soil horizons depending on the information available from soil survey reports for Kenyon, Readlyn, and Floyd soils (USDA-SCS, 1982). For each horizon, bulk density (BD), porosity (estimated with BD and particle density of 2.65 Kg/m^3), and particle size distribution were required as input to the model. BD values for the surface horizon and particle size distribution for all horizons were measured experimentally. BD values for the other horizons were adopted from Sharpley and Williams (1990). Table 2 shows the selected soil properties for Kenyon, Floyd, and Readlyn soils as a function of horizon. Saturated/unsaturated hydraulic conductivity, effective porosity (EP), and bubbling pressure, were estimated by the model based on BD, Θ_{33kPa}, and texture data. Data on water content at field capacity (Θ_{33kPa}) for each horizon were taken from Sharpley and Williams (1990) and specified as input.

Crop Growth Parameters. The crop growth submodel of RZWQM is a generic crop production model capable of predicting the plant growth and production dynamics of corn in response to changes in environment and management practices (Hanson and Hodges, 1992). The default values of the plant growth parameters were used in the model as recommended in the user manual of RZWQM. The planting and harvesting dates for corn, planting depth, and plant density are specified as input to the model and were based on actual field information collected at the research site. Table 3 shows the various crop growth parameters specified as inputs to the RZWQM simulations.

Tillage and Chemical Management Data. Tillage and planting activities were carried out on the fields each year as soon as soil conditions were appropriate for these operations. MP plots were plowed with a moldboard plow and then disked with a disk harrow in the fall, except in 1991 when tillage could not be done in the fall because of wet conditions. Corn was planted directly into stubble in the mNT plots. Both the mNT and MP plots were cultivated using a row crop cultivator for weed control. Therefore, the mNT treatment was not a true no-till system. RZWQM also requires the tillage related data to simulate tillage effects on soil properties (bulk density, macroporosity, and residue incorporation). Corn was planted in rows parallel to the drain lines (Kanwar et al., 1993). Alachlor (2.5 kg/ha), atrazine (2.8 kg/ha), and terbufos (2.8 kg/ha) for rootworm control were applied to the soil during the planting operation, with herbicides sprayed as a tank mix over the entire surface area. Dates of major field operations are provided in table 3.

Table 2. Selected soil properties for Kenyon, Floyd, and Readlyn soil as a function of horizons, used as input for RZWQM simulations*

Horizon No.	Depth (m)	Bulk Density (Mg/m^3)	Porosity (m^3/m^3)	Particle Size Distribution (%)		
				Sand	Silt	Clay
Kenyon Soil						
1	0.0-0.20	1.36	0.49	38	42	20
2	0.20-0.41	1.53	0.43	41	34	25
3	0.41-0.50	1.55	0.42	42	32	26
4	0.50-0.69	1.60	0.40	43	30	27
5	0.69-0.89	1.65	0.38	44	28	28
6	0.89-1.23	1.70	0.36	44	31	25
7	1.23-1.67	1.75	0.34	44	31	25
8	1.67-2.52	1.75	0.34	44	31	25
Floyd Soil						
1	0.0-0.43	1.29	0.51	30	44	26
2	0.43-0.58	1.40	0.47	32	42	26
3	0.58-0.85	1.45	0.45	54	22	24
4	0.85-1.15	1.58	0.40	47	29	24
5	1.15-1.40	1.70	0.36	35	40	25
6	1.40-1.53	1.70	0.36	35	40	25
7	1.53-2.52	1.75	0.34	35	40	25
Readlyn Soil						
1	0.0-0.20	1.34	0.49	31	43	26
2	0.20-0.30	1.45	0.45	31	43	26
3	0.30-0.43	1.45	0.45	37	38	25
4	0.43-0.54	1.50	0.43	37	38	25
5	0.54-0.68	1.60	0.40	55	24	21
6	0.68-0.89	1.65	0.38	46	28	26
7	0.89-1.10	1.70	0.36	46	28	26
8	1.10-1.50	1.70	0.36	46	28	26
9	1.50-2.52	1.70	0.36	46	28	26

* Adopted from Singh et al. (1996).

Table 3. Dates of N fertilization, tillage, pesticide application, planting, and harvesting

Treatment	Year 1990	1991	1992
Nitrogen (200 kg/ha)	23 April	14 May	2 May
Pesticides* and planting	2 May	27 May	5 May
Plant density (#/ha)	60,000	55,000	55,000
Planting depth (mm)	32.0	32.0	32.0
Row crop cultivation	26 May	20 June	5 June
Harvesting	1 Oct.	8 Oct.	16 Oct.
Moldboard tillage	7 Nov.	†	2 April & 10 Nov.

* Alachlor and atrazine were applied at 2.5 kg/ha a.i. and 2.8 kg/ha a.i., respectively (both mNT and MP plots).
† Wet weather delayed tillage until the following spring.

Model Simulations and Evaluations

Initial soil water content and atrazine concentrations of the soil profile were needed as inputs to the model. Initial soil water content was set equal to field capacity, but was adjusted later so that the model predicted the subsurface drain flows at the same time in the beginning of the simulation period as was observed in the field. Soil samples were taken for atrazine analysis each year from 1990 to 1992 before applying herbicides. These field observed atrazine concentrations were used as initial concentrations for model simulations. Some minor adjustments were made in the initial concentrations to predict the same concentrations in the beginning of the simulation period as were observed in the drain water. Initial atrazine concentrations in the soil profile will have an influence on atrazine losses in drainage water in the beginning of the simulation; however, once the atrazine is applied again, the residual atrazine mass will not have much impact on atrazine leaching.

