Calibration of the Root Zone Water Quality Model for Simulating Tile Drainage and Leached Nitrate in the Georgia Piedmont

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ABSTRACT

Calibration procedures and data used to parameterize a model, including model components that may or may not have been addressed, are generally not well documented in modeling studies. A comprehensive description of the process and parameters used for calibrating the Root Zone Water Quality Model, v. 1.3.2004.213, is presented in this article. The model was calibrated to simulate tile drainage and leached nitrate under conventional tillage management practices for maize (*Zea mays* L.) production followed by a rye (*Secale cereale* L.) cover crop in Cecil soils (kaolinitic, thermic, Typic Kanhapludults), and for cotton (*Gossypium hirsutum* L.) development in the Georgia Piedmont. Tile drainage and nitrate leaching were simulated within 15% of the observed values in the calibrated maize scenarios with and without the soil macroporosity option. Simulated and observed tile drainage and leached nitrate were not significantly different, and the simulated values were not significantly different with and without the macroporosity option. Simulated cotton biomass and leaf area index were well correlated with observed biomass and leaf area index until the last 21 d of the reproductive stage. Simulated and observed cotton water use were different by <1 mm d^{-1} based on Δ soil water in a 60-cm profile during the critical peak bloom period. A detailed analysis of the calibration procedure and parameters used in this study will aid subsequent users of the model as well as aid in a subsequent evaluation of the model's performance for simulations of tile drainage and nitrate leaching in Georgia Piedmont cotton production systems.

THE SOIL–PLANT–ATMOSPHERE system is highly complex and difficult to characterize in terms of effective parameters. For complex systems such as this, model calibration and testing may be the only way to estimate those parameters that cannot be easily measured or determined (Hanson, 2000). Calibration of a model is an essential step in the basic protocol for hydrologic modeling, regardless of the scale of the problem (Mulla and Addiscott, 1999). Before simulated values can be expected to accurately represent a system within an acceptable error range, a calibration data set should be used to examine the model under simple sets of initial and boundary conditions, such as upper and lower soil moisture limits and texture, and known parameter values. This process serves to verify whether the model functions properly during execution or simulates values that are outside the range of reasonably acceptable estimates or measurements. It also reveals important information pertaining to model processes and sensitive parameters that may be overlooked when using soils, climate, and management practices different from those under which the model was developed (Mulla and Addiscott, 1999; Gijsman et al., 2002). The calibration process allows refinement of parameters and reveals sensitive parameters that can reveal a model's ability to accurately reflect different scenarios of interest (Hanson, 2000).

Calibration of a model includes parameterization based on direct measurements, pedotransfer functions, or direct or indirect fitting of the model to measured data. Pedotransfer functions (PTFs) provide estimates of parameters such as soil hydraulic properties that are often difficult and time-consuming to measure but accurate enough for many applications (Pachepsky and Rawls, 2005). However, Vereecken et al. (1992) showed that $>90\%$ of the variability in simulations of a soil map unit was due to the variability in the estimated hydraulic parameters using PTFs.

Recently, some modeling studies have begun to provide more details on the calibration approach or procedure that was used (Abrahamson et al., 1999; Cornelis et al., 2004; Zhang, 2004; FAO, 2004). This is due in part to the recognition of the need for standardization of calibration procedures, and subsequent guidelines that have been developed (Clarke et al., 1994; Hanson et al., 1999; Dubus et al., 2002; Saseendran et al., 2003; Bouman and van Laar, 2004). Though the modeling process can be defined procedurally, processes such as calibration and validation are completely subjective and open to best professional judgment, and modelers have no obligation to meet a standardized set of criteria (Corwin et al., 1999). A lack of emphasis on the process used for calibration may have resulted in assumptions or conclusions by readers and subsequent users of a model that may or may not be accurate. It may not be clear in the reported documentation if parameters were based on measured data, if parameters were adjusted during calibration, if all major processes in the model were parameterized, or if sensitivity analyses were performed. The lack of reporting of the calibration process may leave a reader with limited information to discern the model's ability to comprehensively address the system tested. Ad-

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Abbreviations: CI, confidence interval; CT, conventional tillage; EF, tile drain express fraction; LAB, sorptivity factor for lateral infiltration; MSEA, management system evaluation areas; NT, no tillage; PTFs, pedotransfer functions; RRMSE, relative root mean square error; TDR, time domain reflectometry; WT, wetting thickness.

justments made to parameters during calibration may impact other processes in the model that do not concern the current modeler, but may not be suitable under different conditions that would be of interest to another modeler.

This modeling study is based on a current water quality field experiment initiated in 1991 at the USDA-ARS J. Phil Campbell, Sr. Natural Resources Conservation Center in Watkinsville, GA. Objectives of the study included the water quality impacts of maize production based on the effects of conventional tillage (CT) or no tillage (NT), cover crop, and nutrient source. A model that could accurately simulate the sensitivity of drainage and nitrate leaching to these management practices would provide a valuable tool for testing and evaluating different agricultural production scenarios in Cecil and associated series soils which occupy approximately two-thirds of the cultivated land in the southern Piedmont region (Hendrickson et al., 1963).

Using this same study, Johnson et al. (1999) tested the LEACHN model (Hutson and Wagenet, 1992) for maize production for its ability to simulate soil NO_3–N and NH_4–N content, and drainage and leached nitrate under CT or NT management with and without a winter rye cover crop. Using modifications based on laboratory estimates for input parameters, LEACHN generally underestimated soil NH_4–N and NO_3–N during the winter and overestimated soil NH_4–N during the summer. The model also overestimated cumulative drainage and leached nitrate during both seasons (Johnson et al., 1999). The overestimation of leached nitrate in a wetter than normal year was attributed to the absence of a soil macropore–matrix exchange component in the model. We chose to evaluate The Root Zone Water Quality Model (RZWQM) because it includes a macropore component as well as an exchange component between the soil matrix and macropore walls. Visible macropores and preferential flow patterns are found in Cecil soils (Gupte et al., 1996), and we expected that the RZWQM might be able to better simulate drainage and leached nitrate based on the results of the Johnson et al. (1999) study. In addition, the RZWQM includes an option for tile drainage, an important consideration when tile drains have been used in the field due to changes in the soil water dynamics caused by artificial drainage systems (Skaggs, 1978; Ritzema, 1994).

The hydrology, pesticide, and nitrate movement, crop growth, and several agricultural management practices in the original version of the RZWQM model published in 1992 have been tested nationally and internationally with data collected from 1972 to 1996 (Ahuja et al., 2000). Tillage effects on hydraulic properties, manure management, crop yield response to water stress, and tile drainage are just some of the refinements present in the version of the model used in our study (USDA-ARS-GPSR RZWQM development team, personal communication, 2004). Conclusions drawn from some of the early applications in the literature may not be strictly valid, and may not represent typical behavior of the current model (Ma et al., 2001). In addition, soils and climate in the Southeast are very different from the Great Plains and Midwest regions of the USA. This paper reports results of the calibration of the most recent version of the RZWQM (v. 1.3.2004.213) for simulations of tile drainage and nitrate leaching in maize and cotton production with a winter rye cover crop as well an analysis of the effect of macroporosity on tile drainage and nitrate leaching under conventional tillage management practices in the southeastern USA.

The main objective of this study was to calibrate the RZWQM for its ability to simulate tile drainage and nitrate leaching in a Cecil soil in maize and cotton production with a winter rye cover under conventional tillage management practices in the Georgia Piedmont region. A second objective was to evaluate the model's sensitivity to soil macroporosity in relation to tile drainage since regions of preferential flow are found in Cecil soils of the Piedmont region (Gupte et al., 1996). Finally, we aimed to provide a detailed explanation of our calibration procedures for other modelers and user groups who are interested in the process of calibration that might be useful before model evaluation. Clarification of calibration procedures provides a better understanding of the parameterization process, and the sensitive parameter adjustments that are discovered during the process. It may have implications for potential users of the model if any specific parameters or parameter adjustments have significantly influenced test results. In addition, this study contributes toward the standardization of the calibration phase of modeling. A standard calibration protocol supplements the current protocol of parameterization, calibration, and testing with an independent data set, with guidelines that for now are left somewhat arbitrarily up to the modeler (Dubus et al., 2002).

MATERIALS AND METHODS

Field Experiments

The study site is located in northeastern Georgia in the Piedmont region that extends from Virginia to Alabama. The water quality study is located at the USDA-ARS J. Phil Campbell, Sr. Natural Resources Conservation Center in Watkinsville, GA, USA (33°54′ N lat; 83°24′ W long; 229 m elev.). The study was undertaken to evaluate the effects of tillage and winter cover cropping on nitrate leaching from maize production (McCracken et al., 1995). Tillage treatments included CT and NT, and cover cropping treatments consisted of winter rye or fallow conditions. To meet our objectives for the modeling objective of this study, and to simplify the complexity and scope of the calibration for later evaluation of the model, we chose to calibrate the model using only the CT treatment plots in winter rye cover. In addition, the fallow treatment plots were discontinued in 1992 and all plots were planted with a winter rye cover so that continuous complete data sets for one treatment were not available for this modeling study. The NT treatment will be tested in the evaluation study later.

The treatment plots were 10 by 30 m and instrumented with 10 cm i.d. PVC drain tiles installed 2.5 m apart at 75- to 100-cm depths on a 1% slope. The plots were hydrologically isolated from each other with polyethylene sheets extending from the soil surface to a depth of 1 m and with plastic borders 10 cm deep. The volume of water drained from a plot was measured by tipping bucket gauges and digitally recorded by automated dataloggers. The tipping bucket gauges had a sampling slot that subsampled drainage and routed it to a beaker. For every 2 mm of cumulative drainage, a sample was pumped from the beaker into a polyethylene bottle inside a refrigerated sequential waste water sampler (Isco Model 3700 FR, Lincoln, NE). An aliquot of this effluent was stored frozen in polyethylene vials and later analyzed for nitrate using the Griess-Ilosvay method (Keeney and Nelson, 1982). The samples were filtered through a 0.45-μm filter before analysis (McCracken et al., 1995; Johnson et al., 1999).

The soil was a Cecil sandy loam. The pH normally ranged from 5.5 to 5.8 as measured at the study site; therefore, lime was applied approximately every 3 yr to maintain a pH of 6.0 to 6.3 in the surface horizon to avail plant nutrients and prevent aluminum toxicity. Since these soils are variably charged, positively charged soil particles can attract anions such as nitrate that can be weakly held in the soil matrix. Nitrate may bypass the soil matrix via soil macropores. However, Gupte et al. (1996) found regions of preferential flow in dye-stained soil cores from the study site that were not necessarily associated with distinct open macropores observed from the mean cross-sectional areas of the soil columns.

In April 1991, the plots were plowed, disked, and planted to maize. In October 1991, maize was harvested, and six plots were no-till planted to rye and six plots left fallow through the winter. In April 1992, three plots from each of the rye cover and fallow treatments were placed under either CT or NT management. The CT plots were mowed, moldboard plowed, and disked. On 24 Apr. 1992, plots were planted to maize in 76-cm rows at the rate of 60 000 seeds ha^{-1}. Ammonium nitrate fertilizer was applied at a rate of 168 kg N ha^{-1} on 26 Apr. 1992. Maize was harvested on 7 Oct. 1992 and rye was planted on 30 Oct. 1992. Rye was sampled and killed with paraquat (1,1′-dimethyl-4,4′-bipyridinium ion) on 12 Apr. 1993, CT plots were plowed and disked on 13 April, and maize was again planted on 14 Apr. 1993. Maize was harvested on 14 Sep. 1993 and rye was planted on 29 Sep. 1993. Maize and rye yields and N uptake were measured from biomass samples before each field harvest (McCracken et al., 1995). The same procedure of planting maize followed by winter rye was used until Nov. 1994 when winter wheat was planted as the cover crop followed by the first cotton crop in May 1995.

