CALIBRATION AND EVALUATION OF THE ROOT ZONE WATER QUALITY FOR SIMULATING TILE DRAINAGE AND NITRATE LEACHING IN THE GEORGIA PIEDMONT

by

DEBORAH ABRAHAMSON STARK

(Under the Direction of David E. Radcliffe and Gerrit Hoogenboom)

ABSTRACT

Simulation models are used to evaluate the impact of alternative agricultural management practices on soil and water resources that would normally require expensive and labor intensive experimental techniques. However, models must first be evaluated for the system of interest in order to provide a credible account of the impact of different land management practices on these resources. The Root Zone Water Quality Model (RZWQM) was developed to provide a comprehensive simulation of root zone processes that affect water quality, and to respond to a wide range of agricultural management practices. The latest version of the model, v. 1.3.2004, was evaluated in this study for simulating tile drainage and nitrate leaching in maize and cotton production systems under conventional and no tillage management practices. The model accurately simulated tile drainage and nitrate leaching in maize production for conventional tillage management practices in a Cecil soil after calibration. Average cotton production and daily water use were also accurately simulated during the critical peak bloom period for the cotton growth calibration. There were no differences between simulated tile drainage with and without macroporosity in the model, which supports the field research at the study site. When the model was tested with an independent data set for cotton production, tile drainage and nitrate leaching, it over predicted tile drainage and leached nitrate by large amounts under both conventional tillage and no tillage management practices. However, the patterns of tile drainage, leached nitrate, and cotton development were well correlated with observed values. The differences in simulated and observed tile drainage and leached nitrate appeared to be due to 1) the under estimation of simulated ET for the cotton and winter rye crops and, 2) the differences in the amount of soil water and soil nitrogen available for tile drainage and nitrate leaching at the study site during the winter months compared to the period when the model was calibrated. Suggested improvements to the model include a user option to simulate vegetative growth into the reproductive stage for indeterminate crops such as cotton. In addition, model simulations of cover crop development for annual winter cover crop management practices could be improved by processes that allow soil water and nitrogen uptake to respond to various perturbations in soil water and nitrogen under a wider range of rainfall and climate conditions exhibited by annual winter rye from one growing season to the next. Guidelines or standard protocols used for calibrating a model may also be addressed with more interest because of our efforts in this study.

INDEX WORDS: RZWQM, Georgia, Tile Drainage, Leached Nitrate, Piedmont, Kaolinitic, Variably charged, Macroporosity, Preferential flow, Cotton

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DEDICATION

This dissertation is dedicated to my family including my wonderful parents, R.T. (Ted) and Jan Abrahamson, my amazing brothers and sisters-in-law, George and Janice Abrahamson and Steve and Michelle Abrahamson, and my beautiful sister, Melody Abrahamson, to my precious daughter, Heather Michelle Stark, and to my wonderful niece, April Lynn Fricks. It is also in special recognition of Janice C. Abrahamson who died December 12, 2003, because she always pursued her goals of formal as well as spiritual education, smiling down upon this accomplishment now. I thank all of them for their love, support, inspiration and encouragement, and especially my parents for teaching me perseverance and instilling in me the self esteem to reach this goal.

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CHAPTER 1

INTRODUCTION

Purpose of the Study

Our ever-increasing need for food and fiber production from a diminishing land base due to a growing population worldwide carries with it an obligation to protect our natural resources upon which this production depends. Today, agricultural research is focused equally on efficient production of high quality food and fiber and sustaining the water resource due to a growing reliance on ground water for drinking water supplies. One of the primary tools used to assess the impacts of agricultural land management practices on surface and ground water resources is simulation modeling. Simulation models have become valuable tools for aiding in the discovery of the impacts of land management practices on our natural resources particularly in the past two decades. Models have also revealed knowledge gaps in our past and current research as we began to simulate processes such as plant development, soil water movement, and microbial decomposition of plant material based on field and laboratory data and experimentation. Models that can comprehensively and accurately assess the impact of different agricultural management practices on the water resource will provide research scientists as well as land managers and policy makers valuable decision-making information to help preserve our water supplies for the future.

How This Study is Original

This study evaluated the latest version of the Root Zone Water Quality Model (RZWQM), v. 1.3.2004, for simulating tile drainage and nitrate leaching from conventional and no tillage agricultural management practices in the Piedmont of Georgia. The model was developed in the Great Plains region of the U.S. where soils are permanently negatively charged and the climate is much drier than the southeastern U.S. This will be the first use of the model to simulate tile drainage and nitrate leaching as well as the effects of no tillage and macroporosity in the southeastern U.S. where the soils are variably charged and the climate is humid. It will also show whether the generic plant growth submodel can be parameterized to simulate cotton production, a crop that is more complex in its physiology and development than those for which the model has been parameterized (maize, soybean and winter wheat). This model was selected because it was developed as a comprehensive interaction of the soil, water, plant, and nutrient processes that occur in agricultural production systems. In addition, it includes a soil macroporosity option to simulate preferential flow through macropores in the soil profile, which have been observed in Piedmont soils. Tile drains were part of the field experiment in this study to evaluate the impacts of crop production, tillage and cover crop management practices on tile drainage and leached nitrate in Piedmont soils. The RZWQM includes the option to simulate tile drainage using the Hooghoudt equation, an important consideration when modeling drainage in a field with tile drains due to the complexity of flow that occurs when drains are present. Finally, it can be used to simulate a wide range of agricultural management practices and site characteristics such as conventional and conservation tillage, manure and mineral fertilizer applications, and irrigation application.

Chapter 2 of this study will describe the detailed procedure used to calibrate the RZWQM model. It will show how the model was calibrated to simulate tile drainage, nitrate leaching and maize production relative to observed values based on a field study in maize production under conventional tillage management practices in the Georgia Piedmont region. Measured parameters from the study were used if available, and adjustments to parameters that were not measured or that have not been established for southern Piedmont soils were either tested to find the values that most accurately reflected measures of tile drainage and leached nitrate or taken from the literature. Simulation scenarios included tile drainage and nitrate leaching in maize production with and without using the soil macroporosity option in the model, and a separate calibration scenario was used for cotton production with and without the macroporosity option. The same parameters established in the calibrated maize scenarios were used for the cotton calibrations with the exception of the parameters for cotton development, which were taken from a study in cotton adjacent to the maize study or from the literature. Although tile drainage and leached nitrate were not measured in the cotton study used to calibrate the model for cotton production, cotton development in relation to water use based on rainfall and soil moisture measurements were evaluated so that the calibrated model could be used to test tile drainage and nitrate leaching after the original field study in maize production was planted to cotton. The detailed approach described for calibrating the RZWQM will give other researchers and modelers information on all of the parameters and processes addressed during this study in an effort to help guide their calibration process when using the RZWQM or other models. It may also serve as a step towards the establishment of guidelines or a protocol for the calibration process which is now left somewhat arbitrarily up to the modeler, or reported in limited detail in some modeling papers as part of the model testing process.

Chapter 3 describes the evaluation of the calibrated model for simulating tile drainage and nitrate leaching from cotton production using an independent data set from the same field study used for the maize calibrations after it was planted to cotton. It evaluates the results of testing the model for its ability to accurately simulate tile drainage and nitrate leaching under conventional tillage management practices. No tillage management practices are then introduced in the model for testing the model's ability to simulate tillage affects on tile drainage. Finally, it lends further insight into suggested improvements that could be made to the model for simulations of tile drainage, nitrate leaching, and crop production in the Piedmont region and southeastern U.S. where the soils and climate are very different than those under which the model was developed.

LITERATURE REVIEW

The development of the computer has generated a tremendous leap in our ability to conceptually emulate and quantify the processes of nature (Corwin et al., 1999). A model is a simplified representation of an intricate system and a practical way to understand how a system works when experimentation is too costly or time consuming. Simulations with models are also repeatable and nondestructive compared to field studies, and results are often easier to interpret (Zeigler, 1976). A model can be used to increase our understanding of fundamental processes as well as the interactions of these processes under various conditions in agricultural watersheds. Due to the growing reliance upon groundwater as a source for drinking water as well as a source for agricultural production, research in agriculture and other natural resource disciplines use both real-time measurements as well as model predictions in order to determine what must be done to protect and sustain our water resources (Corwin et al. 1999).

Several different criteria have been used to develop a classification system for the different types of models that have been developed over the past several years. However, the basic types used in research and land management applications are physically-based, mechanistic models with many subcategories and derivations for each (Woolhiser and Brakensiek, 1982). Deterministic models are one type of these models that operates so that a given set of events leads to a uniquely definable outcome (Addiscott and Wagenet, 1985). These mechanistic models incorporate descriptions of the key processes in the natural systems based on 'cause-and-effect' relationships that can only be known through experimentation and observation (Corwin et al., 1999).

Recently, there has been a considerable amount of effort by both researchers and natural resource managers to model the impacts of non-point source (NPS) pollution on the water resource at larger scales other than those under which these deterministic or mechanistic models were developed, that being an experimental unit area that consists of relatively homogeneous properties. Deterministic models have been used as the basis for scaling up to the watershed and landscape level by linking them to Geographic Information Systems (GIS) thereby using them in a lumped or distributed manner to account for heterogeneity in the landscape (Corwin et al., 1999). Deterministic models have been developed based on the accumulated knowledge of the soil-water-plant continuum processes in agricultural systems over many years of laboratory and field studies and incorporate key processes from those studies. For any modeling approach to be valid and useful in terms of calibration and prediction, it must be closely related to what can be determined experimentally (Wagenet and Hutson, 1996). Models such as LEACHM (Hutson et al., 1992), PRZM and PRZM3 (USEPA, 2003), GLEAMS (Leonard et al., 1987), OPUS (Smith et al., 1992), CROPGRO (Hoogenboom et al., 1992, Boote et al., 1998), CERES-MAIZE (Jones and Kiniry, 1986, Ritchie et al., 1998) and RZWQM (Ahuja et al., 2000), are examples of field scale, deterministic models. Though these models have been developed based on many years of experimental study, uncertainty associated with model predictions results from all of the errors involved in the process of model formation, calibration, parameter estimations and environmental variability (Gardner et al., 1990). The need for evaluation and improvement of the deterministic, field- and plot-level scale models still exists due to the fact that they serve as the basis for many of the simulation processes used in developing these watershed and landscape level models.