Model Calibration

The hydrology and pesticide components of the model were calibrated by using the daily measured subsurface drain flows and their atrazine concentrations data for the year 1990. Calibration was done for six continuous corn plots on a plot-by-plot basis (three plots each under mNT and MP systems). To calibrate the hydrology component of the model, the criteria used for calibration was to minimize the difference between the predicted and observed cumulative subsurface drain flows during the entire growing season of 1990 [March 11(DOY 70) to November 30 (DOY 334)]. An iterative process was used to determine the best values of lateral saturated hydraulic conductivity (LK_{sat}), saturated hydraulic conductivity of surface layer (K_{sat}), and EP. Table 2 shows selected soil properties for Kenyon, Floyd, and Readlyn soils as a function of horizon. The initial values of K_{sat}, LK_{sat}, and EP were taken from the literature for this site. It was found during the calibration that total subsurface drain flows are sensitive to EP and LK_{sat} while macropore flow is sensitive to K_{sat} of the surface layer which in result affects the atrazine transport to shallow groundwater. A list of calibrated parameters and additional input parameters needed for preferential flow component of the RZWQM is given in table 4. A detailed procedure on calibration of the hydrology component of RZWQM was given by Singh et al. (1996). The additional parameters (not included in table 4) required to run the preferential flow component of the RZWQM are listed in table 5.

Table 4. Calibrated values for LKsat, Ksat, EP, atrazine halflife, and atrazine Koc for each plot

Plot No.	Soil Type	Tillage Treat-ment	LKsat (mm/h)	Surface Layer Ksat (mm/h)	EP (m^3/m^3)	Half Life (days)	Koc
14	Readlyn	mNT*	35.0	20.0	0.20	60.0	80.0
25	Kenyon	mNT	34.0	18.0	0.20	60.0	80.0
31	Floyd	mNT	32.0	18.0	0.20	60.0	80.0
Avg			**33.7**	**18.7**	**0.20**	**60.0**	**80.0**
13	Floyd	MP	23.0	10.0	0.19	60.0	80.0
22	Readlyn	MP	22.0	10.0	0.18	60.0	80.0
35	Readlyn	MP	10.0	10.0	0.17	60.0	80.0
Avg			**18.3**	**10.0**	**0.18**	**60.0**	**80.0**

* mNT = modified no-till; MP = moldboard plowed; Avg = average.

Table 5. A list of parameters used to run preferential flow component of the RZWQM

Description of Parameters	Value	Method of Determination
Sorptivity factor for lateral infiltration (0..1)	0.5	Calibrated
Fraction of macropores directly going to drain flow (0..1)	0.02	Calibrated
Total macroporosity (fraction)	0.00009 (mNT) 0.00013 (MP)	Measured
Avg. radius of cylindrical pores (mm)	1.0	Assumed
Fraction of dead end macropores (%)	5.0	Calibrated

mNT = modified no-till; MP = moldboard plowed.

The pesticide component of the RZWQM was calibrated to obtain the best possible values of parameters such as soil half life and K_{OC}. The criteria used to calibrate the model was to minimize the difference between observed and predicted annual atrazine loss in subsurface drain water. Initial atrazine concentrations of the soil profile has a significant effect on atrazine concentrations in the drain flows in the beginning of the simulation. First, initial concentrations were set equal to the observed data (note that observed initial concentrations were not recorded exactly at the same day when simulations began), but in subsequent trials, initial concentrations for the lower soil horizons were adjusted to make sure that simulated atrazine concentrations in drain flows were approximately the same as the observed values. The model calibration was done with macropore flow allowed to operate.

Model Validation

To validate the model, the predicted results for subsurface drain flows and atrazine concentrations in subsurface drain flows were compared with observed values for 1991 and 1992, for two tillage systems, again on plot-by-plot basis. Initial water content and atrazine concentrations of the soil profile were taken from field data in 1991 and 1992. The rest of the input data were kept the same as for the 1990 simulations. Simulations were made from day of the year (DOY) 70 to 334 for both years, 1991 and 1992. The model simulations were made for each year separately because RZWQM does not have a freeze/thaw component, and thus cannot be used for making simulations during the winter months.

Results and Discussion

Comparison Between the Observed and Predicted Subsurface Drain Flows

Cumulative predicted and observed subsurface drain flows for three years (1990-92) for all six plots are shown in table 6. Simulated subsurface drain flows for the calibration year (1990) were within 10% of observed values for all plots. Subsurface drain flows were simulated using the mean value of macroporosity and no macroporosity. The "no macropore flow case" was created by inputting a zero value for the average volume fraction of macroporosity. This assumes that all the infiltrating water flows through the soil matrix. It is evident from the table 6 that predictions of subsurface drain flows by the model for mNT plots improved slightly when macropore flow was considered as compared to flows predicted without macropores. However, there was no effect of macropore flow on model predictions of subsurface drain flows for MP plots. For 1991 and 1992 (evaluation years), total

Table 6. Observed and predicted subsurface drain flows and macropore flow for 1990, 1991, and 1992