To calibrate the RZWQM for cotton growth, and its ability to simulate tile drainage and leached nitrate from cotton production during the period when the water quality study was planted to cotton, we used parameters from a field experiment in cotton production in 1997 adjacent to the water quality study. The calibration study site was planted on 16 May 1997 on a 1.3-ha watershed using a no-till drill. A winter rye cover crop was planted in late October following cotton harvest. Soil moisture was measured in 15-cm increments to a soil depth of 90 cm using time domain reflectometry (TDR) (Moisture Point, ESI, Victoria, BC, Canada). Ammonium nitrate fertilizer was applied after cotton planting at a rate of 67 kg N ha^{-1}, and winter rye was fertilized after planting with 54 kg N ha^{-1}. Cotton biomass and leaf area samples were collected seven times during the growing season beginning on 16 July 1997 through 23 Sep. 1997. Plant height and populations were also estimated at each sampling date (Schomberg and Endale, 2004).

Model Input and Parameters

The RZWQM model uses a Windows interface and can initially be set up with a minimum dataset using readily available data. The required soil properties are texture and bulk density. Parameters for soil crusting, macroporosity, tile drainage, and various soil hydraulic properties can be supplied by the user or, where data are limited or unknown, the model will use default values based on known research documented in an extensive user help utility. The model has been applied to simulate best management practices for the Management Systems Evaluation Areas (MSEA) research project for maize, soybean, and wheat (Ahuja et al., 2000). The calibrated maize, soybean, and wheat crop parameters in the model can be adjusted during the calibration procedure to simulate crop growth for the area of interest to the modeler. Other crops may be added to the generic plant growth submodel and parameterized by the user. Daily weather data can be generated with the CLIGEN stochastic model (USDA-ARS, 2003) based on nearby historic weather station parameters when measured data is not available. However, we used measured rainfall and weather data from the Georgia Environmental Monitoring Network for Watkinsville located approximately 15 m from the study site (Hoogenboom, 2003).

We parameterized the physical properties of the soil in the RZWQM model from measurements made near the study site by Bruce et al. (1983) and Gupte et al. (1996). Seven distinct layers to a depth of 1.25 m were parameterized based on measured properties of each layer. The initial soil water content at the beginning of the simulation period on 1 Jan. 1991 was set to the measured field capacity for each layer (Table 1). The van Genuchten (1980) equation parameters, α and n were fitted using PROC NLIN (SAS Institute, 2000) based on measured soil water content and pressure head for each depth where residual θ was estimated as that of the wilting point at $h = -15\,000$ cm. The parameters were then converted to the Brooks-Corey parameters, $S2$ and $A2$, the bubbling pressure and pore size distribution index, respectively, based on the RZWQM documentation (Ahuja et al., 2000). We included a soil crusting option with a crust hydraulic conductivity rate set to 0.68 cm h^{-1} based on measurements of a Cecil sandy loam crust under simulated rainfall conditions (Chiang et al., 1993). The initial soil NO_3–N and NH_4–N concentrations used are described in Johnson et al. (1999) from soil data collected from the study site in November 1991. We used 1 Mg ha^{-1} as

Table 1. Physical properties of Cecil sandy clay loam soil used in model. Data for soil cores and horizons compiled from Bruce et al. (1983). Macroporosity and pore radius are average measured values of all pores ≥ 0.2 cm diameter for soil column depths from Gupte et al. (1996).

Model soil layer no.	Model depths	Measured core depths	Core K_s	Core particle density	Core bulk density	Horizon	Horizon depths	Sand	Silt	Clay	Soil column depths	Pore radius	Macroporosity
	cm	cm	cm h^{-1}	g cm^{-3}	g cm^{-3}		cm	%	%	%	cm	cm	%
1	1–5	1–7	18	2.64	1.34	Ap	0–21	78	15	7		0.35	0.014
2	5–15	6–12	20	2.65	1.56			78	15	7	0–20	0.35	0.020
3	15–25	17–23	8	2.72	1.69	BA	21–26	43	20	37		0.35	0.020
4	25–35	27–33	18	2.72	1.43			30	20	50	30–45	0.35	0.020
5	35–65	57–63	10	2.65	1.37	Bt1	26–102	30	20	50		0.35	0.025
6	65–95	87–93	2.6	2.65	1.51			30	20	50	45–60	0.35	0.025
7	95–125	127–133	0.2	2.65	1.55	Bt2	102–131	34	25	41		0.10	0.025

the amount of initial surface residue based on fallow conditions and on one season of maize production before the first winter rye cover crop in October 1991. The fraction of surface residue mass that would be incorporated by natural means was set to 2% based on model references. The field area used was 0.03 ha based on the size of a plot, and the slope was 2%. Input data and initial parameter values used are listed in the Appendix.

Model Processes

The RZWQM is an integrated physical, biological, and chemical process model that simulates plant growth, movement of water, nutrients, and pesticides into the soil and through the root zone at a representative point in an agricultural cropping system. The model is one-dimensional, and designed to simulate conditions on a unit area basis. It was originally developed to provide a comprehensive simulation of the root zone processes that affect water quality, and to respond to a wide range of agricultural management practices and surface processes (Ahuja et al., 2000). It was designed with interactive feedback between soil water, available N, and plant development (Hanson et al., 1999). The RZWQM includes several detailed processes and user options that can affect the simulation results. Descriptions of some of the processes that affect tile drainage and nitrate leaching are described below for the purpose of aiding the reader in discernment of model processes that may have affected the outcome of the calibration performed in this study. Complete descriptions of the processes, equations, and interactions of processes can be found in the model documentation (Ahuja et al., 2000).

Soil Hydraulics

The soil profile can have up to 12 distinct horizons. The profile can be parameterized based on distinct horizons or as distinct layers within horizons. Three grids are then created—one for defining hydraulic properties, a second nonuniform layering system for redistribution of water and nutrients, and a third 1-cm grid that only functions during infiltration. Hydraulic properties in the model are defined by the soil water content–matric suction relationship and the unsaturated hydraulic conductivity–matric suction relationship described by Brooks and Corey (1964) with slight modifications. The model estimates soil hydraulic properties from soil texture, bulk density, and soil water content at a suction of 33 or 10 kPa when measured data for Brooks-Corey parameters are not available. If soil water content at a suction of 33 or 10 kPa is unknown, the parameters for the hydraulic function properties are taken from Rawls et al. (1982) based on the soil texture class and then adjusted based on bulk density. The user has the option of using a minimum description of these properties or a full Brooks-Corey description to account for the effects of trapped air in the soil, which can reduce K_s by as much as 50% during infiltration (Bouwer, 1969). The field saturated K_s is divided by a viscous resistance correction factor of 2.0 so that the infiltration rate at any given time is a function of this reduced K_s in the Green-Ampt infiltration equation (Green and Ampt, 1911). Between rainfall events, soil water is redistributed using the Richards equation minus a sink term for root water uptake and tile drainage flux. These terms are described in more detail in other sections of the paper.

The model includes an option to define soil macroporosity in terms of size and number of macropores present in the soil. The user supplies the macropore number and size (radius) for each soil layer. If data on macroporosity are unavailable, it is best to run RZWQM assuming no macropores (Ahuja et al., 2000). If the user does not select the macroporosity option, then drainage occurs through the soil matrix only.

Water can only enter the macropores at the surface, and the model allows preferential flow through macropores to go directly to the tile drain when the water table resides above the tile drains. Macropore flow may also exchange the soil solution with the soil matrix by miscible displacement through macropore walls. The water solution in the macropore is subject to lateral absorption into the drier soil matrix, and the chemicals in solution are also subject to adsorption or desorption from the macropore walls. Maximum flow-rate capacity of macropores is calculated using Poiseuille's law assuming gravity flow. Lateral absorption into the macropore walls is simulated using Green-Ampt equations (Green and Ampt, 1911; Childs and Bybordi, 1969; Hachum and Alfaro, 1980). The user may also adjust the fraction of microporosity in each soil layer though to not less than 1% of total porosity.

Other than measured values of macroporosity including macropore size and number, the adjustable parameters in the model that can affect macropore flow are the sorptivity factor for lateral infiltration, the effective lateral infiltration wetting thickness, and the tile drain express fraction. To account for the effect that compaction or lining of macropore walls may have in reducing the ability of a soil to absorb water and chemicals, the calculated Green-Ampt radial (lateral) infiltration rate or sorptivity rate will be multiplied by a user-specified sorptivity factor ranging from 0 to 1. The lateral infiltration wetting thickness into a macropore wall can be adjusted to a value between 0 and 2 cm. The tile drain express fraction can be adjusted to a value between 0 and 0.1 to vary the percentage of macropore flow that follows the path into the tile drains and is not subject to absorption into the soil matrix.

Tile Drainage

If the user chooses to simulate tile drainage in the model, flux out of the drains will occur when the water table in the soil profile is above the depth of the drains. The depth of the water table is defined as the depth at which the pressure head first becomes negative, and all heads below that depth are nonnegative. When tile drainage is selected, the system will automatically set the bottom boundary condition for the Richards equation to a constant flux condition described by the Buckingham-Darcy equation (Buckingham, 1907) where the total head is the sum of the matric potential and gravitational heads, $h + z$, in the form:

$$v_w = -K\,(h)(\partial\, h/\partial\, z + 1)$$

for $z = z_w$; $t > 0$; where v_w = water table leakage rate (ground water leakage rate) in cm h^{-1}, $-K(h)$ = unsaturated hydraulic conductivity as a function of matric pressure head in cm h^{-1}, and z = the lower boundary of the soil profile at time (t) greater than zero. The ground water leakage rate can be adjusted during calibration. The Buckingham-Darcy equation is also used as the surface boundary condition set to the evaporative flux rate until the surface pressure head falls below a minimum value (set to $-20\,000$ cm), at which time a constant head condition $h = h(z)$ is used.