The soil-plant-atmosphere system is highly complex, and difficult to characterize in terms of effective parameters. The confidence building process in model prediction is a long-term and iterative process (Hassan, 2003), and model developers continue to test and refine models to improve simulation of physical, biological and chemical processes and systems (Donigian and Huber, 1991). 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), and can provide estimates of those parameters that cannot be easily measured or determined Hanson (2000). Most of the modeling studies in the literature provide only a cursory explanation of the calibration procedure used prior to model testing, which may leave a reader with limited information to discern the model's ability to comprehensively address the system tested. Results of the calibration phase of a model offer insights into observed strengths and weaknesses of the model during the testing phase since testing a model is essentially a process to evaluate the accuracy, uncertainty, and bias in the calibrated model predictions (Mulla and Addiscott, 1999). The process of calibrating and testing a model also reveals important information pertaining to model processes and sensitive parameters which 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 Root Zone Water Quality Model (RZWQM) is a process-based, deterministic model that simulates major physical, chemical and biological processes in crop production systems under a range of common agricultural management practices (Ahuja, et al., 2000). The model was first released in 1992 by USDA-ARS scientists at the Great Plains System Research unit in Fort Collins, Colorado, and was developed in the Great Plains region of the U.S. where soils and climate are very different from those in the Piedmont region and the southeastern U.S. in general. The model includes simulation of tile drainage and runoff as well as predictions of the potential for ground- and surface-water flow and contamination (Ahuja et al., 2000). It includes an option to simulate the effects of soil macroporosity on soil water movement and drainage, and was suited for this study because areas of preferential flow have been found in Piedmont and other well-structured soils (Gupte et al., 1996; Williams et al., 2003). The version of the model used in this study has recently been refined to improve the simulation of runoff and drainage with surface chemical mixing, improved residue processes, and includes more parameterized crops (RZWQM development team, personal communication, 2004).

The objective of this study was to calibrate and test the RZWQM for its ability to simulate tile drainage and nitrate leaching from a field study in the Georgia Piedmont, and to further assess the ability of the model to simulate watershed hydrology of agricultural soils, management practices, and cropping systems common to Georgia. By defining the strengths and weaknesses of the model for simulating tile drainage and nitrate leaching in the Piedmont region, the model may be used to simulate the impact of agricultural management practices on the water resource in southeastern soils and climates. Ground water supplies in the Piedmont region are small, and perennial streams, impoundments, and rainfall are the major sources of water for municipal, industrial, and agricultural use (Smith et al., 1978). Accurate simulations of agricultural production systems of Georgia and the Piedmont region could serve as the basis for assessment of potential non-source pollutants from agricultural watersheds that impact Georgia water resources.

CHAPTER 2

CALIBRATION OF THE ROOT ZONE WATER QUALITY MODEL FOR SIMULATING TILE DRAINAGE AND LEACHED NITRATE IN THE GEORGIA PIEDMONT[1]

[1] D. A. Abrahamson, D. E. Radcliffe, J. L. Steiner, M. L. Cabrera, J. D. Hanson, K. W. Rojas, H. H. Schomberg, D. S. Fisher, L. Schwartz and G. Hoogenboom. Submitted to Agron. J.

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

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ABSTRACT

Water quality models are useful for a wide range of applications, but many model parameters and processes are extremely sensitive to small adjustments and can affect model simulations and final results. This potentially can lead to erroneous conclusions unless the model has first been calibrated to the system of interest. In addition, some parameters that do not significantly affect simulation results may require unnecessary time and effort in further applications. The goal of this study was to calibrate the Root Zone Water Quality Model for simulating tile drainage and leached nitrate under conventional-tillage management practices in the Georgia Piedmont. Several key processes in the model have recently been refined based on studies where soils and climate are very different from the Piedmont region. The current version has not been tested in the Piedmont for tile drainage and nitrate leaching since these revisions. We focused not only on the calibration procedure but also tested the sensitivity of tile drainage and nitrate leaching to parameters such as macroporosity. Tile drainage and leached nitrate were simulated within 15% of observed values in the calibrated maize scenarios with and without macroporsoity. Simulated cotton biomass and leaf area index were well correlated with observed biomass and leaf area index until the last 21 days of the reproductive stage,

when the calibrated model could not accumulate enough cotton biomass to fall within 15% of observed total biomass by the end of the growing season. However, simulated cotton water use based on rainfall minus the change in soil water averaged 5.1 mm d^{-1} and 5.6 mm d^{-1} with and without macroporosity, and observed water use was 5.8 mm d^{-1} during the critical period of peak bloom for cotton. The calibration procedure and analyses used in this study should help us clarify aspects of the model's performance during a subsequent testing phase to include no tillage management systems, and contribute to our analyses of the model's ability to accurately simulate tile drainage and nitrate leaching in Georgia Piedmont cotton production systems.

INTRODUCTION

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 and known parameter values. This process serves to verify that the model functions properly without failing during execution or simulating values that are outside the range of reasonably acceptable estimates or measurements. It also reveals important information pertaining to model processes and sensitive parameters which 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).

Calibration of a model includes parameterization based on direct measurements, pedotransfer functions, or direct or indirect fitting of the model to measured data. Although many models are designed to accomplish the same objectives, they may use different scientific approaches, processes and logic. The purpose of calibrating a model is to insure that the model can adequately represent desired components under the conditions to be tested. The calibration process also allows refinement of parameters that may have a range of values and reveals sensitive parameters that lend insight to a model's ability to accurately reflect different scenarios of interest (Hanson, 2000).

Most of the modeling studies in the literature provide only a cursory explanation of the calibration procedure used prior to model testing. The 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. For instance, it is often unclear if parameters were based on measured data, if parameters were adjusted during calibration and to what extent, if all major processes in the model were parameterized and to what extent, or if sensitivity analyses were performed. All of these processes may or may not have been addressed or performed during the calibration process. The methods used to calibrate the model are usually reported in the same manuscript as the model testing, and slight reference is given to the calibration procedure. This 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. Adjustments 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 water quality field experiment initiated in 1991 at the USDA-ARS J. Phil Campbell, Sr. Natural Resources Conservation Center in Watkinsville, Georgia (Johnson et al., 1999; Endale et al., 2002). The modeling objective 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).

Johnson et al. (1999) tested the LEACHN model (Hutson et al., 1992) for maize production using the same study 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. The over estimation of leached nitrate in a wetter than normal year was attributed to the absence of a soil macropore-matrix exchange component in the model. The Root Zone Water Quality Model (RZWQM) includes a macropore component as well as an exchange component between the soil matrix and macropore walls. We chose to evaluate this model expecting that it might be able to better simulate drainage and leached nitrate because visible macropores and preferential flow patterns are found in Cecil soils (Gupte et al., 1996). It also includes an option for tile drainage, an important consideration when tile drains have been used in the field study due to changes in the soil water dynamics that artificial drainage systems incur.

The hydrology, pesticide and nitrate movement, crop growth, and several agricultural management practices in the original version of the 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 U.S where the model was originally developed and tested. This paper reports results of the first major calibration of the most recent version of the RZWQM for tile drainage and nitrate leaching in the Southeast.

The main goal of this paper was to calibrate the RZWQM for its ability to simulate drainage and nitrate leaching in the Southeast. A second objective was to provide calibration procedures for other modelers and user groups who are interested in the process of calibration that might be useful prior to model evaluation. Clarification of calibration procedures, including more specific information on the parameterization process and sensitive parameter adjustments that were discovered during the process will provide a better understanding of a model's ability to perform during the testing phase. It may have implications for potential users of the model if any of these have significantly influenced test results. In addition, this study contributes towards a standardization of the calibration phase of modeling. A standard calibration protocol would supplement 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.

MATERIALS AND METHODS

Field Experiments

The water quality study consisted of twelve 10 x 30 m plots with drain tiles installed at 75 to 100 cm depths on a 1% slope, 2.5 m apart. 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. A complete description of the study is given by Endale et al. (2002).

The soil was a Cecil sandy loam (fine, kaolinitic, thermic, Typic Kanhapludult). The pH normally ranged from 5.5 to 5.8 as measured at the study site; therefore, lime was applied approximately every three years to maintain a pH of 6.0 to 6.3 in the surface horizon in order 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.

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. 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 9870 seeds ha^{-1}. Ammonium nitrate fertilizer was applied at the rate of 168 kg 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 on 12 Apr 1993, CT plots were plowed and disked on 13 Apr, 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 yield 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 November, 1994 when winter wheat was planted as the cover crop followed by the first cotton crop in May 1995.

In order to calibrate the RZWQM for cotton growth for its ability to simulate tile drainage and leached nitrate from cotton production after the water quality study was planted to cotton, we used parameters from a field experiment planted to cotton in 1997 adjacent to the water quality study. The study site was planted to cotton on 16 May 1997 on a 1.3 ha watershed using a no-till drill. A winter rye cover was planted in late October following cotton harvest. 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 was sampled and leaf area was measured throughout the growing season. Plant height and populations were also estimated at each sampling date. The final sampling date for biomass and leaf area was 3 Oct 1997 (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 upon known research documented in an extensive user help utility. Daily weather data can be generated with the CLIGEN stochastic model (USDA-ARS, 2003) based on nearby historic weather station parameters. The model has been applied to simulate best management practices for the Management Systems Evaluation Areas (MSEA) research project for maize and soybean (Ahuja et al., 2000). The calibrated maize and soybean crop parameters in the model can be adjusted during the calibration procedure to accurately 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.

We parameterized the physical properties of the soil in the RZWQM model from measurements made in or near the field experiment site (Bruce et al., 1983; Gupte et al., 1996). Seven distinct layers to a depth of 1.25 m were parameterized based on measured properties of each layer, and the initial water content at the beginning of the simulation period on 1 Jan 1991 was set to the measured approximate field capacity for each layer (Table 1.1a, 1.1b, and Appendix A). The van Genuchten (1980) pore size distribution index and air-entry parameters for the soil water characteristic were fit based on measured values of saturated and residual soil water content using PROC NLIN (SAS, 2000), and converted to Brooks-Corey parameters based on the procedure described in Ahuja et al. (2000). We included a soil crusting option with a crust hydraulic conductivity rate set to 0.68 cm hr^{-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 Nov 1991. We used 1 t ha^{-1} as the amount of initial surface residue based on fallow conditions and on one season of maize production prior to the first winter rye cover crop in Oct 1991. The fraction of surface residue mass that would be incorporated by natural means was set to 2% based on model references. Rainfall and other weather data were recorded at an automated weather station adjacent to the site (Hoogenboom, 2003).

We used management practices including day of planting, tillage operation, and fertilizer application rates and dates and set initial conditions such as beginning soil moisture and temperature, surface crop residue properties, and field area and slope as required by the model, based on recorded data from the study site. The field area used was 0.03 ha based on the size of a plot, and the slope was 2%. Other input data and initial parameter values used are listed in Appendix A.

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), and was designed with interactive feedback between soil water, available nitrogen 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, and adjustments that were made that could have influenced or significantly impacted the model's ability to simulate the scenarios of 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. They may be homogeneous or distinct layers. Three numerical (transport) grids are created - one for defining hydraulic properties, a second non-uniform 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 Brooks-Corey parameters have been compiled by Rawls et al. (1982) for eleven soil textural classes (Ahuja et al., 2000). The model estimates soil hydraulic properties from soil texture, bulk density, and soil water content at 33 or 10 kPa when measured data for Brooks-Corey parameters are not available. If soil water content 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). If van Genuchten parameters are available, the pore size distribution index and air-entry value (bubbling pressure) parameters of the soil water characteristic curve may be converted to Brooks-Corey parameters and used instead. 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 will occur by way of the soil matrix only.