						Results With Macropore Flow*			Results Without Macropore Flow		
Year	Plot No.	Soil Type	Tillage Treat- ment	Rainfall (mm)	Macro- pore Flow (mm)	Predicted Flow (mm)	Observed Flow (mm)	Percent Differ- ence	Predicted Flow (mm)	Observed Flow (mm)	Percent Differ- ence
1990	14	Readlyn	mNT	1130.0	41.0	304.0	282.0	+7.8	285.9	282.0	+1.3
	25	Kenyon	mNT		46.6	291.0	270.0	+7.7	261.8	270.0	–3.0
	31	Floyd	mNT		89.0	251.8	258.0	–2.4	192.3	258.0	–25.4
	Avg				**58.9**	**282.3**	**270.0**	**+4.5**	**246.7**	**270.0**	**–8.6**
	13	Floyd	MP		8.6	128.5	117.0	+9.8	126.0	117.0	+7.6
	22	Readlyn	MP		33.3	106.5	98.0	+8.6	92.0	98.0	–6.1
	35	Readlyn	MP		32.3	61.0	59.0	+3.3	59.2	59.0	+0.3
	Avg				**24.7**	**98.7**	**91.0**	**+8.4**	**92.4**	**91.0**	**–1.5**
1991	14	Readlyn	mNT	972.0	11.7	338.0	342.0	–1.1	332.0	342.0	–2.9
	25	Kenyon	mNT		12.5	309.8	301.0	+2.9	307.3	301.0	+2.0
	31	Floyd	mNT		31.8	304.0	345.0	–11.8	288.6	345.0	–16.3
	Avg				**18.7**	**317.3**	**329.3**	**–3.6**	**309.3**	**329.3**	**–6.0**
	13	Floyd	MP		2.0	226.0	224.0	+0.9	226.0	224.0	+0.9
	22	Readlyn	MP		2.2	191.1	169.0	+13.0	190.9	169.0	+12.9
	35	Readlyn	MP		12.6	185.4	161.0	+15.1	112.1	161.0	–30.3
	Avg				**5.6**	**200.8**	**185.0**	**+8.5**	**176.3**	**185.0**	**–4.7**
1992	14	Readlyn	mNT	726.8	0.20	164.5	151.2	+8.7	164.3	151.2	+8.6
	25	Kenyon	mNT		1.94	165.0	214.0	–22.8	162.6	214.0	–24.0
	31	Floyd	mNT		25.2	136.0	251.0	–45.8	118.0	251.0	–52.9
	Avg				**9.1**	**155.2**	**205.4**	**–24.4**	**148.3**	**205.4**	**–27.7**
	13	Floyd	MP		0	88.9	159.0	–44.0	88.9	159.0	–44.0
	22	Readlyn	MP		0	69.1	75.0	–7.8	69.1	75.0	–7.8
	35	Readlyn	MP		12.7	88.2	99.0	–10.9	83.8	99.0	–15.3
	Avg				**4.2**	**82.1**	**111.0**	**–26.0**	**80.6**	**111.0**	**–27.3**
Overall two years (evaluation years)						mNT: –11.6%;MP: –4.4%			mNT: –14.4%;MP: –13.2%.		

* Results only with mean macroporosity are shown.
mNT = modified no-till; MP = moldboard plowed.

annual subsurface drain flows predicted by the model were in close agreement with the observed values (average percentage difference for two years: –11.6% for mNT and –4.4% for MP systems).

Figures 1 and 2 show typical examples of measured versus predicted daily subsurface flows for the growing season of 1990 for one mNT and one MP plot, respectively. Similar figures were prepared for other plots but are not shown here due to space limitation. Predicted subsurface drain flows generally agreed well with observed flows. Peak subsurface drain flows were under predicted for some of the rainfall events for both tillage systems. RZWQM predicted higher peak subsurface drain flows for mNT plots when macropore flow was considered as compared to without macropore flow. However, there was no effect of macropore flow on peak subsurface drain flow predictions for the MP tillage system. The model predicted peak subsurface drain flows approximately at the same time as were actually observed in the field. Similar trends were observed for all other individual plots. Some of the discrepancies between observed and predicted peak flows could be due to: (1) the error involved in linear interpolation of observed cumulative subsurface drain flow data; and (2) approximation of breakpoint rainfall data from hourly data. Given the fact that a high degree of spatial variability exists under field conditions, the model predictions of subsurface drain flows were quite good.

Comparison Between Observed and Predicted Atrazine Concentrations in Subsurface Drain Flows

Macropore flow is considered the primary mechanism for pesticide transport to shallow water tables. Therefore, to test the macropore component of RZWQM, atrazine concentrations in subsurface drain flows were predicted and compared with the observed atrazine concentrations in subsurface drain flows. Atrazine concentrations in subsurface drain flows were predicted with and without macropore flow. The predicted concentrations of atrazine from the RZWQM simulations versus observed concentrations of atrazine under different tillage systems are shown in figures 1 through 6. Similar graphs for other individual plots were made but are not shown here due to space limitation.

Figures 1 and 2 show the typical examples of measured versus predicted atrazine concentrations in subsurface flows for 1990 under mNT and MP tillage systems, respectively. As shown in figures 1 and 2, predicted concentrations are in good agreement with observed concentrations with a few exceptions. As indicated in figure 1, the effect of macropore flow on atrazine transport was clearly visible in the mNT system. Extremely low concentrations of atrazine were predicted when macropore flow was not considered. Although the effect of macropore flow was not significant in the MP tillage system (fig. 2), the model predictions of atrazine concentration followed the decreasing trends of observed data with time reasonably well. Both observed and simulated atrazine