Lateral flow to tile drains can introduce error in the measurement of unsaturated zone parameters. However, Radcliffe et al. (1996) found that tile drain breakthrough curves can be used in Cecil soils to determine field-scale unsaturated zone transport parameters if a model accounts for two-dimensional flow in the saturated zone. The drainage rate to the tile drains in the RZWQM is calculated according to the Hooghoudt equation as applied by Skaggs (1978) to correct for the two-dimensional flux to the drains. The RZWQM adds the flux to root

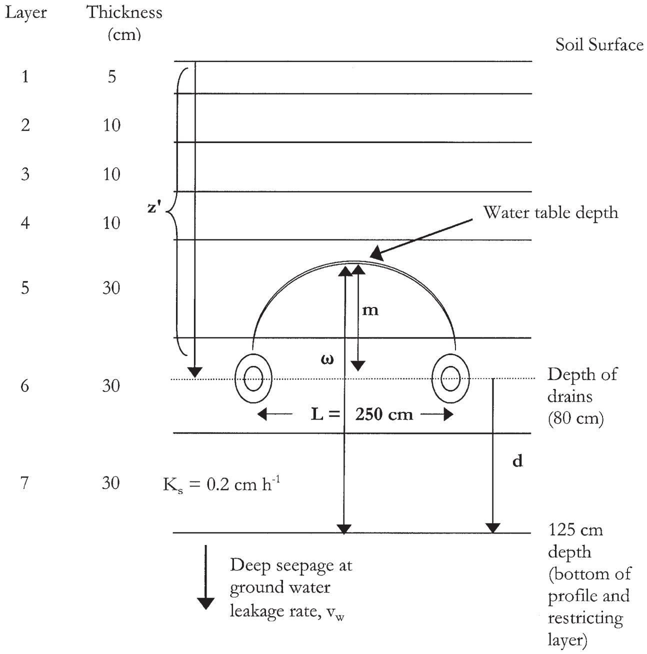

Fig. 1. Tile drainage system as set up in the RZWQM to emulate the design at the study site where z' = depth of drains, ω = distance from the water table to the impermeable layer, m = water table height above the drains, d = distance from the drain to the impermeable layer, and L = distance between drains. Design is based on the Hooghoudt steady state equation to estimate the flux at the center of the drains and correct for two-dimensional flow.

uptake to become a sink term at the equivalent depth of the drains.

There are two restrictive layers in the Cecil soils at the study site beginning at depths of 35 to 40 cm and at depths of 85 to 90 cm (Radcliffe et al., 1996). We set the tile drain depth in the model to 80 cm, which places them in the middle of the 30-cm soil layer that resides directly above the second restrictive layer. The model calculates the effective depth of the tile drains by calculating effective lateral hydraulic conductivity using the K_s of the soil layer where the drain resides as well as the layer beneath the drain layer to represent the transmissivity of both layers. Figure 1 depicts how we implemented the tile drainage system at the study site in the model to best represent the soil profile and tile drainage system for our simulations.

Tillage Effects on Soil

The algorithms used to simulate crop residue incorporation and tillage-induced changes in soil bulk density in the RZWQM were adopted from the USDA–Water Erosion Prediction Project (WEPP) model (Alberts et al., 1989). Tillage eliminates all potential macropore flow until the tilled zone reconsolidates with time as a function of rainfall intensity and amount and reverses the effects of tillage on bulk density, macroporosity, and hydraulic properties. Soil hydraulic property changes due to tillage are based on work by Ahuja et al. (1998) showing no change in the air-entry suction and increased soil water retention in the wet range of the Brooks-Corey soil water retention curve. The RZWQM model also allows for soil crusting after a rainfall event and will default to a value that is an 80% reduction of the first soil layer K_s (Ahuja et al., 2000), or can be user-designated.

Soil Nutrient Cycling

The submodel for Organic Matter and Nitrogen cycling (OMNI) is linked to other related submodels in the RZWQM such as soil chemistry, solute transport, and plant growth. Significant use of concepts and principles found in nutrient models such as NTRM (Shaffer and Larson, 1987), Phoenix (Juma and McGill, 1986), CENTURY (Parton et al., 1983), and Frissel's N model (Frissel and van Veen, 1981) were also used (Shaffer et al., 2000). Organic Matter and Nitrogen cycling (OMNI) accounts for all N and C processes and pools, with a subset of these processes modeled independently by rate equations. The remaining processes are modeled as functions of specified zero-order and first-order rate equations. The user may adjust many of these rates; however, the model documentation recommends against adjustments of these rates without carefully considering the complexity of the process as implemented in the RZWQM (Shaffer et al., 2000).

The initial dry mass of surface crop residue is user-specified. The model determines the mass incorporated into the surface soil residue pools for initializing the nutrient chemistry model. Initialization of microbial and humus pools will determine how most C and N cycling processes function during the first several years of a simulation. During the simulation, flat surface residue is made available for decomposition after incorporation by the specified tillage operation in CT systems. Standing dead residue becomes flat residue using an exponential decay function after the previous harvest. Nitrifying bacteria are assumed to have full access to NH_4 ions (adsorbed + solution). The concentration of NO_3^- increases at the rate of nitrification minus the assimilation rate of NH_4–N for microbial biomass production. The model does not contain a soil anion exchange process, and transport of chemicals under saturated conditions is simulated as piston flow in the mesopore regions of the soil matrix.

Crop Growth

The RZWQM has a single generic plant growth submodel that can be parameterized to simulate different crops. One can choose any of the crops that have already been parameterized for their simulation. Maize, soybean, and winter wheat crops have already been parameterized for the Management Systems Evaluation Areas (MSEA) sites in the midwestern USA (Hanson, 2000). The RZWQM also provides a second option submodel for simulation of crop growth referred to as the Quikplant model. It is a simple grass model that requires inputs such as maximum leaf area index and rooting depth of the crop, total seasonal N uptake, and harvest date. The plant reaches peak LAI, height, and maximum N use in the middle of the growing season. The Quikplant model includes the root input distribution supplied by the user for extraction of water and N from the soil. However, Quikplant is not a detailed growth model and should only be used to simulate water and soil N extraction, and when simulating crop production is not the primary aim of the modeler (Ahuja et al., 2000).

The RZWQM model calculates potential transpiration and soil evaporation using the extended Shuttleworth and Wallace (S-W) model (Farahani and Ahuja, 1996). The extended S-W model includes the effect of surface residue on soil evaporation and partitions evaporation into the bare soil and residue-covered fractions. Actual rates of soil evaporation and canopy transpiration are controlled by the soil water transport and crop growth components of the model (Farahani and DeCoursey, 2000). Water uptake by the roots is evaluated using the approach of Nimah and Hanks (1973), and the equation is solved iteratively by varying the effective root water pressure head until the potential transpiration demand is met based on the ability of the soil to supply the demand. The sum of the sink term cannot exceed the potential transpiration demand. The pressure head reaches a minimum value where it is held steady, and the sum of the sink term for root water uptake from all soil layers then resides below potential demand. The sink term for the Richards equation consists of both the distributed sink due to root uptake, and a point sink arising from tile drainage.

Nitrogen is passively taken up by the plant in proportion to plant transpiration and in quantities necessary to satisfy the present N demand. The amount of N that passively enters the plant is determined by the concentration of N in soil water extracted by the root system from each soil layer. If inadequate N is brought into the plant via transpiration, active N uptake occurs in a manner similar to the Michaelis-Menten substrate model. The total amount of additional N available to the plant through uptake is the sum of passive and active uptake. Available N is hierarchically allocated to roots and then to the other plant organs. Any N remaining after plant demands are met is placed into a storage pool and subtracted from plant N demand the following day (Hanson, 2000).

Model Calibration

General Procedure

After entering all of the model inputs and parameters, we ran the model for a period of 12 yr (3 yr of climate and rainfall data repeated four times) to initialize the organic N pools (rapid, medium, and slow decomposition pools) as suggested in the model documentation. This step is performed before actual calibration begins. The only parameters that we adjusted after the initialization procedure were the soil nitrate and soil ammonium nitrate values for each soil layer beginning on 1 Jan. 1991, the first day of the period for simulating tile drainage and leached nitrate for the analysis period (Table 2). The reason for this was that after the initialization procedure, the model greatly over- or underestimated these values although we had used a value of 1 Mg ha^{-1} and a wheat cover factor type based on model references and conventional till management practices during parameterization before running the initialization procedure. The measured mineral soil N data had been collected immediately after winter rye was planted for the first time as a cover crop at the study site in the fall of 1991 (Johnson et al., 1999; McCracken et al., 1995); therefore, the measurements reflected the previous 2 yr of winter and spring fallow conditions followed by a maize crop in the summer of 1991. Including a winter rye cover crop as part of the management practices during the 12-yr initialization procedure created more residue for simulated decomposition and, therefore, more mineralized soil N than that measured in the Fall of 1991. However, the simulation period for calibration that began after initialization of the model (1 Jan. 1991–14 Apr. 1993) included conventional till and winter rye cover crop management practices. Resetting the initial values of soil mineral N to their measured values after the initialization procedure before we began the simulations of tile drainage and leached nitrate on 1 Jan. 1991 reflected the soil N conditions at the study site just before the introduction of the winter rye cover crop in the fall of 1991.

For the calibration simulations, we used the general procedure recommended in the model documentation by calibrating the water balance, then the nutrient balance, and finally, crop production (Hanson, 2000) with additional details to meet our objectives for tile drainage and nitrate leaching with and without macroporosity (Fig. 2). We ran the simulations from 1 Jan. 1991 through April 1993 based on the availability of measured data for comparison to simulated values of tile drainage, leached nitrate, plant production, and soil N. Model simulations from November 1991 through April 1993 were used to evaluate and adjust the N balance by comparing simulated and observed values for soil N, nitrate leaching, and tile drainage. The period from November 1992 through April 1993 was used to test the sensitivity of tile drainage to the ground water leakage rate, and as the final evaluation period for tile drainage and leached nitrate after adjustments to the N balance. The reason for this was twofold. The tile drains were installed in one of the three conventional till plots that we used for calibration in 1981 and in the other two conventional till plots used for calibration in 1990. Since a winter rye cover crop was first introduced to the study in October 1991, the period from November 1992 through April 1993 allowed the simulation of conventional tillage maize production with winter rye cover after winter rye had been planted for at least one season. This also allowed additional time for the soil around the drains to settle from disturbance due to the installation of tile drains in two of the plots 2 yr earlier.

Table 2. Initial soil nitrogen on 1 Jan. 1991, and the observed and simulated N balance using the calibrated v_w value before and after adjusting the sensitive plant parameter, A_p, for the N balance simulation period, November 1991 to April 1993. No macroporosity model.

Initial soil NO_3–N, kg ha^{-1}	36.5		
Initial soil NH_4–N, kg ha^{-1}	6.25		
N balance (Day 6 Nov. 1991–13 Apr. 1993)		Simulated	
N component, kg ha^{-1}	Observed	Unadjusted	Adjusted
Initial soil NO_3–N	82	65	65
Initial soil NH_4–N	14	0	0
Fertilizer (NH_4NO_3)	168	168	168
Final soil NO_3–N	17	1	1
Final soil NH_4–N	29	0	0
Difference total soil mineral N	50	64	64
Leached NO_3 (tile drains)	63	38	62
Leached NO_3 (below drains)	–	−4	−3
Biomass N	205	227	235
Net N mineralized	50	34	66

Field measurement errors are typically >10%; therefore, it is unrealistic to match the observed data any more closely (Hanson et al., 1999). Our target error rate for the response variables in all periods was ±15% or less of measured values based on the goodness-of-fit test or the percentage difference recommended in the model documentation calculated as:

$$\%D = [(P - O)/O] \times 100$$

where P is the predicted value and O is the observed value.

We first calibrated the model without the macroporosity option, and then with macroporosity because measurements of macroporosity were available from the study site (Gupte et al., 1996). We ran the model with the macroporosity option to determine whether or not the model could simulate tile drainage more accurately with macropores since work by Gupte et al. (1996) showed preferential flow in Cecil and related soils of the Piedmont that was not necessarily associated with distinct open macropores but also occurred by way of infilled macropores. We followed the same general procedure for calibration with and without the macroporosity option, and compared the results of simulated tile drainage and leached nitrate with and without macroporosity.