Water can only enter the macropores at the surface, but the model also 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 adjust the fraction of microporosity in each soil layer though to not less than 1% of total porosity. The model defines micropores as pores less than 1.5 mm in diameter, and will calculate microporosity, if not adjusted by the user, as the ratio of soil water content at 200 kPa to saturated water content. As a result, the mesopore region of the soil matrix includes pore sizes between 1.5 mm diameter and the minimum macropore diameter size supplied by the user.

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, and 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 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 non-negative. 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 uptake to become a sink term at the equivalent depth of the drains (Appendix B).

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 placed 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 (Appendix B). Fig. 1.1 depicts how we implemented the tile drainage system from the field study 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 Simulation Project (WEPP) model (Alberts et al., 1989). Tillage eliminates all continuous macropore channels and changes them to dead-end macropores. 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 Organic Matter and Nitrogen cycling (OMNI) process is linked to other related submodels in 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). RZWQM 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 intitial 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 carbon and nitrogen 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 input requirements for crops depend on which plant growth submodel is chosen. The generic plant growth submodel can be fully parameterized with specific physical and physiological parameters if these parameters are known. If only a few parameters are known, default values may be used based on similar crops (i.e., maize versus sorghum) or from data available in the literature. The model has been fully parameterized and calibated for maize and soybean for the Management Systems Evaluation Areas (MSEA) sites in the midwestern USA (Hanson et al., 2000). The RZWQM also provides a second option submodel for simulation of crop growth referred to as the Quikplant model. It is a simple growth and yield model that requires parameters such as maximum leaf area index and rooting depth of the crop, total seasonal nitrogen uptake, and harvest date. The plant reaches peak LAI, height and nitrogen use in the middle of the growing season and uses the root input distribution for extraction of water and nitrogen from the soil. However, Quikplant is not a detailed growth model and should only be used to simulate water and soil nitrogen 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 total 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 nitrogen 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 et al. 2000).

Model Calibration

General Procedure

After entering the required model inputs and parameters, we ran the model for a period of 12 years (three years of climate and rainfall data iterated four times) to initialize the organic nitrogen pools (rapid, medium, and slow decomposition pools) as suggested in the model documentation.

The only parameters that we adjusted after the initialization procedure were the initial soil nitrate and soil ammonium nitrate values for each soil layer on 1 Jan 1991 (Table 1.2). The reason for this was that after the initialization procedure, the model over- or under estimated these values although we had used a value of 1 t ha^{-1} of 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 nitrogen 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) so the measurements reflected the previous two years 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 twelve-year initialization procedure created more residue for simulated decomposition and, therefore, more mineralized soil nitrogen than was measured the first year from the study site. However, the simulation period for calibration that began after initialization of the model included conventional till and winter rye cover crop management practices. By re-setting the initial values of soil mineral N back to their measured values before we began the calibration simulations on 1 Jan 1991, the simulations would be able to reflect the soil N conditions at the study site just prior to the introduction of the winter rye cover crop in the Fall of 1991, and yet still account for the affects of a winter rye cover during the calibration process.

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 et al., 2000) with additional details to meet our objectives for tile drainage and nitrate leaching with and without macroporosity (Fig. 1.2). We ran the simulations from 1 Jan 1991 through Apr 1993 based on the availability of measured data for comparison to simulated values of tile drainage, leached nitrate, plant production and soil nitrogen. Model simulations from Nov 1991 through Apr 1993 were used to evaluate and adjust the nitrogen balance since observations for soil N, nitrate leaching, and tile drainage were available for the entire period. However, the period of Nov 1992 through Apr 1993 was used to test the sensitivity of tile drainage to the ground water leakage rate, and also used for the final calibration and evaluation of tile drainage and leached nitrate after adjustments to the nitrogen balance. The reason for this was twofold. The tile drains were installed in one of the conventional till plots used for calibration in 1981 and in the other conventional till plots used for calibration in 1990. Since a winter rye cover crop was first introduced to the study in Oct 1991, the period from Nov 1992 through Apr 1993 provided a period of time when all plots used to simulate conventional tillage maize production with winter rye cover to be in winter rye for at least one season. This also allowed additional time for the soil above the drains to settle from disturbance due to the installation of tile drains in some of the plots two years prior to this time.

Field measurement errors are typically greater than 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 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.

Water Balance Calibration for Tile Drainage

No Macroporosity

In order to calibrate the water balance, we chose to adjust the ground water leakage rate (water table leakage rate), v_z, 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 measurements of it available for our soils under the conditions set forth in this study. We increased the rate beginning with a value of 0 cm hr^{-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 tile drainage stayed within a range that we could reasonably use for leached nitrate. The period used for this adjustment was Nov 1992 through Apr 1993 when all conventionally-tilled plots were in winter rye cover and drain tiles had been installed for at least two years.

With Macroporosity

We ran the model with the macroporosity option to determine if macropores affected total or event drainage based on work by Gupte et al. (1996) that showed preferential flow in Cecil and related soils of the Piedmont. The calibration of the model with the macroporosity option was actually performed after we calibrated tile drainage, leached nitrate and maize production without macroporosity but is described here for organizational purposes of this paper.

The parameters for adjusting the amount of macropore flow that occurred in the soil included 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 were 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 analyses 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 just 9% of macropore water flowing into the tile drains. However, there would be no absorption into the macropore wall. The parameter set 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 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 or parameter combination's 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 could provide us with 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 above-ground biomass N of the maize crop within, or as close as possible to 15% of the measured value. We then evaluated the simulated nitrogen balance relative to N mineralization to begin refining the calibration for leached nitrate in drainage if needed. In plots with tile drains, Groffman et al. (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:

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

Where N_{net} = net mineralization; $Soil\ N_{final}$ = final soil mineral N on 13 Apr 1993; $Crop\ N_{uptake}$ = above-ground 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 was over or under predicting a nitrogen 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 then adjusted the nitrification and/or 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 re-evaluated the N balance after each adjustment. Iterative adjustments to sensitive plant parameters and the nitrification / 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 nitrogen balance and tightly coupled to the other processes, we followed the procedure for calibrating plant growth recommended for the model by Hanson et al., (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 on the values used for calibration of the MSEA sites (Hanson et al., 2000), (Appendix A). The calibration for cotton development included adjustments of these 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. 1.2 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 (University of Georgia College of Agricultural and Environmental Sciences, 1998; Blount et al., 2000). The parameters included total seasonal N uptake, length of growing season (days), maximum crop height, leaf area index, and rooting depth, stover after harvest, C:N ratio of fodder material, and winter dormancy recovery day of year (Appendix A).

After calibrating for maize and winter rye, we held all parameters constant and added cotton to the generic plant growth submodel. Parameters were obtained from the 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; University of Georgia College of Agricultural and Environmental 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 C). 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 from the weather station near the study site. A simple water balance was calculated by subtracting the change in observed or simulated soil moisture in a 60 cm soil profile from rainfall for each day that soil moisture was measured.

Observed soil moisture in cotton showed little or no flux below 60 cm in the field study used for calibration (Schomberg and Endale, 2004). In addition, cotton is one of the most sensitive crops to aluminum toxicity, which frequently occurs in acid subsoils such as those in Georgia (Gascho and Parker, 2001; Sumner, 1994). Maximum observed rooting depth for cotton in Piedmont and Coastal Plains soils of Georgia has been shown to be less than 60 cm in some studies (Endale, personal communication, 2003).

Model Evaluation

We tested for the main effects and interactions of the three parameters used 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, PROC GLM, 2000). Based on this information, we idenitified the parameter or combination of parameters with the highest correlations for simulated and observed tile drainage as well as the highest probabilities associated with them. Based on our analysis, we determined whether further testing was needed within a more narrow range of the parameter(s). Since one of our objectives was to try and simulate how macropore flow may contribute to drainage in Cecil soils, we chose to refine the range of the parameter(s) as much as possible to improve our understanding of the drainage process for these soils.

We regressed the final values of observed tile drainage and leached nitrate on simulated tile drainage and leached nitrate using linear regression analysis (SAS, 2000), in order to compare measured and simulated r-square values, slopes and intercepts. We also calculated the relative root mean square error (RRMSE) (Loague et al., 1991), standard error of the mean difference (Addiscott et al., 1987), maximum error, average and standard deviation between measured and simulated drainage and leached nitrate to characterize systematic over- or under-prediction, and used graphical displays to show trends and distribution patterns (Loague et al., 1991). These types of analyses are normally used to evaluate results of simulated versus measured values at the end of the evaluation phase of a model. Our goal was to carefully analyze the outcome of the calibration before testing with an independent data set to insure that model strengths and weaknesses were reflected as accurately as possible before drawing our conclusions during the testing phase.

RESULTS AND DISCUSSION

Calibration - No Macroporosity

Increasing the ground water leakage rate from 0 cm h^{-1} to 0.004 cm hr^{-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 to the other rates that were tested (Fig. 1.3). A higher K_s for a soil layer above a layer with lower K_s as depicted in Fig. 1.2 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. However, though the ground water leakage rate turned out to be a very small value, 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 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 ten percent of irrigation water applied. Measured values of Ks in these two layers were 0.2 cm h^{-1} 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} versus 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, which could decrease the rate of soil water movement below the measured value of 0.035 cm h^{-1}.

Though we chose the ground water leakage rate that best simulated total tile drainage when compared to total observed drainage, simulated leached nitrate was not within 15% of observed leach nitrate for the period used to evaluate the N balance from Nov 1991 through Apr 1993. Simulated leached nitrate was 25 kg ha^{-1} less than observed leached nitrate and simulated above-ground biomass N for maize was 30 kg ha^{-1} greater than observed above-ground 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 under predicted and above-ground biomass N was over predicted by almost the same amount, we decreased the A_p parameter (propagule age effect) in the model. A decrease in this parameter will reduce yield and therefore reduce the crop N demand. In addition, our target error range for yield was large (5716 to 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 system would simply allocate the nitrogen balance components differently with this adjustment. The adjusted A_p parameter increased simulated leached nitrate to within less than 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 but within 15% of total observed biomass N for all three crops (winter rye 1992, maize 1992, and winter rye 1993) (Table 1.2).

The analysis of simulated and observed soil mineral N for each day of twelve field-measured values revealed that three of the twelve simulated soil mineral N predictions were outside the 95% confidence interval (C.I.) of observed soil mineral N. Total simulated tile drainage and leached nitrate for the final analysis period of Nov 1992 through Apr 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%, we considered the calibration acceptable as the final calibrated version for maize production 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. 1.4a) although seven of twelve simulated drainage events were outside of the 95% C.I. of observed tile drainage events (Fig. 1.5a). 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. 1.4b). Six out of twelve simulated leached nitrate events was outside the 95% C.I. of observed leached nitrate (Fig. 1.5b). The relative root mean square error (RRMSE), or the percent deviation of the simulated values with respect to the mean of the observed values, shows a large percent deviation from the mean observed values, reflecting the fact that the majority of simulated events for both tile drainage and leached nitrate were outside of the 95% C.I. (Table 1.3). However, linear regression analysis of total observed tile drainage on total simulated tile drainage, and total observed leached nitrate on total simulated leached nitrate revealed that the slopes were not significantly different from one, and the intercepts were not significantly different from zero at the 0.05 probability level (Table 1.4).