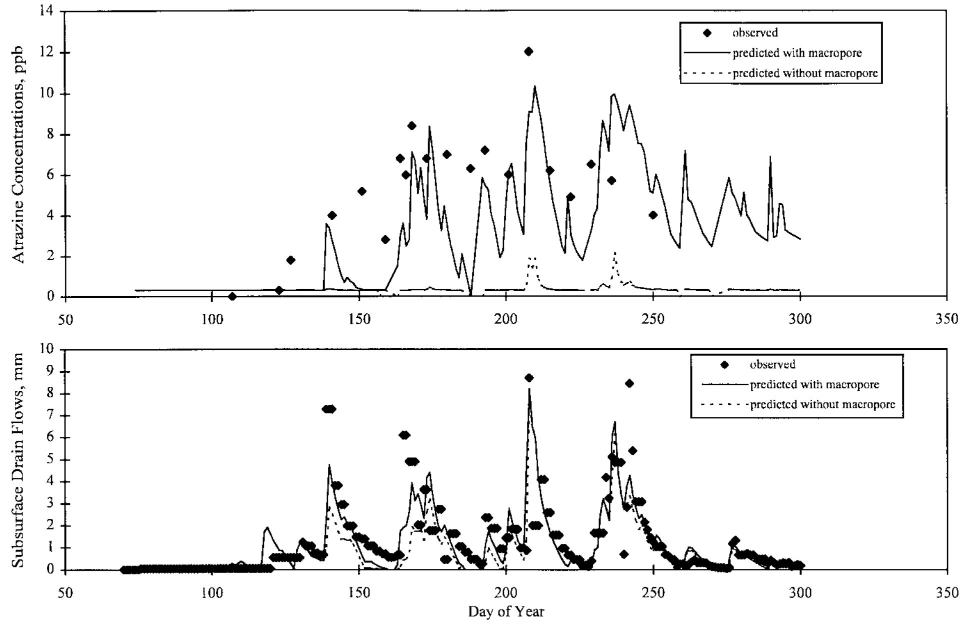

Figure 1–Daily observed and predicted subsurface drain flows and atrazine concentrations with and without macropore flow for plot 32 (modified no-till) for 1990.

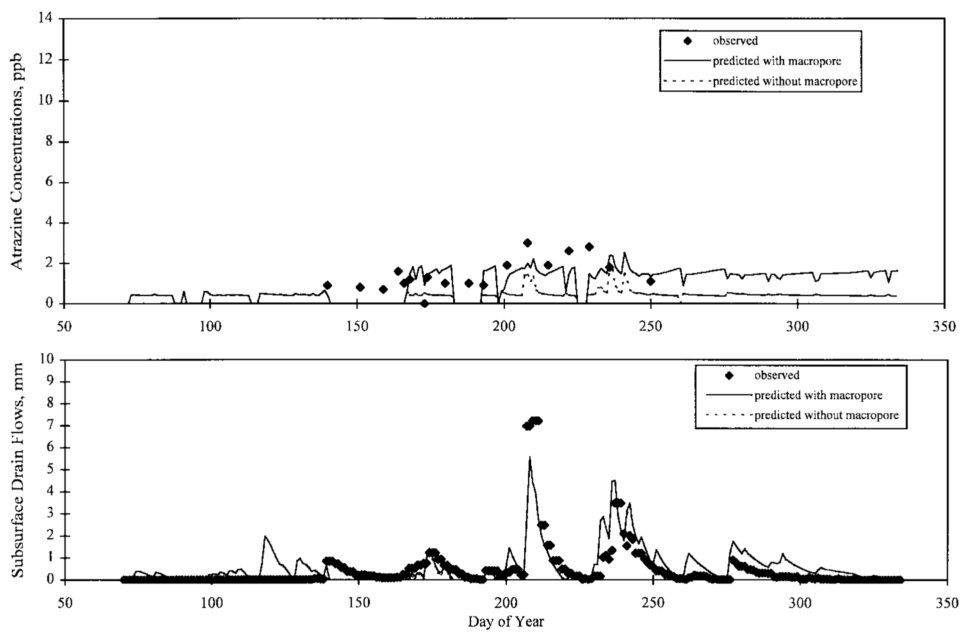

Figure 2–Daily observed and predicted subsurface drain flows and atrazine concentrations with and without macropore flow for plot 13 (moldboard plow) for 1990 (subsurface drain flows with and without macropore were identical).

concentrations in subsurface drain flows for the MP tillage system were consistently lower (quantitatively) throughout the growing season. Although measured macroporosity for the MP plots was higher, atrazine transport to drain lines was less compared to the mNT system. This could be due to higher LK_{sat} for mNT compared to MP system. The LK_{sat} is the most sensitive parameter affecting the total flow to drain lines.

The observed values of atrazine concentrations were not available for all days of the growing season for all three years because water samples were analyzed on a weekly basis due to cost involved. Therefore, simulated atrazine concentrations were compared with observed values for storm events to have a better idea of the accuracy of the model predictions. The predicted flux of atrazine versus observed discharge of atrazine in subsurface drain flows under mNT and MP tillage systems are shown in figures 3 and 4, respectively. As figures 3 and 4 show, the observed atrazine fluxes were greater than predicted fluxes (except on Day 236 when simulated value has a higher peak than the measured). For both tillage systems, the highest predicted flux of atrazine was observed on Day 208 (0.745 g ha^{-1} and 0.111 g ha^{-1}, for NT and MP plots, respectively). Also, the timing of the peaks in observed and

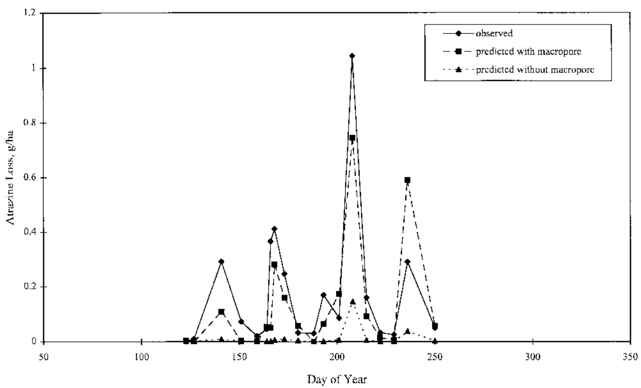

Figure 3–Observed and predicted atrazine losses in subsurface drainage water for storm events for plot 31 (modified no-till) for 1990.