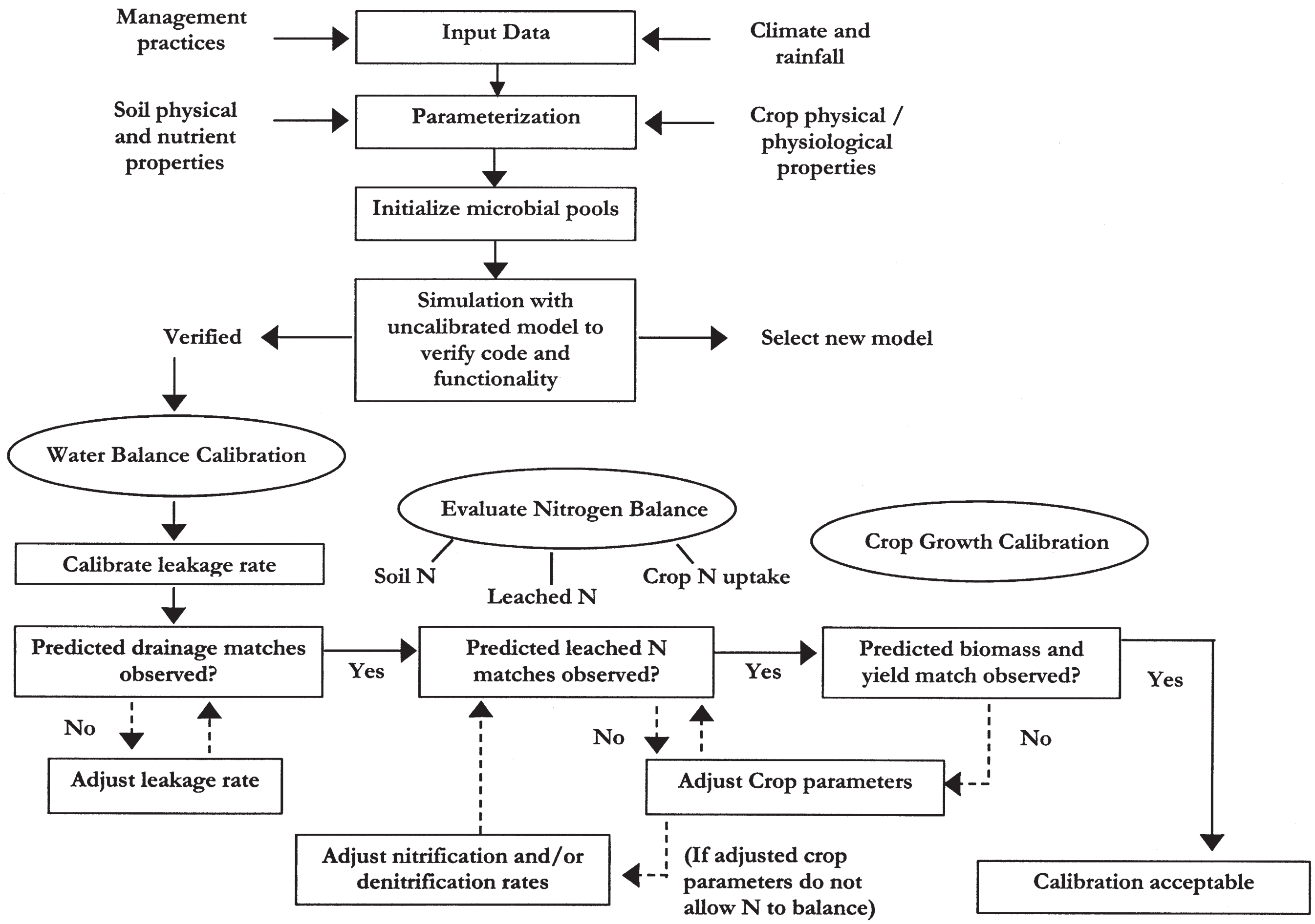

Fig. 2. Flow chart of procedure used to calibrate and evaluate the Root Zone Water Quality Model.

Water Balance Calibration for Tile Drainage

No Macroporosity

To calibrate the water balance, we chose to adjust the ground water leakage rate (water table leakage rate), v_w, or the water that will flow out of the bottom of the user-designated soil profile. We used this parameter for calibration because there were no available measurements of it from the study area. We chose a parameter that had not been measured because one of the strengths of our study was the number of field measurements that were available. According to Corwin et al. (1999), the definition of calibration is a test of a model with known input and output information that is used to adjust or estimate parameters for which there is no measured data. We increased the ground water leakage rate beginning with a value of 0 cm h^{-1} until total simulated tile drainage was within the prescribed 15% range of total observed tile drainage. During this step, we also observed the effect this adjustment had on leached nitrate since chemicals in the soil move with the soil solution. In addition, this assured that simulation of leached nitrate stayed within our target error range of ±15% of mean measured leached nitrate. The measurement period used for comparison after this adjustment was November 1992 through April 1993, after all conventionally tilled plots were in winter rye cover for 1 yr and all of the drain tiles had been installed for at least 2 yr.

With Macroporosity

After we calibrated the model without macroporosity, we calibrated the model with macroporosity by first testing three adjustable macroporosity parameters in the model. The parameters for adjusting the amount of macropore flow that occurs in the soil include the wetting thickness or effective lateral infiltration into the macropore wall (WT), the tile drain express fraction (EF), or the proportion of macropore water that flows to the tile drains, and the sorptivity factor for lateral infiltration (LAB), an adjustment to the calculated Green-Ampt lateral infiltration rate. These parameters were chosen because there was no measured data available for predetermination of possible values, and preliminary runs of the model that showed tile drainage was sensitive to them.

One of the most common forms of sensitivity analysis is to vary model parameters around their base values by some fixed percentage (Silberbush and Barber, 1983; Ma et al., 2000). We chose values of each of the three macroporosity parameters based on the range of values allowed by the model and created a matrix parameter set varying each parameter by approximately 50%. In the case of EF and LAB, initial and final values were increased or decreased from the 50% target value to avoid unreasonable combinations of parameter values. For example, a wetting thickness of zero and an absorption rate of zero with an express fraction of 0.09 would result in 9% of macropore water flowing into the tile drains. However, there would be no absorption into the macropore wall. The parameter set that we used consisted of values of WT ranging from 0.5 cm to 2.0 cm by 0.5 cm; EF values of 0.01, 0.05, and 0.09; and LAB values of 0.1, 0.5, and 1.0, which would reduce lateral absorption calculated with Green-Ampt by either 10, 50, or 0%, respectively, for a total of 36 simulations. The results of each parameter set on total simulated tile drainage and leached nitrate were compared to find the best combination for reducing errors between simulated and measured tile drainage and leached nitrate. Our target error rate of ±15% or less was used for differences between total simulated and total measured tile drainage and total simulated and total measured leached nitrate. We tested each macroporosity parameter and parameter combination set for its sum of squares contribution to the model sum of squares, described below in the model evaluation section, to determine if parameter values needed to be adjusted to a more narrow range of values. Final adjustments of these parameters to best simulate tile drainage for our study in conjunction with crop development provided a better understanding of how macroporosity functions and influences drainage in Cecil soils under conditions modeled, e.g., conventional tillage in maize or cotton production.

Leached Nitrate Calibration

After total simulated and measured drainage were within the 15% error range, we adjusted the sensitive plant parameters in an attempt to bring the simulated aboveground biomass N of the maize crop within, or as close as possible to, 15% of the measured value. We then evaluated the simulated N balance relative to N mineralization to begin refining the calibration for leached nitrate in drainage if needed. In plots with tile drains, Groffman (1984) found that tile drainage in Cecil soils increased aeration and thereby increased mineralization while decreasing gaseous N losses, resulting in a greater supply of nitrate in the drains. Based on available measured data, we evaluated simulated net mineralization for the period from 6 Nov. 1991 through 13 Apr. 1993 as follows:

$$N_{net} = (\text{Soil } N_{final} + \text{Crop } N_{uptake} + N_{leached}) - (\text{Soil } N_{init} + N_{fert})$$

where N_{net} = net mineralization; Soil N_{final} = final soil mineral N on 13 Apr. 1993; Crop N_{uptake} = aboveground biomass N; $N_{leached}$ = leached N in tile drains; Soil N_{init} = initial soil mineral N on 6 Nov. 1991; and N_{fert} = fertilizer N applied. If the model over- or under-predicted a N component in the system, we first adjusted the plant parameters to improve the simulation of N uptake, which in turn would affect the other N components. If simulated N_{net} could not be achieved within ±15% of observed N_{net}, or the system was producing too much or too little nitrate, we adjusted the nitrification and denitrification rates to bring Soil N_{final}, Crop N_{uptake}, and $N_{leached}$ to within ±15% of, or as close as possible, to observed values. We reevaluated the N balance after each adjustment. Iterative adjustments to sensitive plant parameters and the nitrification and denitrification rates were made until $N_{leached}$ and Crop N_{uptake} were as close as possible to their measured values.

Crop Growth Calibration

Since plant production was part of the N balance and tightly coupled to the other processes, we followed the procedure for calibrating plant growth recommended for the model by Hanson (2000) when using the generic plant growth submodel. This procedure is based on adjustments to five sensitive plant parameters including active N uptake rate (μ_1), daily respiration as a function of photosynthesis (Φ), the biomass to leaf area conversion coefficient (C_{LA}), and the age effect for plants during the propagule stage and the seed development stage (A_p and A_s). We used the generic plant growth submodel for both the maize and cotton calibrations, and based adjustments of these parameters for maize within the range of values used for calibration of the MSEA sites (Hanson, 2000). The calibration for cotton development included adjustments of these same sensitive parameters as well as changes to some of the physiological and phenological parameters described below and used in the plant production input file. The calibration for each crop then proceeded by varying each of the sensitive parameters until total biomass and yield were within the 15% range of measured values. During adjustment of these parameters to improve yield simulations to reflect the observed values, we also checked the effect on simulated tile drainage and leached nitrate. This process was used iteratively as depicted in Fig. 2 until simulated tile drainage, leached nitrate, and maize yield were within, or as close as possible, to the desired 15% error range of observed values.

The parameters for the Quikplant model to simulate the winter rye cover crop were obtained from local crop measurements or estimates based on measurements of rye crops (Univ. of Georgia College of Agric. and Environ. Sciences, 1998; Blount et al., 2000). The parameters included total seasonal N uptake, length of growing season (days), maximum crop height, leaf area index, rooting depth, stover after harvest, the C/N ratio of fodder material, and winter dormancy recovery day of year (Appendix A).