Calibration with Macroporosity

Results of the thirty-six 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 more narrow range of each. The new matrix consisted of seventy-five combinations of these three parameters based on the range of each between their maximum and minimum values from the highest correlations of simulated versus observed tile drainage. After running the model for each of the new seventy-five combinations of WT, EF, and LAB, we again chose the highest correlations of simulated with observed tile drainage and the highest probabilities. We narrowed these further by choosing those combinations with the smallest errors between simulated and observed tile drainage and simulated and observed leached nitrate for the period from Nov 1992 to April 1993. The final values used for these parameters for calibrating the model with macroporosity were WT = 1, EF = 0.01, and LAB = 0.4.

With these three parameters selected for macroporosity, the system produced 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 1.5). 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 (Nov 1992 to Apr 1993). In each case, net mineralization increased, and too much nitrate was produced in the system 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. 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 N uptake. This would then create a situation that required an endless number of iterative adjustments in order to bring simulate leached nitrate, tile drainage and yield back to within 15% of observed values. After several attempts to adjust the macroporosity components and the sensitive plant parameters to simulate leached nitrate and net mineralization accurately 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 both of these rates to zero decreased soil nitrate N and increased soil ammonium N. Leached nitrate was reduced, 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 defaults, and increased the denitrification rate incrementally to decrease the amount of nitrate in the system (Table 1.6b). Using a Latin Hypercube Sampling technique to determine the sensitivity of 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 Nov 1992 through Apr 1993.

The analysis of simulated soil nitrate and twelve measured values of soil nitrate revealed that three of twelve simulated values were outside the 95% C.I. of measured values as was the case for the calibration without macroporosity. However, leached nitrate and biomass N for all three crops were still over predicted for the period from Nov 1991 to Apr 1993 initially used to test the N balance (Table 1.5), 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 for the calibrated scenario with macroporosity revealed that cumulative simulated tile drainage followed the pattern of cumulative observed tile drainage (Fig. 1.4a) with eight of twelve simulated drainage events outside the 95% C.I. of observed tile drainage events (Fig. 1.5a). 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 five of twelve drainage events following the same pattern as simulated leached nitrate without macroporosity (Fig. 1.4b). Six of the twelve simulated leached nitrate events were outside the 95% C.I. of observed leached nitrate as was the case with no macroporosity (Fig. 1.5b.) The RRMSE shows a large percent deviation from the mean observed values reflecting the fact that the majority of simulated events for tile drainage and one half of the simulated leached nitrate events were outside of the 95% C.I. of measured events (Table 1.3). Linear regression analysis of total observed tile drainage on total simulated tile drainage, and total observed leached nitrate on total simulated leached nitrate revealed that the slopes were not significantly different from one, and the intercepts were not significantly different from zero at the 0.05 probability level (Table 1.4). 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 indicate 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 influence of macroporosity.

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/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 effective in the case of calibration for nitrate leaching for one scenario or one study. However, based on our experience, it is likely the model will not perform consistently if the conditions 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

The sensitive parameters, μ1, Ap, As, Φ, 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 1.6a). 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 less than 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 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 due to the fact that the model could not produce the large increase in observed biomass between day 245 and day 266 (Fig. 1.6) without adjusting the plant parameters to rapidly increase total biomass early in the season (before the first bloom period for cotton). 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 days for the vegetative stage and 40 days 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 the accumulation and allowing it to continue to increase until the last 21 days of observed cotton boll development (Fig. 1.6).

Simulated biomass developed according to observed biomass based on the days that biomass was measured until the period from day 246 to 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, which occurred 21 days prior to the maximum observed value of 4.83 cm^3 cm^{-3} on day 266. Simulated cotton yield was 2559 kg ha^{-1} without macroporosity, and 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 entire period of measured biomass (day 197 through day 266) was 1250 kg ha^{-1} without macroporosity and 1538 kg ha^{-1} 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 to 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. 1.7). Total simulated PET for the period was 42 mm and showed good agreement with a total calculated PET of 47 mm, or 4.7 mm d^{-1} and 5.2 mm d^{-1} respectively. These values of PET could indicate that actual water use was slightly higher than calculated and simulated water use. Daily average termperatures were normal for the period (Hoogenboom, 2003), and cotton water use ranges from 2.5 mm d^{-1} to 6.4 mm d^{-1} during this time from first square to first bloom in the development period (NCSU-CES, 2004). However, at the end of this period 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. Calculated and simulated water use relative to measured and simulated biomass values indicated that the model may not be 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.

During the critical peak bloom period in 1997 (day 197 through day 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. During this critical period just prior to peak bloom, cotton requires approximately 7 to 8 mm of water per day to reach potential yield (Bednarz et al., 2002). Total simulated PET was 149 mm and calculated PET was 145 mm or 4.5 mm d^{-1} and 4.4 mm d^{-1} respectively, which indicates that calculated and simulated water use could be somewhat high for this period, and that roots did not extract all of the soil water from the 60 cm profile during the period. In either case, low values for calculated and simulated cotton water use compared to the potential water use for this period might be due to the effect that temperatures had on cotton development.

During the 1997 growing season, temperatures ranged from 0.3 ºC to 2.6 ºC below the long-term monthly means for the area (Schomberg and Endale, 2004). The authors attributed the low cotton seed lint yield to the lower-than-average daily temperatures for the cotton growing season. The optimum mean maximum temperature for cotton growth is approximately 32 ºC (Nyakatawa et al., 2000). The mean maximum daily temperature during the entire period of critical peak bloom was 28 ºC based on measurements at the weather station adjacent to the study site (Hoogenboom, 2003). Simulated cotton biomass was accumulating more rapidly during the peak bloom period from day 197 until day 231 when simulated and observed cotton biomass values were nearly equal. The average difference between observed and simulated biomass on day 231 and day 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 day 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 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 prior to peak bloom when water use can range from 6.4 mm d^{-1} to 10 mm d^{-1} (NCSU-CES, 2004; Bednarz, 2002). 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 day 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 days of reproductive development and likewise, greater water use for measured cotton boll biomass during the final reproductive stage of cotton development.

Miley and Oosterhuis, (1990), Mauney (1986) 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, 1980). Although we parameterized the generic plant growth model for cotton based on locally measured values and values from the literature for the southeastern U.S, 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 days of the growing season. This is in part due to the fact that the model does not allocate carbon to leaves and stems after completion of the vegetative growth stage (Hanson et al., 2000). Another factor that could be affecting the model's ability so simulate the large amount of carbon allocated to reproductive growth at the end of the growing season is that the timing of carbon 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 to crops such as maize and sorghum, due in part to the fact that the net assimilation rate, or dry weight per unit leaf area is somewhat lower for cotton than for other crops. Cotton also does not cycle respiration CO_2 to photosynthate 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 carbon 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 carbon 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 to a cotton plant.

The model was not able to simulate the large increase in biomass from day 245 to day 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 days 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 for the Piedmont region, we considered the simulation of cotton water use adequate, particularly for a model that is not specifically developed to address the complexity of cotton growth.

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.

All of the major processes for soil water and chemical movement in and through the root zone as well as plant growth are tightly coupled in the model (Ahuja et al., 2000). Based on our experience in this study, one of the strengths of the RZWQM is its ability to simulate these interdependent processes in our soils and climate as accurately as we have shown for tile drainage, nitrate leaching, soil nitrogen and maize yield. However, by the same token, 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 those processes are examined under different soil and climate regimes than those used to develop the model.

There were no differences between simulated tile drainage with and without macroporosity in the model. This is supported by the field study 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 days 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 carbon 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 carbon 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.

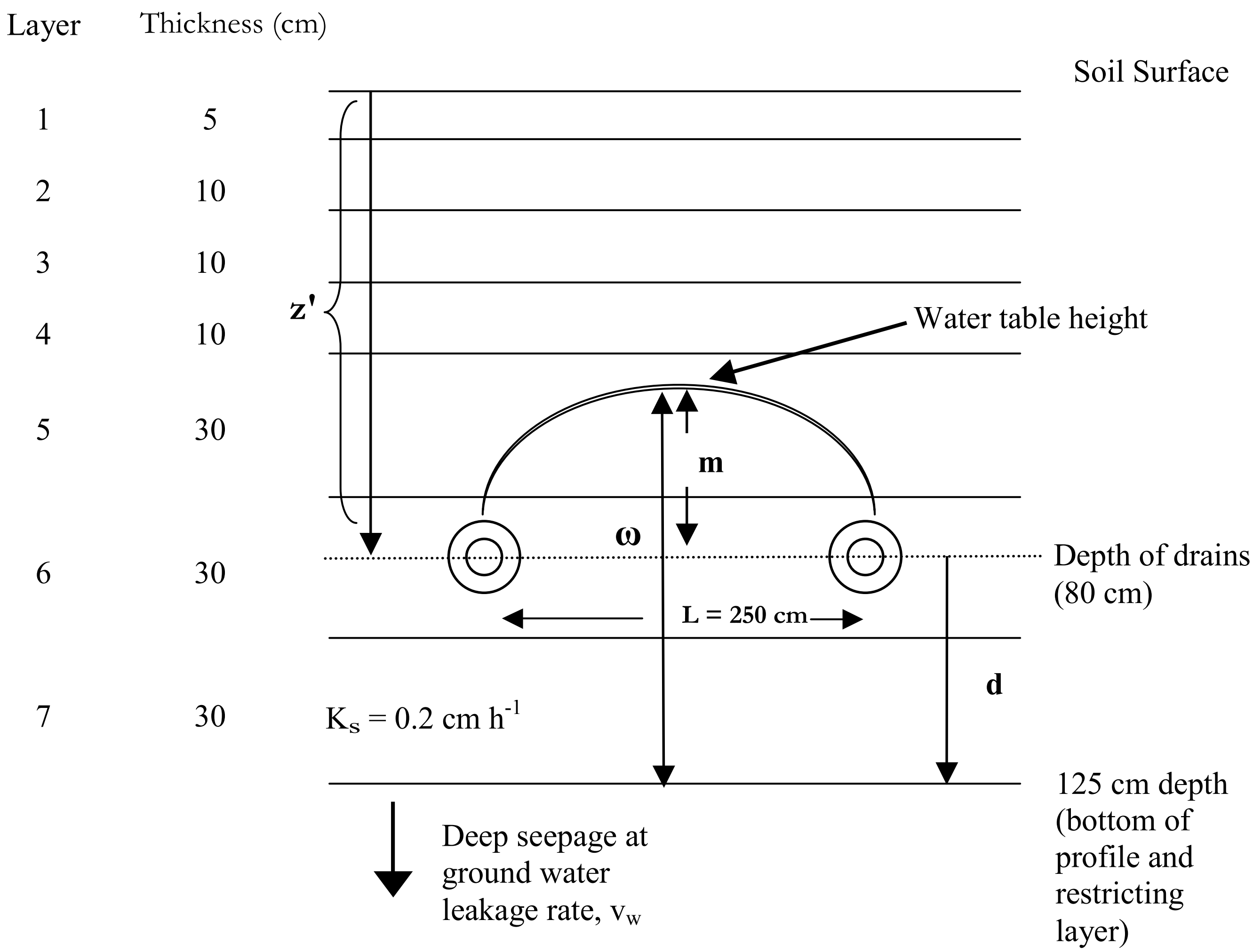

Fig. 1.1. Tile drainage system as set up in the RZWQM to emulate the design at the study site where z' = depth of drains, ω = distance from the water table to the impermeable layer, m = water table height above the drains, d = distance from the drain to the impermeable layer, and L = distance between 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.