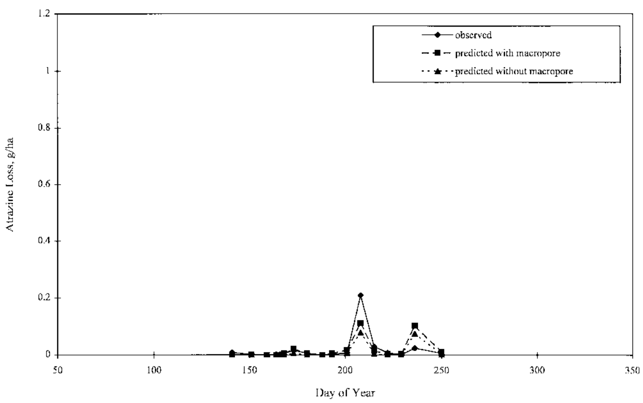

Figure 4–Observed and predicted atrazine losses in subsurface drainage water for storm events for plot 13 (moldboard plow) for 1990.

simulated fluxes occurred at the same time with few exceptions in the beginning. Figures 3 and 4 indicate that the simulation of atrazine transport to subsurface drainage by the RZWQM model with appropriate macroporosity and other climatological data is possible and predicted results are similar to those observed in the field.

Simulated daily atrazine concentrations in subsurface drain flows for 1991 showed a similar pattern as were observed in the field (figs. 5 and 6). However, peak atrazine concentrations were underpredicted several times for both mNT and MP plots. A close look at figures 5 and 6 revealed that the effect of macropore flow was not so prominent in 1991 as was observed in the year 1990. However, scattered peaks of atrazine concentrations in the observed data for MP system suggest that atrazine moved to lower depths in the soil profile quicker in 1991 than was observed in 1990. Visual observation of figures 5 and 6 showed that simulated atrazine concentrations were directly proportional to the flows predicted by the model.

Simulated daily atrazine concentrations in subsurface drain flows for 1992 (figs. 7 and 8) did not match with the observed trends. The majority of the time when atrazine losses occurred, the model predicted no concentrations, since it predicted zero flows. Overall losses were very low, however, and so the underpredictions are less “serious” from that standpoint. For the year 1992, observed and simulated values of atrazine concentrations in the subsurface drain water were consistently lower than the previous year and no macropore flow effect was observed on atrazine transport to subsurface drain flows.

Comparison Between Predicted and Observed Total Annual Atrazine Losses with Subsurface Drain Flows

Table 7 shows the observed and predicted values of atrazine losses with subsurface drain flows for both tillage systems for 1990, 1991, and 1992. The values in table 7

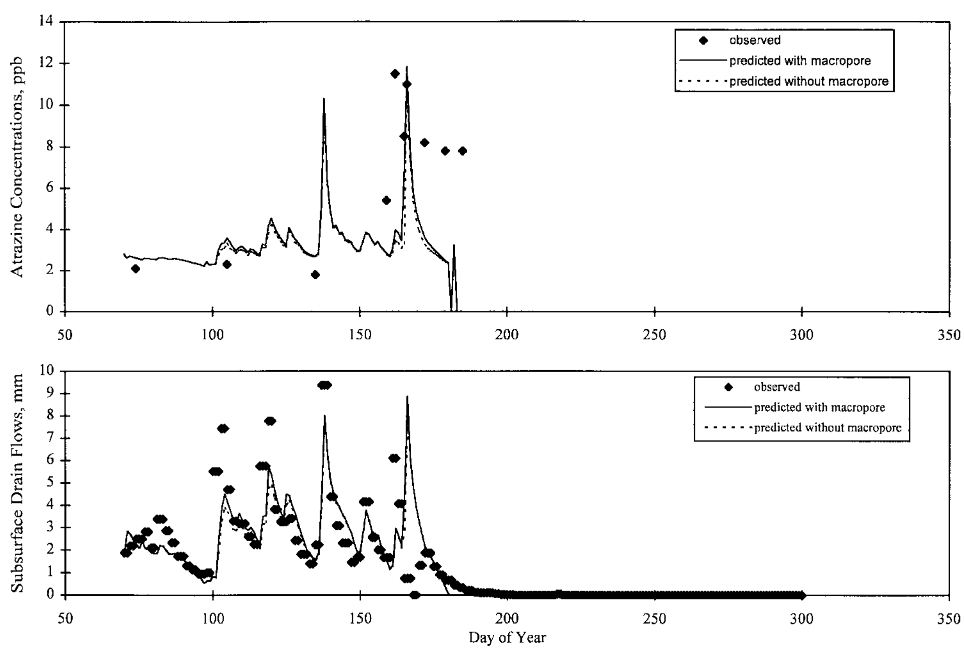

Figure 5–Daily observed and predicted subsurface drain flows and atrazine concentrations with and without macropore flow for plot 31 (modified no-till) for 1991.

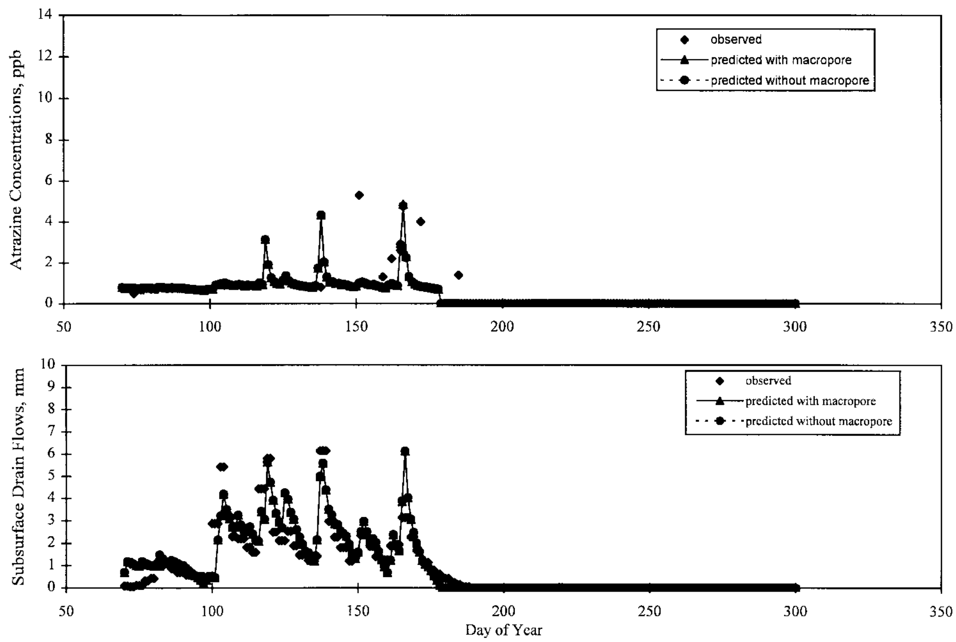

Figure 6–Daily observed and predicted subsurface drain flows and atrazine concentrations with and without macropore flow for plot 13 (moldboard plow) for 1991.