After the model was calibrated for tile drainage and leached nitrate in maize and winter rye production, we held all parameters constant and added cotton to the generic plant growth submodel. Parameters were obtained from the cotton field study conducted adjacent to the water quality site (Schomberg and Endale, 2004), and from literature values (Carns and Mauney, 1968; Miley and Oosterhuis, 1990; Univ. of Georgia College of Agric. and Environ. Sciences, 2000; Nyakatawa and Reddy, 2000; Nyakatawa et al., 2000; Reddy et al., 2004). The cotton calibration simulation period was 1 Jan. 1997 through 31 Dec. 1997. The parameters adjusted for cotton in the generic plant growth input file included the physical dimensions of the plant; the maximum, minimum and optimum temperature for growth; maximum leaf area index; and the minimum number of days the plant required to transect each physiological growth stage (Appendix A7). Through iterative adjustments of these parameters, we compared simulated and observed cotton total biomass until simulated values were within 15% of observed values. Since we did not have measures of tile drainage or leached nitrate from the study used to calibrate for cotton, we compared simulated and calculated PET and water use to ensure that the model could simulate both reasonably well as a basis for later evaluating simulated tile drainage in the water quality study. Calculated PET was based on the Priestley-Taylor equation (Priestley and Taylor, 1972) from the weather station near the water quality study site, approximately 100 m from the cotton calibration study site (Hoogenboom, 2003). We calculated observed and simulated water use for cotton as:

$$\text{Water use} = \text{Rainfall} - \text{Observed or simulated } \Delta \text{ Soil Water}$$

where Rainfall = measured rainfall at the weather station adjacent to the water quality study site, Δ Soil Water = Soil water$_{i+1}$ − Soil water$_i$, where soil water was measured or simulated in a 60-cm profile, and i = day of year. Observed soil moisture in cotton showed little or no change below 60 cm in the field study used for calibration (Schomberg and Endale, 2004). The rooting depth for cotton is shallow in acid soils because it is one of the most sensitive crops to aluminum toxicity, which frequently occurs in acid subsoils such as those in Georgia (Mitchell et al., 1991; Sumner, 1994; Gascho and Parker, 2001).

Evaluation of Simulation Results

For the analysis of the macroporosity parameters, we tested for the main effects and interactions of the three parameters for macroporosity and selected the most significant effects based on the Type I sum of squares each contributed to the model sum of squares (SAS Institute, 2000). Based on this information, we identified the parameter or combination of parameters with the highest correlations and highest probabilities for simulated and observed tile drainage. We determined at this point whether further testing was needed within a more narrow range of parameters. Since one of our objectives was to try to simulate how macropore flow may affect drainage in Cecil soils, we chose to refine the range of the parameters as much as possible to improve our understanding by way of the simulation process.

For the analysis of simulated and observed values of tile drainage and of nitrate leaching, we regressed the final observed values on simulated values using linear regression analysis (SAS Institute, 2000), to compare r^2 values, slopes, and intercepts. We calculated the relative root mean square error (RRMSE), standard error of the mean difference (Addiscott and Whitmore, 1987), maximum error, average and standard deviation of measured and simulated values to characterize systematic over- or under-prediction, and used graphical displays to show trends and distribution patterns (Loague and Green, 1991). The RRMSE, which is the RMSE relative to the mean of the observed values, is calculated as follows:

$$\left[\sum_{j=1}^{N}(s_j - o_j)/N\right]^{0.5} \times (100/O)$$

where N = number of observations; o_j = observed value j; s_j = simulated value j; and O = mean of the observed values. The RRMSE standardizes the RMSE, and is expressed as a percentage that represents the standard variation of the estimator. The RRMSE assigns equal weight to any overestimation or underestimation of the statistic (S.P. Weschsler, www.csulb.edu/~wechsler; verified 18 Aug. 2005).

For the cotton water use analyses, we compared observed and simulated water use for the period of peak water use in cotton from first square to first bloom and from first bloom to peak bloom. Our criteria for the acceptable differences between daily simulated and observed water use was ±15% or less based on a minimum daily value of 6.4 mm of water use for cotton during these periods, a total of approximately 55 d in July and August (NCSU-CES, 2004).

RESULTS AND DISCUSSION

Calibration: No Macroporosity

Increasing the ground water leakage rate from 0 to 0.004 cm h^{-1} decreased simulated tile drainage linearly. The final ground water leakage rate used for calibrating the model for tile drainage and leached nitrate was 0.0039 cm h^{-1} because simulated values were in good agreement with observed values compared with the other rates that were tested (Fig. 3). A higher K_s for a soil layer above a layer with lower K_s as depicted in Fig. 2 for the two bottom layers of the profile could create unsaturated conditions in the lower layer due to negative pressure at the interface of the two layers. This would result in very slow soil water movement from the upper layer into the lower layer over time and create a perched water table. However, though the ground water leakage rate turned out to be very small, simulated tile drainage was sensitive to very small changes in the ground water leakage rate. Our analysis indicates that adequate flow occurred in the RZWQM simulation of drainage through

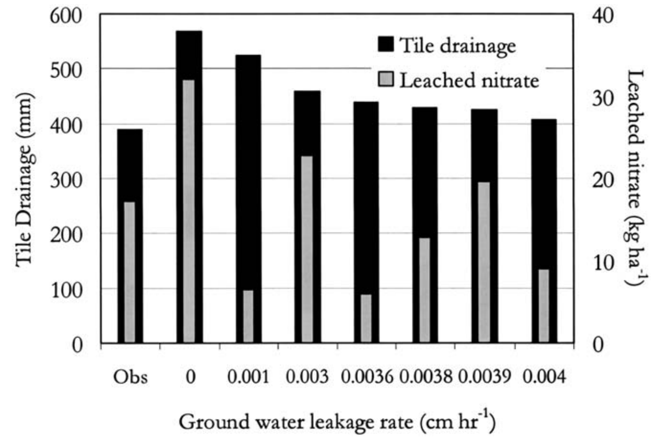

Fig. 3. Simulations using values of ground water leakage rate, v_w, for sensitivity analysis of simulated tile drainage and leached nitrate.

the lower layer into ground water to warrant calibration of the ground water leakage rate when the model is used to simulate tile drainage. In a study of tile drain breakthrough curves on two plots adjacent to the water quality study in 1991, Radcliffe et al. (1996) found that seepage through the two layers below the tile drains accounted for approximately 10% of irrigation water applied. Measured values of K_s in these two layers were 0.2 and 0.035 cm h^{-1}, respectively, at a site near the water quality study without tile drains (Bruce et al., 1983). The bottom of the first layer in that study (133-cm depth) corresponds to the bottom layer of the soil profile (125-cm depth) in our study. The difference in the K_s of the layer below 133 cm and our calibrated ground water leakage rate (0.035 cm h^{-1} vs. 0.0039 cm h^{-1}) could be due to the mechanical compaction of the soil around the drains that was performed after installation in the water quality study. The compaction of the soil below the installation depth during the process could have decreased the rate of soil water movement below the measured value of 0.035 cm h^{-1} as well.

Though we chose the ground water leakage rate that best simulated total tile drainage when compared with total observed drainage, simulated leached nitrate was not within ±15% of observed leached nitrate for the period used to evaluate the N balance from November 1991 through April 1993. Simulated leached nitrate was 25 kg ha^{-1} less than observed leached nitrate and simulated aboveground biomass N for maize was 30 kg ha^{-1} greater than observed aboveground biomass N, and both were outside the ±15% error range. Simulated soil mineral N was 45 kg ha^{-1} less than observed but within ±15% of observed soil mineral N, and simulated maize yield was within ±15% of observed yield. Since leached nitrate was underpredicted and aboveground biomass N was overpredicted by almost the same amount, we decreased the A_p parameter (propagule age effect). A decrease in this parameter will reduce yield in relation to total biomass and therefore reduce the crop N demand. This is due to the fact that propagule N demand is met first when the plants are in the reproductive stage in the hierarchical scheme for N allocation in the generic plant growth submodel (Hanson, 2000). In addition, our

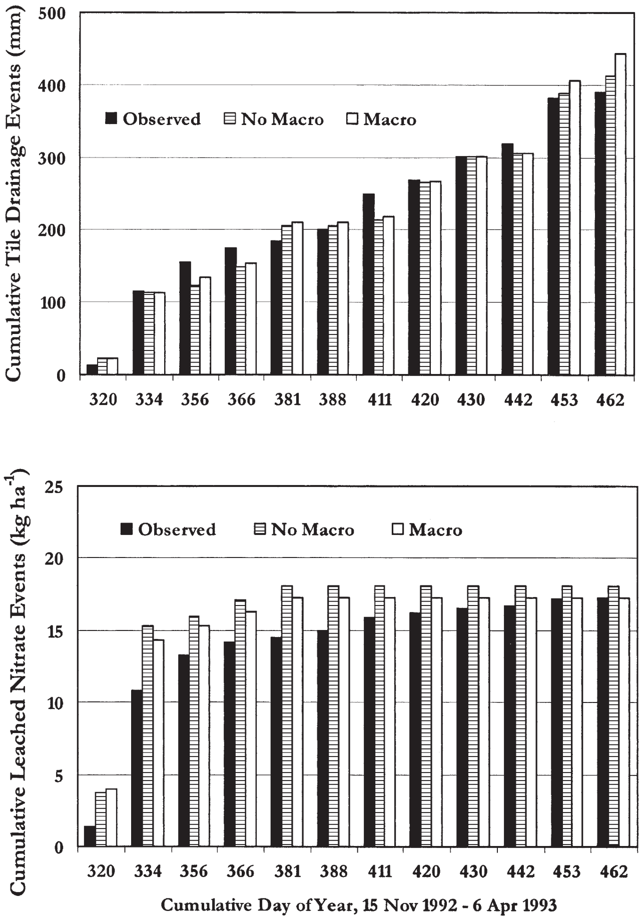

Fig. 4. Cumulative observed and simulated tile drainage (top) and leached nitrate (bottom) with and without macroporosity for the simulation period November 1992 through April 1993 for maize.

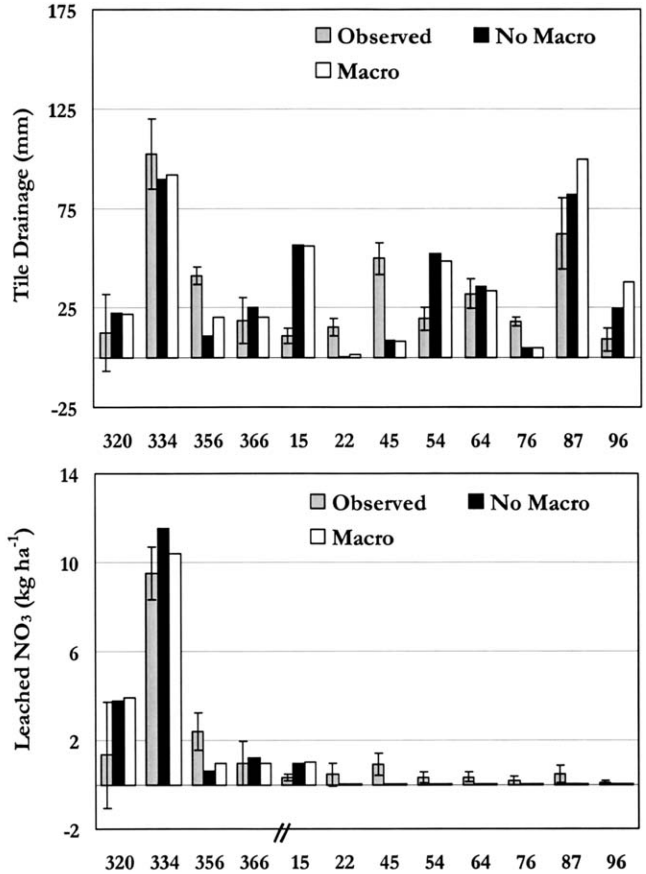

Fig. 5. Measured and simulated event tile drainage (top) and leached nitrate (bottom) for the simulation period from November 1992 through April 1993 with and without the macroporosity option for maize. Observed drainage events shown with 95% C.I. bars.

target error range for yield was large (5716–7734 kg ha^{-1}) so that a slight reduction in yield would be acceptable. Our previous experience of adjusting the sensitive plant parameters by trial and error showed that the model would allocate the N balance components differently with this adjustment. The adjusted A_p parameter increased simulated leached nitrate to within <1% of observed leached nitrate while simulated maize yield remained within 15% of observed yield, though it decreased slightly. The remaining sensitive crop parameters for maize were left unadjusted from their original values. Total simulated N uptake was slightly higher in the adjusted model than in the unadjusted model. However, total simulated aboveground biomass N for all three crops (winter rye 1992, maize 1992, and winter rye 1993) was within 15% of total observed aboveground biomass N for all three crops (Table 2).