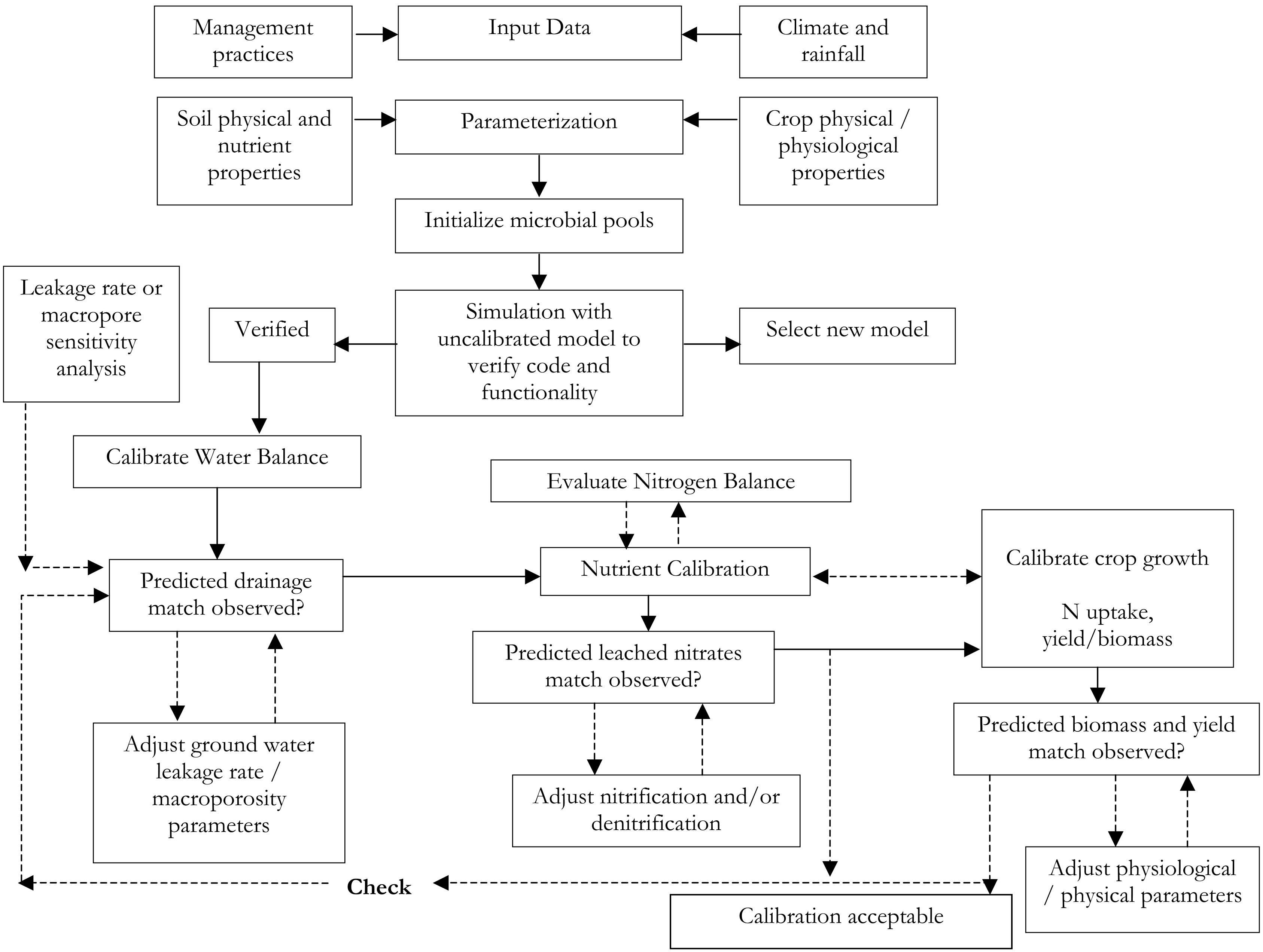

Fig. 1.2. Flow chart of procedure used to calibrate and evaluate the Root Zone Water Quality Model.

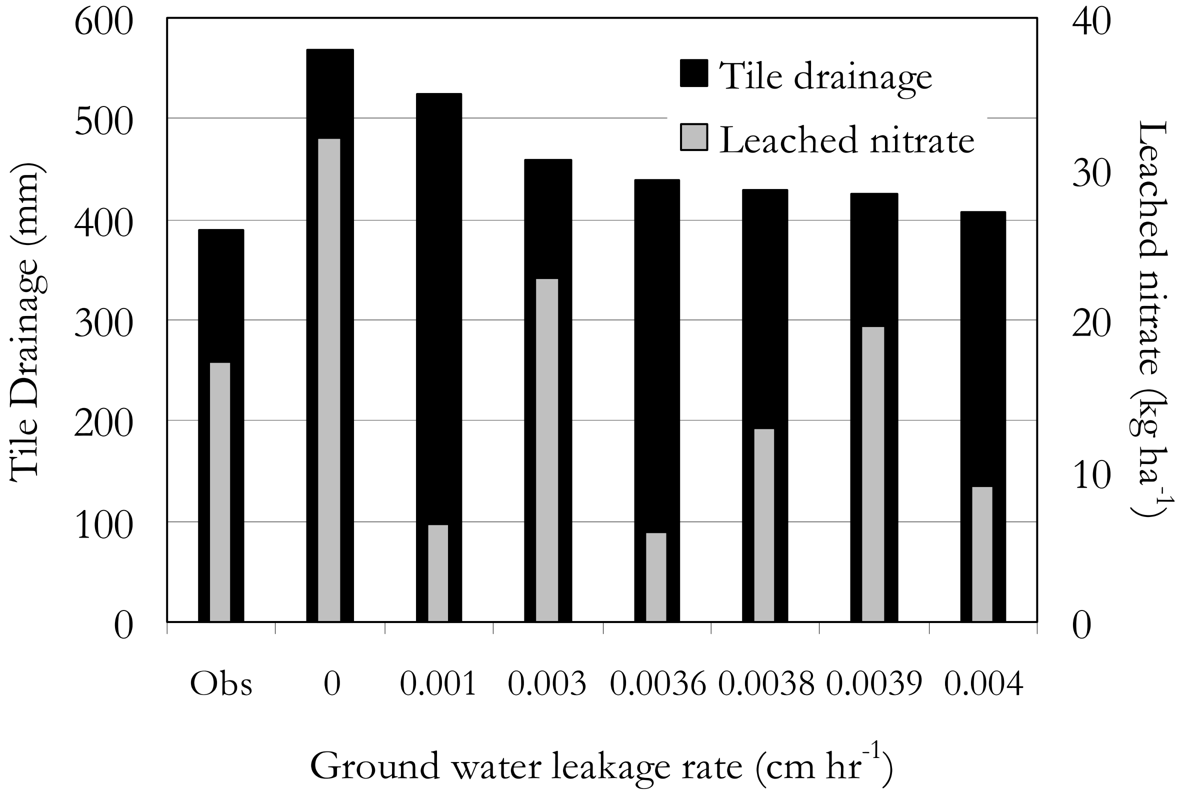

Fig. 1.3. Sensitivity of simulated tile drainage and leached nitrate to adjustments of ground water leakage rate, v_w, in relative to observed tile drainage.

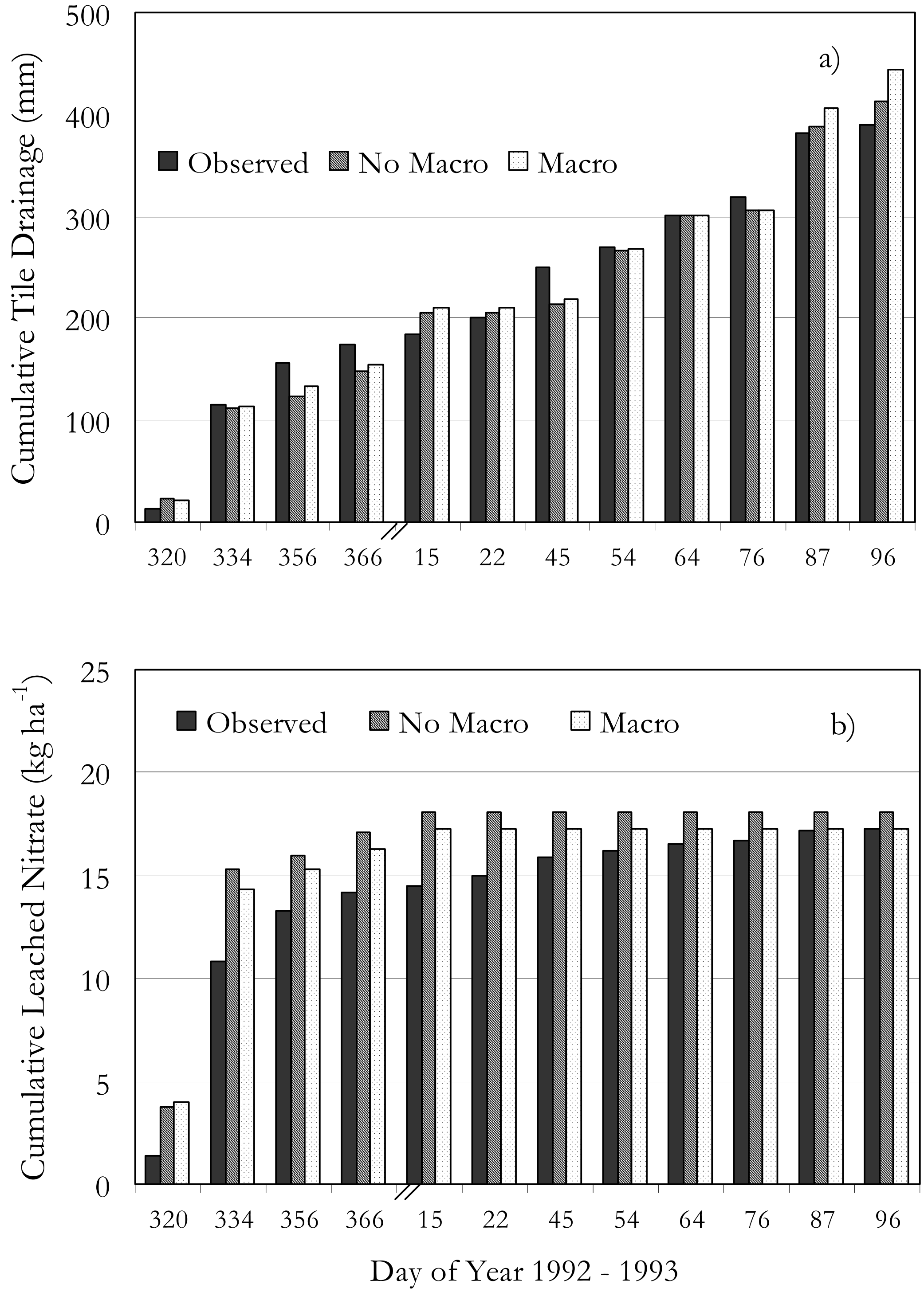

Fig. 1.4. Cumulative observed and simulated a) tile drainage and b) leached nitrate with and without macroporosity for the simulation period Nov 1992 through Apr 1993 for maize.