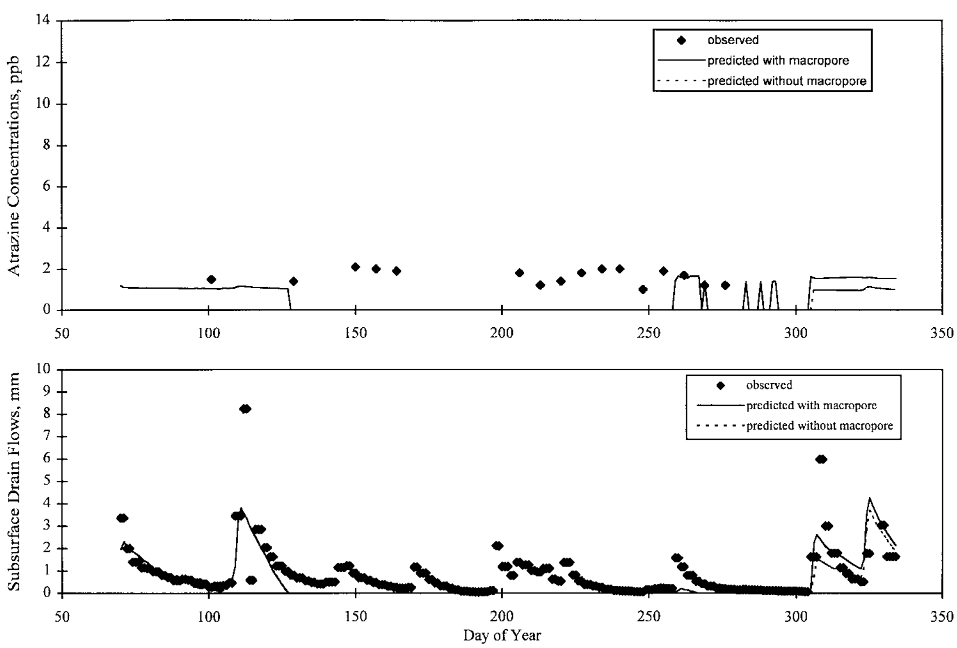

Figure 7–Daily observed and predicted subsurface drain flows and atrazine concentrations with and without macropore flow for plot 31 (modified no-till) for 1992.

indicate that the RZWQM simulated values close to the observed values for mNT plots when macropore flow was used (maximum average % difference was +17.64), however, the model did not predict annual losses close to the observed values without macropore flow (maximum average % difference was −66.55). For MP plots, the simulated and observed losses were in close agreement for 1991, but model predictions for individual plots were not very good for 1990 and 1992. However, overall atrazine losses (evaluation years, 1991 and 1992) predicted by the model were close to the observed values (percentage difference for two years: –9.9% for mNT and +12.0% for MP). For 1991 and 1992, macropore flow did not make much difference on the predictions of atrazine losses. The year 1992 was a dry year (drier than normal). The drier than normal conditions resulted in low or zero drainage after pesticide application, resulting in trace losses of atrazine in 1992.

SENSITIVITY ANALYSIS

A sensitivity analysis was conducted for atrazine losses with subsurface drain flows. Since atrazine losses with

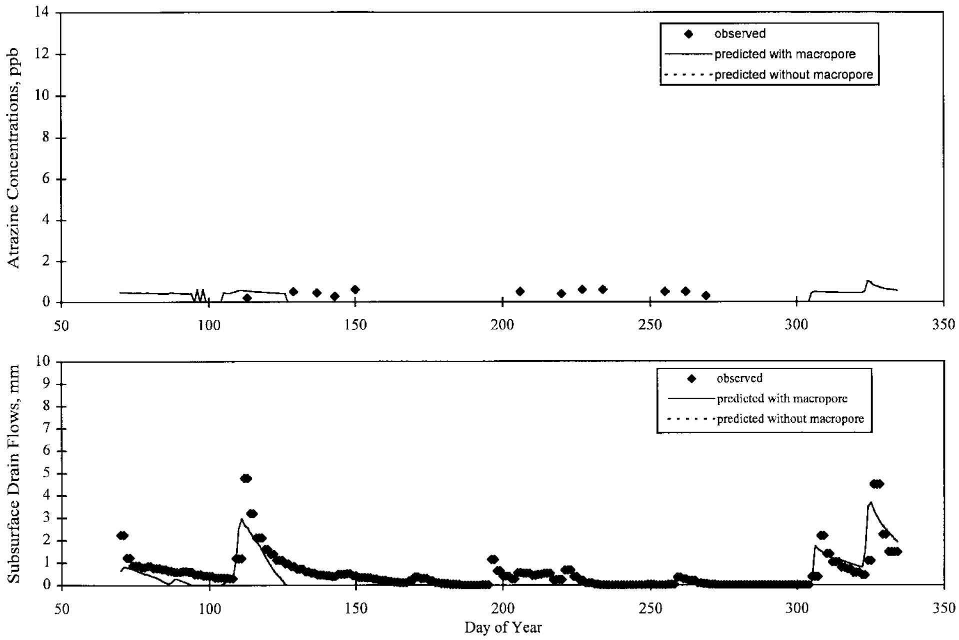

Figure 8–Daily observed and predicted subsurface drain flows and atrazine concentrations with and without macropore flow for plot 13 (moldboard plow) for 1992 (simulated values with and without macropore were identical).