The analysis of simulated and observed soil mineral N for each day of 12 field-measured values from November 1991 through April 1993 revealed that 3 of the 12 simulated soil mineral N predictions were outside the 95% confidence interval (CI) of observed soil mineral N. Total simulated tile drainage and leached nitrate for the final analysis period of November 1992 through April 1993 were 6 and 5% of total observed values, respectively. Since we met our objective of obtaining a difference between simulated and observed values for tile drainage, leached nitrate and maize yield of 15% or less for the final analysis period, we considered the calibration acceptable as the final calibrated scenario for maize production with a winter rye cover crop without macroporosity.

The analysis of simulated tile drainage and leached nitrate for the calibrated scenario revealed that cumulative simulated tile drainage followed the pattern of cumulative observed tile drainage (Fig. 4). However, 7 of 12 simulated drainage events were outside of the 95% CI of observed tile drainage events (Fig. 5). Simulated leached nitrate increased at the same rate as observed leached nitrate during the first five drainage events and then leveled out at or near zero for the remaining seven events while observed leached nitrate continued to increase slightly (Fig. 4). Six out of 12 simulated leached nitrate events were outside the 95% CI of observed leached nitrate (Fig. 5). The RRMSE showed a large percentage deviation from the mean observed values, reflecting the fact that the majority of simulated events for tile drainage and half of the events for leached nitrate were outside of the 95% CI (Table 3). Linear regression analysis of total observed tile drainage on total simulated tile drainage revealed that simulated tile drainage explained 37% of the variation in observed tile drainage. Analysis of total observed leached nitrate on total simu-

Table 3. Simulated and observed tile drainage and leached nitrate for (a) no macroporosity model and (b) with macroporosity for maize production during the calibration period November 1992 through April 1993.

Component	Observed mean	Simulated mean	Mean difference	Standard error mean difference	Max error	RRMSE†
(a)			No macroporosity			
	mm					%
Tile drainage	32.5	34.4	−1.9	7.3	40.9	74.6
	$kg\ ha^{-1}$					%
Leached nitrate	1.4	1.5	−0.1	0.7	1.8	78.3
(b)			With macroporosity			
	mm					%
Tile drainage	32.5	36.9	−4.4	7.6	41.8	78.8
	$kg\ ha^{-1}$					%
Leached nitrate	1.4	1.4	−0.0	1.4	1.4	68.6

† RRMSE, relative root mean square error.

lated leached nitrate revealed that simulated leached nitrate explained 90% of the variation in observed leached nitrate. The slopes of the regressions for both response variables were not significantly different from one, and the intercepts were not significantly different from zero at the 0.05 probability level (Table 4).

Calibration with Macroporosity

Results of the 36 parameter matrix analysis for the macroporosity parameters WT, EF, and LAB revealed that the interaction of all three parameters contributed a large enough Type I sum of squares to the model sum of squares to warrant further testing within a narrower range of each parameter. The new parameter matrix set consisted of 75 combinations of these three parameters based on the range of each between their maximum and minimum values and from the highest correlations of simulated vs. observed tile drainage. After running the model for each of the new 75 combinations of WT, EF, and LAB, we again chose the highest correlations and the highest probabilities of simulated with observed tile drainage. We narrowed these further by choosing those combinations that simulated the smallest differences between simulated and observed tile drainage, and simulated and observed leached nitrate for the period from November 1992 to April 1993. The final values used for these parameters for calibrating the model with macroporosity were WT = 1 cm, EF = 0.01, and LAB = 0.4.

With these three parameters selected for macroporosity, the model simulated a very large amount of nitrate with large increases in leached nitrate and net mineralization and smaller increases in the other N balance components for the N balance analysis period (Table 5). We tried six other combinations of the macroporosity parameters that also showed high correlations between simulated and observed tile drainage and leached nitrate for the final analysis period (November 1992–April 1993). In each case, simulated net mineralization increased, and the system produced too much nitrate and increased one or more of the N components by large amounts. The N balance became very volatile with the inclusion of the macroporosity option, and we were not able to simulate the N balance components, including net mineralization, to within ±15% of observed values during the N balance analysis period. Adjustments to one or more of the other sensitive plant parameters such as N uptake (μ_1) or the proportion of photosynthate to respire (Φ) could cause the model to suddenly generate unreasonably high amounts of nitrate in one or more N components such as leached nitrate. We also found that more than one combination of values for the sensitive plant parameters would simulate yield and possibly simulate one other N component such as leached nitrate within 15% of observed values, but again would create large changes in other components of the N balance such as crop N uptake. This would then create

Table 4. Regression statistics for tile drainage and leached nitrate with and without the macroporosity option for the calibration period November 1992 through April 1993.†

Model	Observed	Simulated	RMSE	*r*	Intercept	Slope
	total mm					
			Tile drainage			
No macro	390	413	23.0	0.61	12.8*	0.6**
With macro	390	443	22.7	0.62	12.8*	0.5**
			NO_3 in tile drainage			
	$kg\ ha^{-1}$					
No macro	17.2	18.1	0.85	0.95	0.3*	0.75**
With macro	17.2	17.3	0.90	0.94	0.3*	0.81**

* Intercepts not significantly different from 0 at $p < 0.05$.
** Slopes not significantly different from 1 at $p < 0.05$.
† RMSE, root mean square error; *r*, correlation coefficient; intercept and slope of measured vs. simulated values.

Table 5. Initial soil N on 1 Jan. 1991, and observed and simulated N balance using calibrated v_w before and after adjustment to the denitrification rate for the simulation period of November 1991 to April 1993. Macroporosity model.

Initial soil NO_3–N, $kg\ ha^{-1}$	36.5		
Initial soil NH_4–N, $kg\ ha^{-1}$	6.25		
N balance (day 6 Nov. 1991–13 Apr. 1993)		Simulated	
N component, $kg\ ha^{-1}$	Observed	Unadjusted	Adjusted
Initial soil NO_3–N	82	102	103
Initial soil NH_4–N	14	0	0
Fertilizer (NH_4NO_3)	168	168	168
Final soil NO_3–N	17	1	1
Final soil NH_4–N	29	0	0
Difference total soil mineral N	50	101	102
Leached NO_3 (tile drains)	63	538	178
Leached NO_3 (below drains)	–	−9	−30
Biomass N	205	342	259
Net N mineralized	50	611	167

a situation that required an endless number of iterative adjustments to bring simulate leached nitrate, tile drainage, and yield back to within a reasonable range of observed values. After several attempts to adjust the macroporosity components and the sensitive plant parameters to simulate leached nitrate and net mineralization within our 15% target error range without success, we set both the nitrification and denitrification rates to zero to allow the model to produce mineral N by way of organic matter decay and microbial biomass N mineralization and decay (Shaffer et al., 2000). Under these conditions, the OMNI submodel will test for sufficient NH_4^+ and NO_3^- in the system and shut down the decay process if net immobilization is occurring, limiting the amount of NH_4^+ that can be released by the microbial biomass decay process. In contrast, nitrifying autotrophic bacteria have full access to NH_4^+ in the model in both adsorbed and solution phases so that as long as mineralization is occurring, NH_4^+ will be nitrified. Setting the nitrification and denitrification rates to zero decreased soil nitrate N and increased soil ammonium N. This also reduced leached nitrate, although it was still 48 kg ha^{-1} greater than observed leached nitrate, and N uptake by the second winter rye crop increased 17 kg ha^{-1}. Finally, we set the nitrification and denitrification values back to the model default values, and increased the denitrification rate incrementally to decrease the amount of nitrate in the system (Table 5). Using a Latin Hypercube Sampling technique to determine the sensitivity of crop N uptake, silage yield, and nitrate leaching below the root zone in the RZWQM, Ma et al. (2000) found that all of the responses were negatively related to the denitrification constant. In addition, the authors found that a combination of mean irrigation and manure application rates simulated leached nitrate concentrations from 0 to 755 kg N ha^{-1}. They described the outcome of combining irrigation and manure rates as the worst scenario for simulating their response variables. By using the model default nitrification rate and increasing the denitrification rate, we were able to stabilize the N balance components, and to simulate leached nitrate, tile drainage, and maize yield more accurately for the final analysis period of November 1992 through April 1993. However, we were not able to simulate any of the response variables to within ±15% of observed values during the N balance analysis period (Table 5).

The analysis of simulated soil nitrate and 12 measured values of soil nitrate revealed that 3 of 12 simulated values were outside the 95% CI of measured values as was the case for the calibration without macroporosity. However, leached nitrate and biomass N for all three crops were still overpredicted for the period from November 1991 to April 1993 initially used to test the N balance (Table 5), but simulated tile drainage and leached nitrate were within 15% of observed values for the final analysis period. Due to the volatile nature of the N balance with macroporosity after numerous attempts to improve the N balance, we accepted the scenario as the final calibration of the model in maize production with macroporosity.

The analysis of simulated tile drainage and leached nitrate with macroporosity for the calibrated scenario revealed that cumulative simulated tile drainage followed the pattern of cumulative observed tile drainage (Fig. 4) with 8 of 12 simulated drainage events outside the 95% CI of observed tile drainage events (Fig. 5). There were no significant differences in the means or the variances between tile drainage simulated with or without macroporosity. Simulated leached nitrate increased at the same rate as observed leached nitrate during the first 5 of 12 drainage events following the same pattern as simulated leached nitrate without macroporosity (Fig. 4). Six of the 12 simulated leached nitrate events were outside the 95% CI of observed leached nitrate, as was the case with no macroporosity (Fig. 5). The RRMSE showed a large percentage deviation from the mean observed values, reflecting the fact that the majority of simulated events for tile drainage and half of the simulated leached nitrate events were outside of the 95% CI of measured events (Table 3). Linear regression analysis of total observed tile drainage on total simulated tile drainage, and total observed leached nitrate on total simulated leached nitrate revealed nearly the same relationship as the regressions without macroporosity. The slopes were not significantly different from one, and the intercepts were not significantly different from zero at the 0.05 probability level (Table 4). There were no significant differences between the means or the variances with and without macroporosity for simulated leached nitrate.

Though it was more difficult to calibrate the model with macroporosity than without macroporosity due to the volatile nature of the N balance with macroporosity, the differences between simulated tile drainage and leached nitrate relative to macroporosity indicated that macroporosity did not have a significant influence on the amount of tile drainage that occurred in these soils. In a study of intact dye-stained soil cores from the study area in conventional tillage, Gupte et al. (1996) found little evidence of preferential flow in the upper 45 cm of the cores. Preferential flow often occurred in regions of soil and in-filled macropores at depths between 45 and 60 cm rather than through open macropores. In addition, the presence of tile drains below 60 cm in our study would influence the way drainage occurs both in the field and in model simulations due to the difference in the flow patterns created when tile drains are present (Skaggs, 1980; Ritzema, 1994). Any preferential flow that occurs due to the presence of macropores near the depth of the tile drains would be difficult to quantify separately from the impact of tile drains on soil water flow.