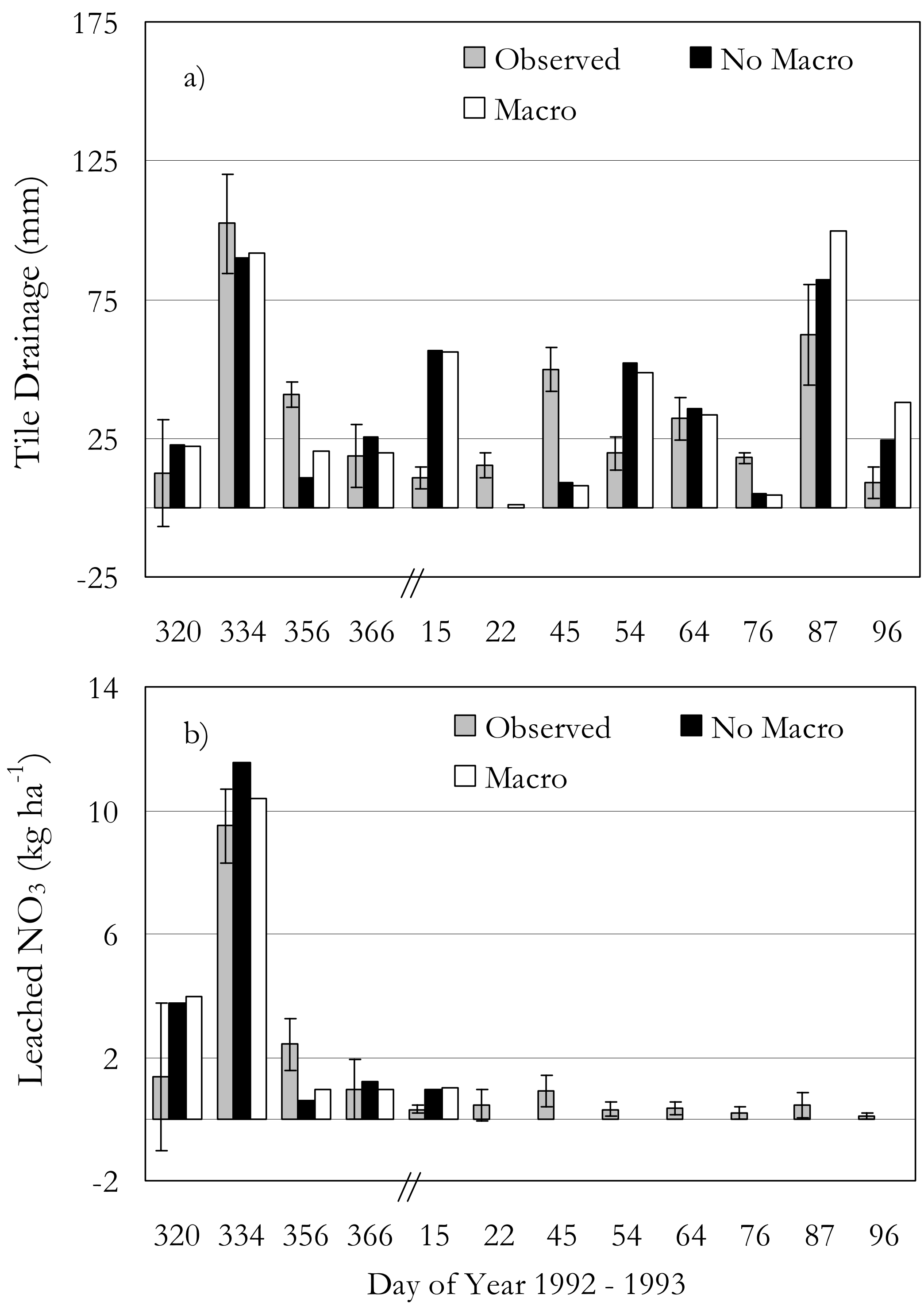

Fig 1.5. Measured and simulated event a) tile drainage and b) leached nitrate for simulation period from Nov 1992 through Apr 1993 with and without macroporosity option for maize. Observed drainage events shown with 95% C.I. bars.

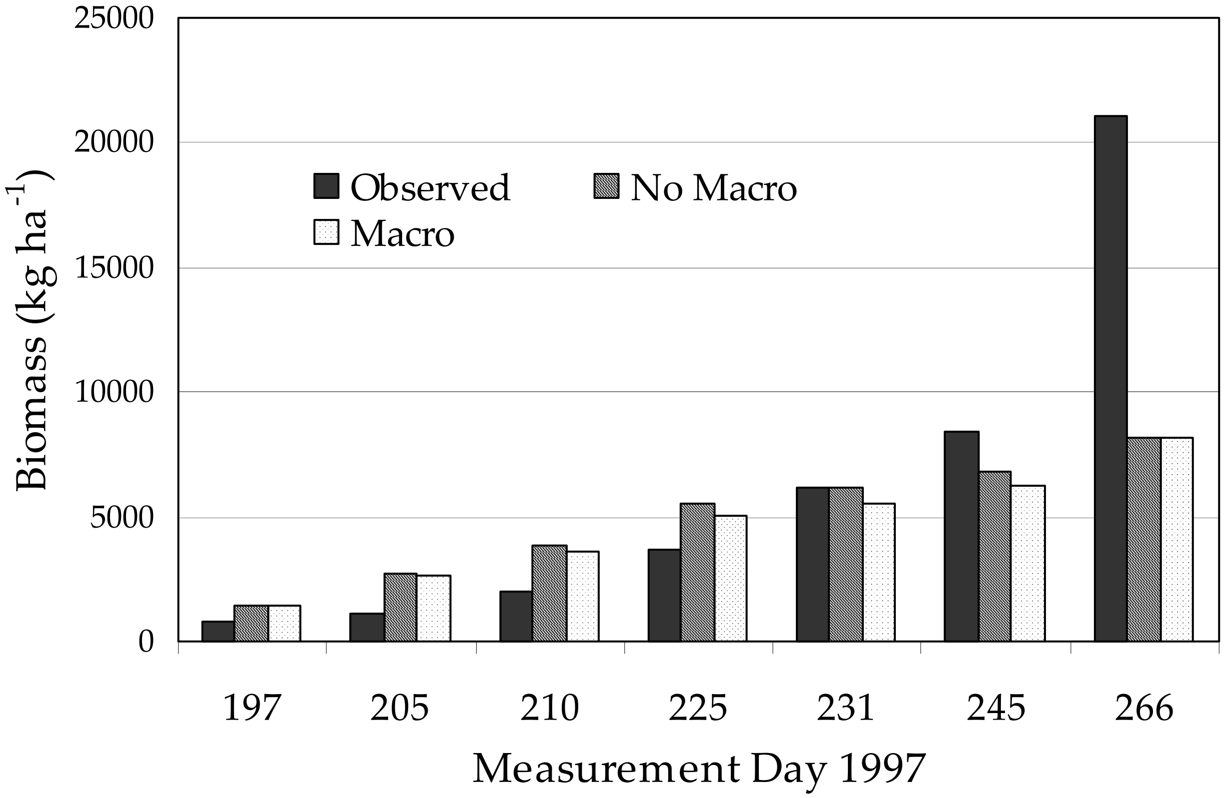

Fig. 1.6. Observed and simulated cotton biomass development with and without the macroporosity option in the model.

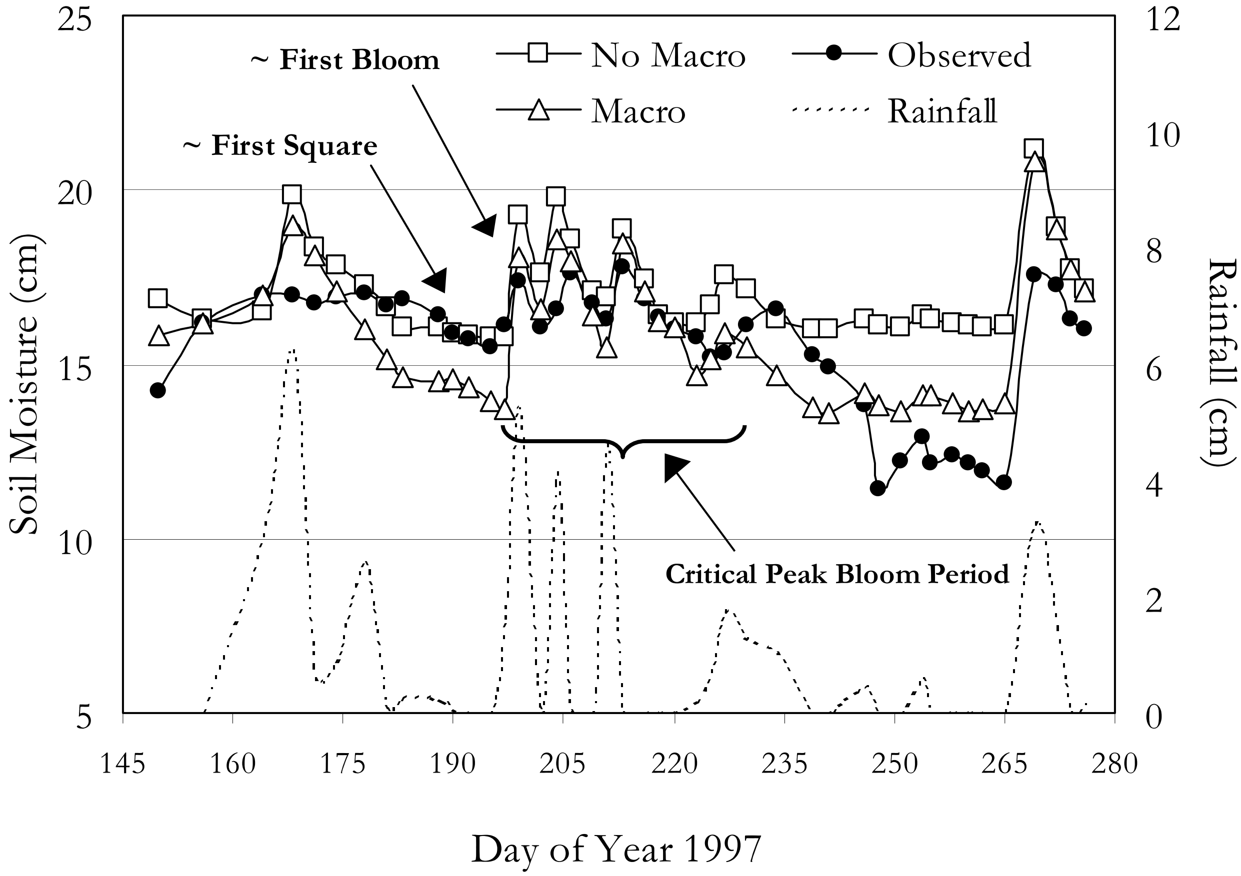

Fig. 1.7. Observed soil moisture and rainfall and simulated soil moisture with and without macroprosity for the cotton growing season in 1997.