Table 7. Observed and predicted atrazine losses with subsurface drain flows for 1990, 1991, and 1992

				Atrazine Losses With Macropore Flow*			Atrazine Losses Without Macropore Flow		
Year	Tillage	Plot No.	Soil Type	Predicted Loss (g/ha)	Observed Loss (g/ha)	% Differ-ence	Predicted Loss (g/ha)	Observed Loss (g/ha)	% Differ-ence
1990	mNT	14	Readlyn	15.30	14.30	+6.99	2.90	14.30	–79.72
	mNT	25	Kenyon	32.50	26.93	+20.68	13.42	26.93	–50.17
	mNT	31	Floyd	13.82	11.15	+23.95	1.20	11.15	–89.23
		Avg		**20.54**	**17.46**	**+17.64**	**5.84**	**17.46**	**–66.55**
	MP	13	Floyd	2.29	1.64	+39.63	1.06	1.64	–35.36
	MP	22	Readlyn	3.00	1.88	+59.57	0.09	1.88	–95.21
	MP	35	Readlyn	3.20	2.77	+15.52	0.80	2.77	–71.12
		Avg		**2.83**	**2.10**	**+34.76**	**0.65**	**2.10**	**–69.05**
1991	mNT	14	Readlyn	7.60	11.70	–35.04	6.90	11.70	–41.02
	mNT	25	Kenyon	15.25	16.07	–5.10	14.58	16.07	–9.27
	mNT	31	Floyd	12.27	11.05	+11.04	10.90	11.05	–1.36
		Avg		**11.71**	**12.94**	**–9.50**	**10.79**	**12.94**	**–16.62**
	MP	13	Floyd	2.96	2.54	+16.53	2.95	2.54	+16.14
	MP	22	Readlyn	2.15	1.98	+8.58	2.12	1.98	+7.10
	MP	35	Readlyn	2.13	2.27	–6.16	2.00	2.27	–11.89
		Avg		**2.41**	**2.26**	**+6.64**	**2.36**	**2.26**	**+4.42**
1992	mNT	14	Readlyn	0.60	0.95	–36.84	0.59	0.95	–37.89
	mNT	25	Kenyon	1.70	1.50	+13.33	1.70	1.50	+13.33
	mNT	31	Floyd	1.80	2.30	–21.74	1.26	2.30	–45.22
		Avg		**1.37**	**1.58**	**–13.29**	**1.18**	**1.58**	**–25.32**
	MP	13	Floyd	0.51	0.32	+59.37	0.51	0.32	+59.37
	MP	22	Readlyn	0.14	0.12	+16.66	0.14	0.12	+16.66
	MP	35	Readlyn	0.51	0.29	+75.86	0.45	0.29	+75.86
		Avg		**0.39**	**0.24**	**+62.50**	**0.37**	**0.24**	+54.2
Overall two years (evaluation years)				mNT: –9.9%; MP: +12.0%			mNT: –17.6%; MP: +9.2%.		

* Mean macroporosity value was used.
mNT = modified no-till.
MP = moldboard plowed.

subsurface drainage depends on hydrology and chemical parameters, sensitivity analysis was conducted using hydrology and chemical parameters together. Sensitivity analysis was conducted on calibrated parameters (annual values) for plot 31 (mNT) for 1990. Figure 9 shows the results of the sensitivity analysis for chemical properties (initial atrazine concentrations, K_{OC}, and atrazine half life).

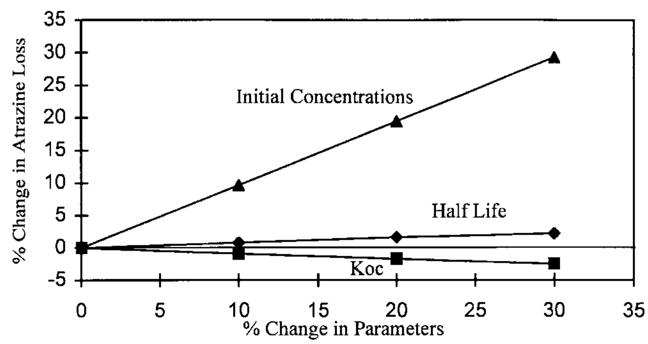

Figure 9–Parameter sensitivity to atrazine loss for 1990 for plot 31.

The percent change in initial atrazine concentrations was directly proportional to percent change in annual atrazine losses. Both half life and K_{OC} values were not very sensitive to atrazine losses, but increased K_{OC} value decreased atrazine losses with subsurface drainage. This is due to the fact that an increase in K_{OC} value will result in more adsorption of atrazine to the soil and less availability of atrazine for leaching. Based on these results, it can be concluded that prediction of pesticide leaching losses with subsurface drain flow can be improved by using site specific K_{OC} values and initial atrazine concentrations in the soil profile.

Figures 10 and 11 show the sensitivity analysis for hydrology parameters (macroporosity, lateral flow from macropore, initial water content, and K_{sat} of surface layer). Results of this sensitivity analysis indicate that total macropore flow was highly sensitive to K_{sat}, lateral flow from macropore, and initial water content in decreasing order (fig. 10). During sensitivity analysis, it was found that a small change in macroporosity (within 30%) did not show any effect on total macropore flow. However, atrazine losses were sensitive to lateral flow from macropores (fig. 11). A 30% increase in lateral absorption of atrazine from macropores caused approximately 70%

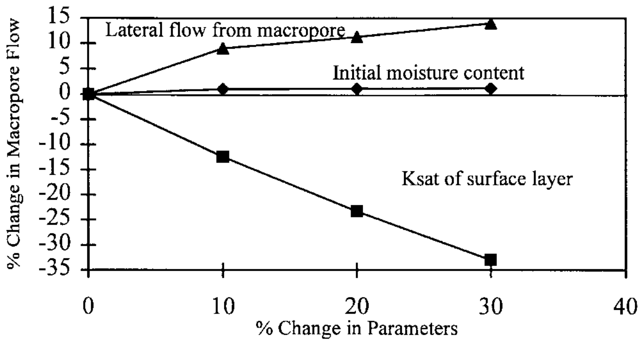

Figure 10–Parameter sensitivity to macropore flow for 1990 for plot 31.