The contribution of macropore flow to simulations of nitrate leaching was also difficult to quantify because the amount of nitrate leached was greatly affected by changes to other parameters such as the plant parameters, the nitrification and denitrification rates, and the macroporosity parameters. This was in spite of the fact that we narrowed the combination of adjustable parameters for macroporosity to those that best simulated our response variables before adjustments to any of the plant parameters. A sensitivity analysis using all of the combined parameters that appeared to affect nitrate leaching with the macroporosity option might be effec-

Table 6. Final adjusted values used for the sensitive parameters for cotton calibration of the RZWQM.

Parameter	Definition	Value	Units
μ_1	maximum active N uptake	3.5	g plant^{-1} d^{-1}
Φ	daily respiration as a function of photosynthesis	0.005	d^{-1}
C_{LA}	biomass to leaf area conversion coefficient	12	g leaf area^{-1}
A_p	age effect for plants in propagule development stage	0.97	–
A_s	age effect for plants in seed development stage	0.97	–
–	minimum leaf stomatal resistance	50	s m^{-1}
–	maximum rooting depth	1.0	m
–	N sufficiency index (trigger for timed application of fertilizer)	0.9	–
–	luxurious N uptake factor (increases or reduces uptake)	1	–

tive in the case of calibration for nitrate leaching for one scenario or one study. However, based on our experience in this study, it is likely the model will not perform consistently if the conditions tested are different than those under which the model was calibrated due to the volatile nature of the N balance once macroporosity is introduced. Ma et al. (2000) concluded that the interdependency of various parameters can introduce high variability in response variables that are tested with the RZWQM, but that model output responses can be much less sensitive to variations in one parameter than in the other. A closer examination of this variability is needed where the model produces large amounts of nitrate with minor changes to crop parameters or N rates before the model can be expected to perform in a reliable manner in subsequent simulations of nitrate leaching with the macroporosity option.

Cotton Calibration

After cotton was included in the generic plant growth submodel, the sensitive parameters, μ_1, A_p, A_s, Φ, and C_{LA}, and leaf stomatal resistance were iteratively adjusted as well as the minimum number of days required for the vegetative and reproductive growth stages to simulate cotton biomass development as closely as possible to observed development (Table 6). We also adjusted the albedo of a mature plant to 0.2 based on model references to bring total simulated PET at the end of the cotton growth period as close as possible to total calculated PET from the weather station near the study site (Hoogenboom, 2003). The result of this adjustment was a difference of $<$3 mm between total simulated and total calculated PET for the cotton growth period. Adjustments to the minimum number of days for each of the vegetative and reproductive growth phases were particularly sensitive in our efforts to achieve a growth pattern and values for simulated cotton biomass and leaf area index that matched observed values on measurement days. It was not possible to simulate total biomass to within 15% of total observed biomass despite numerous iterative adjustments and combinations of the phenology parameters. This was because the model could not produce the large increase in observed biomass between Day 245 and Day 266 without adjusting the plant parameters to rapidly increase total biomass early in the season (before the first bloom period for cotton) (Fig. 6). When we adjusted the parameters to rapidly accumulate biomass early in the season, after simulated vegetative growth peaked, biomass accumulation would begin to decline as the simulated plant entered the reproductive stage followed by leaf senescence. The optimum balance for the number of days in each of the vegetative and reproductive growth stages to achieve a simulated pattern of development that matched observed development for cotton resulted in a period of 115 d for the vegetative stage and 40 d for the reproductive stage. This allowed the model to simulate cotton biomass accumulation and leaf area similarly to observed biomass and leaf area during the majority of the growing season by slowing biomass accumulation until the last 21 d of observed cotton boll development when simulated biomass began to decline (Fig. 6).

Simulated biomass developed according to observed biomass based on the days that biomass was measured until Day 246 through the final measurement on Day 266 when total observed biomass was 21 100 kg ha^{-1}, and total simulated biomass was 8148 kg ha^{-1} without macroporosity and 8180 kg ha^{-1} with macroporosity. The maximum simulated leaf area index for the cotton growth period was 3.9 cm^3 cm^{-3} without macroporosity and 3.4 cm^3 cm^{-3} with macroporosity, and occurred 21 d before the maximum observed value of 4.83 cm^3 cm^{-3} on Day 266. Simulated cotton yield was 2559 kg ha^{-1} without macroporosity, 3448 kg ha^{-1} with macroporosity, and observed seed lint yield was 1205 kg ha^{-1}. The final observed weights for the cotton bolls were 55% of the final observed total biomass, and simulated cotton yields were 31% of total simulated biomass without macroporosity and 42% of total simulated biomass with macroporosity.

The mean difference between observed and simulated biomass for the seven measurement days in 1997 was 1250 kg ha^{-1} without macroporosity and 1538 kg ha^{-1}

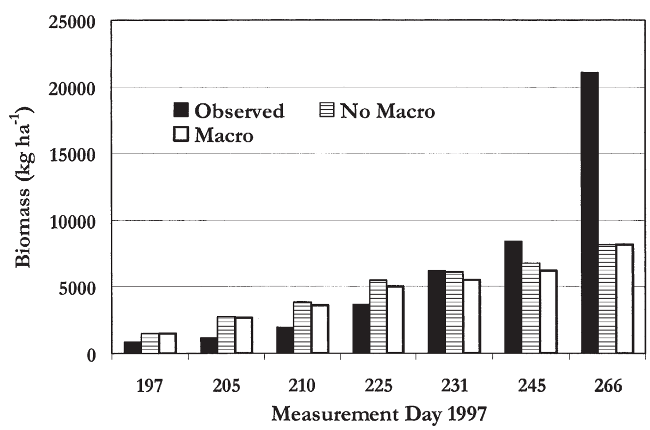

Fig. 6. Observed and simulated cotton biomass development with and without the macroporosity option in the model.

with macroporosity. The mean observed water use for the entire period was 3.1 mm d^{-1} and the mean simulated water use was 3.2 mm d^{-1} without macroporosity and 3.1 mm d^{-1} with macroporosity. Simulated water use was positively correlated with observed water use. For the period from first square to first bloom in cotton development (Day 188–197), observed water use was 3.0 mm d^{-1} and simulated water use was 2.5 mm d^{-1} without macroporosity and 3.3 mm d^{-1} with macroporosity (Fig. 7). Greater soil water depletion in a 60-cm profile with macroporosity from Day 180 through 190 was a result of simulated tile drainage during the period of rainfall from Day 150 through 190 after the soil became saturated. Tile drainage from Day 150 through 190 was 70 mm without macroporosity and 94 mm with macroporosity. Simulated ET without macroporosity was 7 mm greater than with macroporosity for the same period with an average of 2.7 mm d^{-1} and 2.5 mm d^{-1}, respectively. During the period of greatest cotton water use and when temperatures were the warmest during the growing season (mid to end of July, Day 197–210), 111 mm of rainfall recharged the profile. Simulated ET for this period was 4.4 mm d^{-1} with and without macroporosity, reflecting no difference in simulated cotton water use. However, simulated tile drainage without macroporosity was 33 mm greater than simulated tile drainage with macroporosity due to greater antecedent soil moisture without macroporosity before rainfall began on Day 197. Daily average temperatures were normal for this period (Hoogenboom, 2003), and total simulated and calculated PET for the period were each 66 mm. Cotton water use normally ranges from 2.5 to 6.4 mm d^{-1} during this time from first square to first bloom in the development period (NCSU-CES, 2004). However, on Day 197 measured biomass was 831 kg ha^{-1}, and simulated biomass was 1480 kg ha^{-1} without macroporosity and 1466 kg ha^{-1} with macroporosity. Although calculated and simulated PET values were the same, large differences in observed and simulated biomass accumulation during the period revealed that the model was not accurately simulating water use efficiency, or the number of units of water required to produce a relative number of units of cotton biomass at this stage of development. In addition, simulated and measured soil moisture depletion were nearly equal from Day 211 until 223 when rainfall began, and simulated and observed biomass accumulation for the period were different by only 25 kg ha^{-1}, although total simulated biomass on Day 225 was 5522 kg ha^{-1} and observed biomass was 3717 kg ha^{-1}.

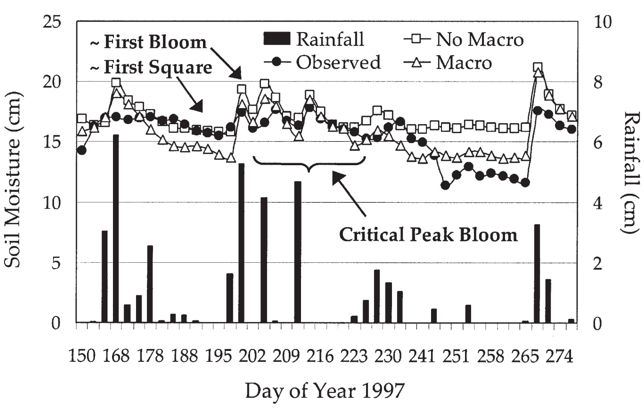

Fig. 7. Observed soil moisture and rainfall and simulated soil moisture with and without macroporosity for the cotton growing season in 1997.

From Day 223 through 231, total rainfall was 38 mm and simulated ET with and without the macroporosity option was 36 mm. A dry period followed from Day 232 through the end of the cotton growing season on Day 265, during which time measured soil moisture showed greater depletion than simulated soil moisture with and without macroporosity. Total measured biomass accumulation was 14 900 kg ha^{-1}, and simulated biomass accumulation was 2010 kg ha^{-1} without macroporosity and 2600 kg ha^{-1} with macroporosity during this period, and explained the lower values of simulated soil water depletion compared with measured depletion.

During the critical period just before peak bloom, cotton requires approximately 7 to 8 mm of water per day to reach potential yield (Bednarz et al., 2003). During the critical peak bloom period in 1997 (Day 197–228), mean observed water use was 5.8 mm d^{-1} and mean simulated water use was 5.6 mm d^{-1} without macroporosity and 5.1 mm d^{-1} with macroporosity. Total simulated PET was 149 mm and calculated PET was 145 mm or 4.5 and 4.4 mm d^{-1}, respectively, indicating that both calculated and simulated water use could be somewhat high for this period. Lower values of calculated and simulated PET relative to calculated and simulated soil water use would mean that the roots did not extract all of the soil water in the 60 cm soil profile. Low values of actual cotton water use compared with the potential water use might be due to the effect that temperatures had on cotton development for this period in contrast to the period from first square to first bloom. During the 1997 growing season, temperatures ranged from 0.3 to 2.6°C below the long-term monthly means for the area (Schomberg and Endale, 2004). The authors attributed the low cotton seed lint yield on Day 265 to the lower-than-average daily temperatures for the cotton growing season. The optimum mean maximum temperature for cotton growth is approximately 32°C (Nyakatawa et al., 2000). The mean maximum daily temperature during the entire period of critical peak bloom was 28°C based on measurements at the weather station next to the study site (Hoogenboom, 2003).