Table 1.1a. Physical properties of Cecil sandy clay loam soil used in the 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 dia. for soil column depths from Gupte et al.,

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	Macro-porosity
	--- cm ---	--- cm ---	cm h^{-1}	------- g cm^{-3}-------			--- cm ---	-------- % -------			------- cm -------		%
1	1-5	1-7	18	2.64	1.34	Ap	0-21	78	15	7		0.014	0.014
2	5-15	6-12	20	2.65	1.56			78	15	7	0-20	0.020	0.020
3	15-25	17-23	8	2.72	1.69	BA	21-26	43	20	37		0.020	0.020
4	25-35	27-33	18	2.72	1.43			30	20	50	30-45	0.020	0.020
5	35-65	57-63	10	2.65	1.37	Bt1	26-102	30	20	50		0.025	0.025
6	65-95	87-93	2.6	2.65	1.51			30	20	50	45-60	0.025	0.025
7	95-125	127-133	0.2	2.65	1.55	Bt2	102-131	34	25	41		0.025	0.025

Table 1.1b. Initial volumetric water content on 1 Jan 1991 set equal to approximate field capacity from Bruce et al. (1983) for model simulations.

Depth	θ
----- cm -----	---- $cm^3\ cm^{-3}$ ----
8	0.18
23	0.22
38	0.25
53	0.28
69	0.36
84	0.41
99	0.43
114	0.43
125	0.43

Table 1.2. Initial soil nitrogen on 1 Jan 1991, and the observed and simulated nitrogen balance using the calibrated v_w value before adjusting the sensitive plant parameter, Ap, and after adjustment for the nitrogen balance simulation period, Nov 1991 to Apr 1993. No macroporosity model.

Initial soil NO_3-N (kg ha^{-1})	36.5		
Initial soil NH_4-N (kg ha^{-1})	6.25		
Nitrogen Balance (Day 6 Nov 1991 to 13 Apr 1993)	Observed	Simulated	
Nitrogen Component (kg ha^{-1})		Unadjusted	Adjusted
Initial soil NO_3-N	82	65	65
Initial soil NH_4-N	14	0	0
Fertilizer ($NH4_4NO_3$)	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

Table 1.3. Simulated and observed tile drainage and leached nitrate for (a) no macroporosity model and (b) with macroporosity for maize production during the calibration period Nov 1992 through Apr 1993.

(a)	No Macroporosity					
	Observed Mean	Simulated Mean	Mean Difference	Std. Error Mean Difference	Max Error	RRMSE†
	---------- 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					
	Observed Mean	Simulated Mean	Mean Difference	Std. Error Mean Difference	Max Error	RRMSE†
	---------- 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.

Table 1.4. Regression statistics for a) tile drainage and b) leached nitrate with and without the macroporosity option for the simulation period Nov 1992 through Apr 1993.

(a)	Tile Drainage					
Model	Observed	Simulated	RMSE	r	Intercept	Slope
	--------- mm ---------					
No Macro	390	413	23.0	0.61	12.8*	0.6**
With Macro	390	443	23.0	0.62	12.8*	0.5**

(b)	NO_3 in Tile Drainage					
Model	Observed	Simulated	RMSE	r	Intercept	Slope
	-------- 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**

RMSE, root mean square error; r, correlation coefficient; intercept and slope of measured vs simulated values.

* Intercepts not significantly different from 0 at $p < 0.05$.

** Slopes not significantly different from 1 at $p < 0.05$.

Table 1.5. Initial soil nitrogen on 1 Jan 1991, and observed and simulated nitrogen balance using calibrated v_w before and after adjustment to the denitrification rate for the simulation period of Nov 1991 to Apr 1993. Macroporosity model.

Initial soil NO_3-N (kg ha^{-1})	36.5		
Initial soil NH_4-N (kg ha^{-1})	6.25		
Nitrogen Balance (Day 6 Nov 1991 to 13 Apr 1993)	Observed	Simulated	
Nitrogen Component (kg ha^{-1})		Unadjusted	Adjusted
Initial soil NO_3-N	82	102	103
Initial soil NH_4-N	14	0	0
Fertilizer ($NH4_4NO_3$)	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

Table 1.6a. Final adjusted values used for the sensitive parameters for cotton calibration of the RZWQM with and without macroporosity.

Parameter	Definition	Value	Units
μ_1	Maximum active nitrogen 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
-	Nitrogen sufficiency index – trigger for timed application of fertilizer	0.9	-
-	Luxurious nitrogen uptake factor – increases or reduces uptake	1	-

Table 1.6b. Organic matter decay rates and rate coefficients for some of the major processes to simulate the carbon and nitrogen pools in the OMNI submodel of the RZWQM. The final adjusted value for denitrification was 4.34e-013 in the model simulations with macroporosity.

OM Decay Rates		
Residue		
	Slow	1.673e-007
	Fast	8.14e-006
Humus		
	Fast	2.5e-007
	Transition	5.0e-008
	Stable	4.5e-010
Arrhenius Rate Coefficients		
	OM Decay	8.187e-009
	Nitrification	1.0e-009
	Denitrification	1.0e-013
	Urea Hydrolysis	0.00025
Biomass Decay Coefficients		
	Aerobic Heterotrophs	5.0e-035
	Autotrophs	4.77e-040
	Anaerobic Heterotrophs	3.4e-033

CHAPTER 3

EVALUATION OF THE ROOT ZONE WATER QUALITY MODEL FOR SIMULATING TILE DRAINAGE AND LEACHED NITRATE IN THE GEORGIA PIEDMONT[1]

[1] D. A. Abrahamson, D. E. Radcliffe, J. L. Steiner, M. L. Cabrera, D. M. Endale and G. Hoogenboom. To be submitted to Agron. J.

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

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ABSTRACT

Modeling non-point source pollution has become a widely used analysis tool to test the impact of different agricultural management practices on water quality. The goal of this project was to evaluate the Root Zone Water Quality Model (v. 1.3.2004) for simulating tile drainage and nitrate leaching under conventional tillage and no tillage management practices in cotton production in the southern Piedmont region of the USA. The model was recently refined to improve the simulations of drainage, nitrate leaching and the effects of tillage in the Great Plains region of the U.S. where the climate is much drier and the soils are permanently negatively charged. In an earlier study, we calibrated the model for tile drainage and nitrate leaching, and for cotton development and water use based on experimental data collected at the J. Phil Campbell, Sr. Natural Resource Conservation Center in the southern Piedmont at Watkinsville, Georgia in 1991 through 1993. The evaluation of the model with an independent data set with data from 1997 through 1998 revealed large differences in measured and simulated tile drainage and leached nitrate during the cotton and winter cover crop growing seasons. There were 30 observed drainage events from total rainfall during the period which allowed us to compare the differences between simulated and observed tile drainage and leached nitrate. Measured and simulated tile drainage values were different by 1074 mm for the

conventional tillage treatments and by 843 mm for the no tillage treatments. Measured and simulated values of leached nitrate in tile drains were different by 30 kg ha^{-1} and 37.5 kg ha^{-1} for the conventional and no tillage treatments. In spite of the large differences in simulated and observed tile drainage, the model predicted deep drainage plus tile drainage reasonably well. The model is also very sensitive to the ground water leakage rate. Although the calibrated value for the ground water leakage rate worked well for the model calibration period, differences in simulated ET and the effect of annual cover crop management practices during the four-year period since the model was calibrated appeared to have influenced the amount of soil water that was available for drainage and the amount of soil nitrate that was available for nitrate leaching at the study site.

INTRODUCTION

Only within the past decade has the attention of the public, policy makers, regulators, and the scientific community shifted from point source to non-point source pollution (NPS) of subsurface soil and water resources. This has been due to the growing reliance upon groundwater as a source for drinking water as well as a source for agriculture (Corwin et al. 1999). The assessment and remediation of NPS groundwater contamination from the past, present and future use of agrochemicals has posed problems that have significantly greater economic impacts than those which have long been recognized for point sources (Loague and Corwin, 1996). Agricultural research traditionally focused on the efficient use of water for improving the productivity of food and fiber, but is now equally focused on the quality of the water resource as it impacts drinking water supplies.

An effective methodology to develop agricultural management systems that address NPS pollution is through interactive use of selective experimentation and modeling (Ahuja et al. 2000). A model is a synthesis of the current and accumulated state of knowledge and a tool that can be used to increase our understanding of fundamental processes as well as the interactions of these processes under various conditions in agricultural watersheds. Research in agriculture and other natural resource disciplines use both real-time measurements as well as model predictions in order to determine what must be done to ensure that our water resources are sustainable. However, for any modeling approach to be valid and useful in terms of calibration and prediction, it must be closely related to what can be determined experimentally (Wagenet and Hutson, 1996).

While there is a considerable amount of effort by both researchers and natural resource managers to model NPS pollution at the watershed scale, there continues to be a need for evaluation and improvement of the deterministic, field- and plot-level scale models that serve as the basis for these watershed models. Models such as LEACHM (Hutson and Wagenet, 1992), PRZM and PRZM3 (USEPA, 2003), GLEAMS (Leonard et al., 1987), OPUS (Smith et al., 1992), CROPGRO (Hoogenboom et al., 1992, Boote et al., 1998), CERES-Maize (Jones and Kiniry, 1986, Ritchie et al., 1998) and the RZWQM (Ahuja et al., 2000), are examples of field scale, deterministic models. They were developed based on the accumulated knowledge of the soil-water-plant continuum processes in agricultural systems over many years of laboratory and field studies. Distributed parameter models such as AGNPS (Young et al., 1989) use model components from field scale models such as CREAMS (Knisel et al., 1983) to predict soil erosion and nutrient transport/loadings from agricultural watersheds. The SWAT model (Arnold et al., 1993) incorporates features of several agricultural models and is a direct outgrowth of the SWRRB model (Simulator for Water Resources in Rural Basins) (Williams et al., 1985; Arnold et al., 1990), using components from the CREAMS, GLEAMS and EPIC models (Williams et al., 1984) (SWAT, 2004). Deterministic models, though originally developed as research models, have been linked or interfaced with Geographical Information Systems such as GRASS (Geographic Resources Analysis Support System), (GRASS Development Team, 1999-2002) and decision support systems such as DSSAT (Decision Support System for Agrotechnology Transfer, Tsuji et al., 1996, Hoogenboom et al., 1992). Scientific components and submodels of these models are also currently being linked to the Object-Oriented Modeling System (OMS), a framework which facilitates the assembly of a modeling package and shares different model resources (OMSCentral, 2004). Though deterministic models have been developed based on many years of experimental study, uncertainty associated with model predictions results from all of the errors involved in the process of model formation, calibration, parameter estimations and environmental variability (Gardner et al., 1990). The confidence building process in model prediction is a long-term and iterative process (Hassan, 2003), and model developers continue to test and refine deterministic models to improve simulation of physical, biological and chemical processes and systems (Donigian and Huber, 1991).