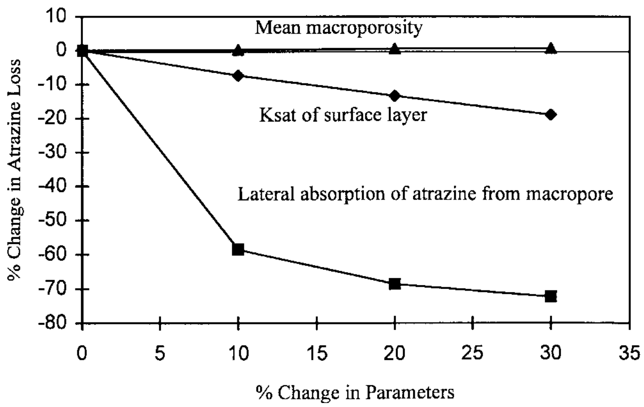

Figure 11–Parameter sensitivity to atrazine loss for 1990 for plot 31.

decrease in atrazine losses in the subsurface drain water. This is due the fact that lateral absorption of atrazine reduces the leaching of atrazine to subsurface drains. K_{sat} of surface layer was the next most sensitive parameter. Figure 12 shows that although atrazine losses with subsurface drain water are not very sensitive to a small change in macroporosity (from no macroporosity to minimum macroporosity), atrazine losses are sensitive to a significant change in macroporosity. This may be true in actual field conditions where macroporosity varies both in time and space. In this study, the same value of macroporosity was assumed for all years throughout the growing season, which is probably not true under field conditions.

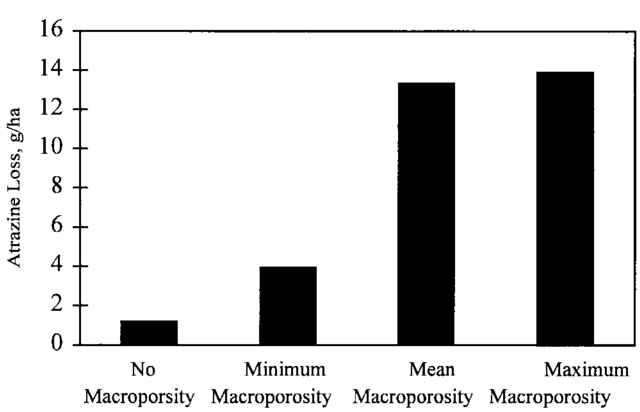

Figure 12–Effect of field measured macroporosity on atrazine loss in subsurface drain flows for 1990 for plot 31.

The spatial variability in soil properties even on a plot scale can contribute to disparities between observed and predicted values, therefore, spatial variability should be considered for future modifications in the model. Although the model is capable of showing a good response to rainfall pattern, it does not take into account the spatial variability in soil properties. The temporal changes in the soil properties due to tillage practices are incorporated in the RZWQM but weather induced changes are not considered.

Summary and Conclusions

The RZWQM (ver. 3.25) was calibrated to simulate atrazine concentrations and losses with subsurface drain flows for two tillage systems (mNT and MP) by using field observed data from a water quality site for 1990. The calibrated model was then used to validate its ability to predict atrazine concentrations and losses with subsurface drain flows for 1991 and 1992. The model simulations were conducted both with and without macropore flow to investigate the effects of surface macroporosity on atrazine movement to subsurface drain flow. The results of this study show that there was a good agreement between the predicted and observed subsurface drain flows when macropore flow was used for all plots for all years. Simulations using the macropore flow component slightly improved the predicted magnitude and timings of peak subsurface drain flows for mNT plots. Overall, the simulated subsurface drain flows were within –11.6% for NT plots and –4.4% for MP plots (average for 1991 and 1992). It can be concluded from this study that the macropore flow component does not change predicted total subsurface drain flows significantly.

The model simulated atrazine concentrations and annual losses with subsurface drain flows were close to the observed values for the two tillage systems for 1990, 1991 and 1992. The timings of peak atrazine concentrations simulated by the model also agreed well with observed data. The simulated atrazine losses with subsurface drain flows were also in close agreement with the observed values. Simulated values were within –9.9% of observed values for mNT plots and were within +12.0% for MP plots (two year average percentage difference).

The results of this study also indicate that a single value of macroporosity for all years (as used in this study) may not produce accurate results. The results of this study also suggest that not all rainfall events produce macropore flow. For example, in 1991, both simulated and observed subsurface drain flows were higher than in 1990, but much less macropore flow was predicted in 1991 (table 6). In addition to macroporosity of the surface layer, other parameters that had a significant effect on atrazine movement were: lateral absorption of atrazine from macropore, K_{sat}, and initial atrazine concentrations of the soil profile. It was concluded from this study that atrazine losses with subsurface drain water were not very sensitive to small changes in macroporosity (within 30%), but were sensitive to a significant change (from minimum macroporosity to mean macroporosity: fig. 12). This suggests that accurate estimation of macroporosity and initial chemical concentrations is necessary for valid model simulations.

Although overall evaluation of the RZWQM indicates that the model has the capability to simulate pesticide concentrations and losses with subsurface drain flow satisfactorily as affected by physical and chemical properties of the soil, the sensitive parameters such as LKsat, Ksat, and macroporosity must be measured or calibrated accurately.

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