Simulated cotton biomass accumulated more rapidly than measured biomass during the peak bloom period from Day 197 until 231 (Fig. 6). On Day 231, simulated and observed cotton biomass values were nearly equal. The average difference between observed and simulated biomass on Day 231 and 246 was 841 kg ha^{-1} without macroporosity and 1428 kg ha^{-1} with macroporosity. The average observed water use was 2.5 mm d^{-1} from Day 231 to 246, and the average simulated water use was 1.6 mm d^{-1} without macroporosity and 1.9 mm d^{-1} with macroporosity, indicating the difference between observed and simulated biomass accumulation and water use during the period. Calculated PET was 72 mm for the period or 4.8 mm d^{-1}, and simulated PET was 74 mm or 4.9 mm d^{-1}. This is the period of development in cotton just before peak bloom when water use can range from 6.4 to 10 mm d^{-1} (Bednarz et al., 2003; NCSU-CES, 2004). Based on calculated values of PET, actual water use may have been higher, and more extraction of water below 60 cm occurred in the field. On Day 246, observed values of biomass began to surpass simulated values of biomass. From Day 246 through 266 when final observed biomass was greater than simulated biomass by more than 10 000 kg ha^{-1}, observed water use was 2.2 mm d^{-1}, and simulated water use was 0.5 mm d^{-1} with no macroporosity and 0.4 mm d^{-1} with macroporosity. Calculated PET was 71 mm or 3.4 mm d^{-1}, and simulated PET was 87 mm or 4.1 mm d^{-1} for this period. This indicates lower simulated water use congruent with lower rates of simulated biomass accumulation during the last 21 d of reproductive development and, likewise, greater measured water use for measured cotton boll biomass production during the final reproductive stage of cotton development.

Mauney (1968), Miley and Oosterhuis (1990), and others agree that the cotton plant has perhaps the most complex structure of any major field crop because of its complex growth habit and sensitivity to adverse environmental conditions. Cotton physiology responds to perturbations in its environment with a dynamic growth response that is often unpredictable, and must be managed to balance the vegetative and reproductive growth stages. This balance is often achieved by using plant growth regulators and other cultural practices (Oosterhuis and Robertson, 1985). Although we parameterized the generic plant growth model for cotton based on locally measured values and values from the literature for the southeastern USA, and balanced the number of days in each of the vegetative and reproductive stages to best simulate cotton development by the model, we could not simulate the large increase in cotton biomass during the last 21 d of the growing season. This is in part due to the fact that the model does not allocate C to leaves and stems after completion of the vegetative growth stage (Hanson, 2000). In addition, the timing of C allocation in cotton development is different than that for crops such as maize and sorghum. Cotton is indeterminate, and the fruiting branches are produced by the main stem and vegetative branches from the time of first square. However, cotton biomass and leaf area accumulate more slowly early in the season compared with some other crops such as maize and sorghum, due to a net assimilation rate, or dry weight per unit leaf area that is somewhat lower for cotton than for other crops. Cotton also does not cycle respiration CO_2 back to the photosynthesis process as efficiently as some crops (Carns and Mauney, 1968). Though both cotton and crops such as maize follow a sigmoid growth curve, maize will allocate more C to leaf area biomass earlier in the season than cotton. The result is more rapid biomass accumulation in maize early in the season and allocation of only enough C for leaf structure to maintain adequate leaf area for photosynthesis during the reproductive stage. In addition, the reproductive components of maize do not contain the weight relative to mass that the fruiting structures of cotton do. The result is lower total biomass production in a maize plant compared with a cotton plant.

The model was not able to simulate the large increase in biomass from Day 245 to 266 based on our parameterization of the generic growth model for cotton production. However, small differences in average simulated and average calculated water use from a 60-cm soil profile during the critical period of peak bloom—and similar patterns of development in biomass accumulation over the growing season until the last 21 d of cotton reproduction—reveal that the RZWQM model was able to respond reasonably well to cotton production for the purposes of this study. Based on our objective to simulate cotton water use as part of the total water balance for later testing the model for tile drainage and nitrate leaching in cotton production, we considered the simulation of cotton water use adequate, particularly for a model that is not specifically developed to address the complexity of cotton development.

CONCLUSIONS

Using a detailed calibration and sensitivity analysis approach with the RZWQM, we were able to simulate tile drainage, leached nitrate, and maize production within 15% of observed values without using the macroporosity option in the model. With the macroporosity option, we were able to simulate our target response variables of tile drainage and leached nitrate in maize production within 15% of observed values for the final analysis period. However, we found that macroporosity confounded the generation of leached nitrate by the model, and would often produce very large amounts of nitrate that could not be managed using the same parameters that were used to calibrate the model without macroporosity. We were able to accurately simulate tile drainage and nitrate leaching with macroporosity for the final analysis period by increasing the denitrification rate in small increments until a stable simulation of the N balance could be achieved.

Based on our experience in this study, one of the strengths of the RZWQM is its ability to simulate interdependent processes in soils and climate. However, the flexibility to adjust parameters in such a complex and comprehensive model as the RZWQM may also result in unpredictable behavior of the model when these processes are examined under different soil and climate regimes than those used to develop the model.

There were no significant differences between simulated tile drainage with and without macroporosity in the model. This is supported by the field research that showed most of the preferential flow in these soils occurs in the soil matrix and through in-filled macropores in the depths above the tile drains rather than through distinct open macropores. However, tile drains may also be influencing the model's ability to simulate preferential flow through macropores due to the difference in the flow patterns that are created when tile drains are present in the soil.

The model was able to simulate the pattern of biomass accumulation and leaf area of cotton development relative to the observed pattern with and without macroporosity until the last 21 d of reproduction. This appears to be due to the inability of the model to simulate vegetative growth after the crop enters the reproductive stage. It may also be due to the method by which the model partitions C during the various stages of crop development that cannot be adjusted except by way of the minimum number of days required to complete each growth stage. We were able to simulate average daily cotton water use to within less than 1 mm of average observed daily water use during the period of peak critical bloom with and without the macroporosity option. An option to adjust C allocation to the different plant components as well as allow vegetative growth to continue into the reproductive stage may improve the model's ability to simulate biomass accumulation as well as daily water use for indeterminate crops such as cotton.

By carefully outlining our calibration procedure along with relevant details often absent in modeling studies that test a model or that may only describe a sensitivity analysis, we hope to have contributed to the understanding of how a calibration may proceed, particularly for such a complex and comprehensive model as the RZWQM. Guidelines or standard protocols used for calibrating a model may also be addressed with more interest because of our efforts in this study. We will test the model under conventional as well as no tillage management practices in cotton production in a follow-up study to this paper that we hope will lend further insight into our ability to simulate tile drainage and nitrate leaching for cotton and other crops in Piedmont soils and climate.

APPENDIX

Table A1. Soil hydraulic properties used in model. Soil water content from Bruce et al. (1983), with Brooks-Corey h_a (air-entry pressure) and λ (pore size distribution index) derived from soil water characteristic fit with van Genuchten parameters and converted to Brooks-Corey parameters.

Soil layer no.	Depth	Soil water content, $cm^3\ cm^{-3}$ at pressure in kPa: Saturation	10	30	100	1500	Brooks-Corey parameters: K_s	h_a	λ fraction
	cm						$cm\ h^{-1}$	kPa	
1	5	0.49	0.21	0.16	0.11	0.05	18	1.61	0.49
2	15	0.41	0.16	0.13	0.10	0.05	20	0.68	0.41
3	25	0.38	0.25	0.22	0.20	0.14	8	0.45	0.18
4	35	0.47	0.35	0.32	0.30	0.24	18	0.45	0.44
5	65	0.48	0.40	0.37	0.35	0.27	10	0.77	0.26
6	95	0.43	0.40	0.38	0.36	0.27	2.6	9.62	0.40
7	125	0.43	0.41	0.39	0.36	0.27	0.2	9.90	0.54

Table A2. Initial soil temperatures and field capacity volumetric water content on 1 Jan. 1991 used for model calibration.

Soil layer no.	Depth	Soil temp.	Water content
	cm	°C	$cm^3\ cm^{-3}$
1	5	6	0.22
2	15	6	0.16
3	25	6	0.25
4	35	10	0.26
5	65	10	0.29
6	95	10	0.38
7	125	10	0.41

Table A3. Soil nutrient parameters with units per kilogram of soil as used in model. Data compiled from Franzluebbers (personal communication, 2001) and Johnson et al. (1999).

Soil layer no.	Depth	Total organic C	Fast residue	Humus: Fast	Humus: Transition	Humus: Stable	Aerobic heterotrophs	Autotrophs	Anaerobic heterotrophs	NO_3–N	NH_4–N
	cm	$mg\ kg^{-1}$	mg C kg^{-1}				no. organisms $kg^{-1} \times 10^6$†			mg N kg^{-1}	
1	5	6960	1044	1044	2088	2784	1083	285	285	2.85	1.58
2	15	5800	725	725	2030	2320	632.7	161.5	161.5	2.85	1.58
3	25	4060	406	406	1624	1624	383.8	76	76	2.85	1.58
4	35	3480	261	261	1218	1740	273.6	57	57	2.50	1.11
5	65	2900	145	145	870	1740	228	47.5	47.5	2.50	1.00
6	95	2320	116	116	696	1392	182.4	38	38	3.22	1.38
7	125	2320	116	116	696	1392	146.3	28.5	28.5	3.22	1.38

† Multiply value in table by 10^6 for actual value.

Table A4. Management options for all crops used in model calibration.

	Planting date			Fertilization	
Crop	1991	1992	1997	Tillage operation(s)	kg ha^{-1}
Maize	24 April	24 April	–	moldboard plow tandem disk	168
Winter rye	18 October	30 October		row planter/coulter	–
Cotton	–	–	16 May	moldboard plow	66

Table A5. Generic plant growth submodel parameters used for calibration of specific crop. The first five parameters were used to capture varietal differences for maize growth calibration at the MSEA sites (Hanson, 2000), and were used for calibrating maize and cotton for the current study.

Parameter	Definition	Value range	Units
μ_1	maximum active N uptake	1.5–3.0	g plant^{-1} d^{-1}
Φ	daily respiration as a function of photosynthesis	0–1	d^{-1}
C_{LA}	biomass to leaf area conversion coefficient	9.5–24	g leaf area^{-1}
A_p	age effect for plants in propagule development stage	0–1	–
A_s	age effect for plants in seed development stage	0–1	–
–	minimum leaf stomatal resistance	40–200	s m^{-1}
–	maximum rooting depth	crop dependent	m
–	N sufficiency index–trigger for timed application of fertilizer	0–1	–
–	luxurious N uptake factor–increases or reduces uptake	0–1	–

Table A6. Parameters used for winter rye and Quikplant submodel.

Parameter	Value
Length of growing season, days	150
N uptake, kg ha^{-1}	95
Crop height, cm	150
Leaf area index	8
Rooting depth, cm	125
Stover after harvest, kg ha^{-1}	3000
C/N ratio of fodder	30
Winter dormant recovery date (day of year)	1

Table A7. Parameters used for cotton in generic plant growth submodel. Physical parameters from Schomberg and Endale (2004) and physiological parameters from Carns and Mauney (1968).

Root depth	Stem diam.	Stem height	Aboveground biomass when height = 1/2 max height		4-leaf stage	Mature	LAI max
cm			g plant^{-1}				cm^3 cm^{-3}
			Physical parameters				
100	60	112	23		10	244	5.0
			Phenological/physiological parameters				
Air temp. for plant growth, °C			Minimum days spent transecting growth stage				
Max	Min	Optimum	Germ.	Emergence	4-leaf	Vegetative	Reproductive
40	16	21	3	3	7	115	40

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