The RZWQM is an integrated physical, biological and chemical process model that simulates plant growth, movement of water, nutrients and pesticides over and through the root zone at a representative area of an agricultural cropping system. The model was originally developed to provide a comprehensive simulation of root zone processes that affect water quality, and to respond to a wide range of agricultural management practices and surface conditions (Ahuja et al., 2000). It was designed with interactive feedback between soil water, available nitrogen and plant production (Hanson et al., 1999). The RZWQM is one-dimensional, and designed to simulate conditions on a unit area basis. It includes several detailed processes and user options that can affect the simulation results.

The goal of this project was to evaluate the performance of the calibrated RZWQM model (Abrahamson et al., in review) for simulating tile drainage and leached nitrate in cotton production under conventional tillage (CT) and no-till (NT) agricultural management practices. The model was originally selected for its ability to simulate soil water movement through macropores because regions of preferential flow have been found in Piedmont and other well-structured soils (Gupte et al., 1996, Williams et al., 2003). Preferential flow is particularly important in agricultural soils where the rapid transport of nutrients and chemicals that bypass the soil matrix can result in groundwater contamination (Williams et al., 2003). However, based upon the calibration analyses, 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 we used to calibrate the model without macroporosity. In addition, we did not find significant differences between simulated tile drainage with and without the macroporosity option in the calibration study. These results support research from the study site that shows most of the preferential flow in these soils occurs in the soil matrix and through in-filled macropores rather than through distinct open macropores (Gupte et al., 1996). Based upon the calibration analyses, we did not include the macroporosity option for simulation of tile drainage and leached nitrate in the current study to test the calibrated model.

Johnson et al. (1999) tested the LEACHN model for simulating tile drainage and leached nitrate at the current study site in 1991 and 1992 where tile drains are present. The authors attributed the overestimation of cumulative tile drainage and leached nitrate to the absence of a soil macropore-matrix exchange component in the model. However, LEACHN does not include a tile drainage component. Tile drains introduce a different soil water flow pattern when present in the soil, and convergence of soil water flow near the drains must be considered (Skaggs, 1978, Ritzema, 1994). Tile drainage is implemented in the RZWQM model using the Hooghoudt equation as applied by Skaggs (1978).

If the RZWQM can be applied in a region of the country where soils and climate differ greatly from the region in which it was developed, it will allow wider applicability of the model for simulating the effects of agricultural management practices such as CT and NT on groundwater supplies. It may then be reliably linked to larger scale models with application for the Piedmont region. The RZWQM is currently being linked to the DSSAT model system (Ma et al., in review), and a geographic information system to study spatially distributed systems at the watershed scale.

MATERIALS AND METHODS

Field Experiments

The experimental data for the evaluation of the RZWQM were collected as part of a water quality study initiated in 1991 at the USDA-ARS J. Phil Campbell, Sr. Natural Resources Conservation Center in Watkinsville, Georgia. The major objective of the water quality study initiated in 1991 was to quantify and compare potential impacts of CT and NT and winter cover crop management practices on leached nitrate in maize production from 1991 to 1994. After the plots were planted to cotton in 1995, the study included mineral and poultry litter fertilizer treatments in a factorial combination with tillage treatments. The current study to evaluate the model includes tile drainage and leached nitrate data collected from the plots from May 1997 to May 1998 while in cotton production under CT and NT management with a winter rye cover crop.

The study consisted of twelve 10 m x 30 m plots with drain tiles installed at 75 to 100 cm depths on a 1% slope, 2.5 m apart. Drain tiles were installed in half of the plots in 1981, and in the remainder of the plots in 1990 to examine nutrient and pesticide losses in tile drainage from the entire study site after 1990. 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. A complete description of the study is given by Johnson et al. (1999) and Endale et al. (2002).

The management practices for the cotton study included light disking in the CT plots for seed bed preparation and after incorporation of fertilizer in winter rye. Winter rye was grown as the cover crop during the fall and winter months (November through April). Deep chisel plowing, followed by disc harrowing, and subsequent disking to smooth the seed bed were performed in the CT plots prior to planting cotton. The only tillage operation performed in the NT plots was the use of a coulter disk for planting (Endale et al., 2002). Cotton was fertilized with ammonium nitrate at a rate of 60 kg N ha^{-1}, and winter rye with 54 kg N ha^{-1} at planting. Cotton yield and biomass and winter rye biomass were sampled at the end of each growing season.

The soil was a Cecil sandy loam (fine, kaolinitic, thermic, Typic Kanhapludult), deeply weathered, kaolinitic, acidic and variably charged. Kaolinite clay makes up over 50% while vermiculite and chlorite make up 10-30% (Endale et al., 2002). The pH normally ranged from 5.5 to 5.8 in the upper layers of the soil profile as measured at the study site; therefore, lime was applied approximately every three years to maintain a pH of 6.0 to 6.3 in the surface horizon in order to avail plant nutrients and prevent aluminum toxicity. Soil moisture was collected in each plot to a depth of 50 cm in 1997 using Time Domain Reflectometry (TDR) (Evett, 2000) and to a depth of 150 cm using TDR in 1998 (MoisturePoint, ESI, Vic., BC, Canada). Rainfall and other weather data for evaluating the model were recorded at an automated weather station adjacent to the site (Hoogenboom, 2003). Average annual rainfall from 1996 through 2003 at the study site was 1195 mm. With the exception of the introduction of poultry litter as a fertilizer treatment in the water quality study on half the plots where mineral fertilizer had previously been applied, the site was assumed to have maintained the same basic soil properties and crop growth potential that were present during the calibration of the model.

Model Simulations

We previously calibrated the RZWQM model for simulating tile drainage and leached nitrate in CT management systems in maize production with and without the macroporosity option in the model, and separately calibrated cotton production with and without macroporosity. The calibrated model simulated tile drainage and leached nitrate within 15% of observed values without the macroporosity option for maize production under CT management practices. In addition, the model accurately simulated average cotton biomass production to within 20% of average observed values, and daily cotton water use was different by less than 1 mm d^{-1} during the period of peak critical bloom with and without the macroporosity option (Abrahamson et al., in review). Our main objective for calibrating the model for cotton was to simulate cotton water use during the period of peak water use in order to compare simulated and observed tile drainage and nitrate leaching for the current study. This in turn gave us a reasonable basis for evaluating the model's ability to simulate tile drainage after the water quality study was placed in cotton production, and measurements of tile drainage and leached nitrate were available.

Changes to the calibrated cotton model for the current study included rainfall and climate data for the years simulated (1997-1998) and the management practices. Management practices included the number and type of tillage operations performed in the CT plots during the period, and a no-till coulter planter for cotton for the NT simulations. We did not include an option for soil crusting in the NT simulations.

The simulation period for the current study at the water quality study site was 1 Jan 1997 through May 1998. We compared observed and simulated tile drainage and leached nitrate from 3 May 1997 through 9 May 1998 when measurements of each response variable were available using linear regression analysis (SAS, 2000). We also tested for differences between observed and simulated slopes and intercepts for both CT and NT scenarios and for simulated tillage effects on simulated tile drainage and leached nitrate. In order to account for drainage and leached nitrate below the depth of the tile drains (80 cm), we calculated the daily observed and simulated water balance for the entire evaluation period and for the cotton growing season in 1997. The observed daily water balance was calculated as:

$$Rainfall - ET - Tile\ Drainage - Runoff - \Delta\ SW50 = Deep\ Drainage + \Delta\ SW50\_125$$

where *Rainfall*, *Tile Drainage*, and *Runoff* were measured values, and $\Delta\ SW50 = SW50_{i} - SW50_{i\text{-}1}$ was equal to the change in measured soil moisture in a 50 cm profile on day *i*. The Ref-ET software was used to calculate daily reference ET (ET_0) based on the FAO Penman-Monteith equation (Allen, 2000), and daily ET_c was calculated using the procedure for calculating crop water requirements based on the growth stages for cotton and for annual cover crops (Allen et al., 1998). We used winter wheat as a surrogate for winter rye for calculating *ET* for the observed water balance. The term, ($\Delta\ SW50\_125 + Deep\ Drainage$) served as the remaining water after accounting for all other terms in the water balance. The daily simulated water balance was calculated as:

$$Rainfall - ET - Tile\ Drainage - Runoff - \Delta\ SW50 - \Delta\ SW50\_125 - Deep\ Drainage = Balance$$

based on measured rainfall and each simulated component from the model. If we assumed that the differences in daily calculated $\Delta\ SW50\_125$ and the daily simulated values of $\Delta\ SW50\_125$ were small, then we could compare the differences in simulated (*Tile Drainage* + *Deep Drainage*) and (observed *Tile Drainage* + calculated *Deep Drainage*). The difference in total simulated leached nitrate in simulated (*Tile Drainage* + *Deep Drainage*) and total observed leached nitrate in observed tile drainage would also give us an estimate of the amount of nitrate that leached below the root zone in the field study.

RESULTS AND DISCUSSION

Total measured rainfall for the entire simulation period was 1805 mm. A drought ensued in June 1998 and there was no measurable drainage after 9 May 1998. There were 30 observed drainage events from the total rainfall during the period (Endale et al., 2002), which allowed us to compare the differences between simulated and observed tile drainage and leached nitrate.

Total observed drainage for the measurement period was 229 mm and total simulated drainage was 1303 mm for the CT treatments. Total measured drainage was 448 mm and simulated drainage was 1291 mm for the NT treatments. The maximum observed drainage volume was 88.4 mm for the CT treatment and 86.7 mm for the NT treatment from a two-day rain event of 132 mm in Oct 1997. Simulated drainage for the same event was 111 mm for CT and 103 mm for NT. Simulated and observed cumulative drainage followed the pattern of cumulative rainfall in spite of the fact that there were large differences in simulated and observed drainage volumes (Fig. 2.1). The linear regression analyses of observed values of drainage on simulated drainage revealed high correlations and slopes that were significantly different from zero and significantly different from one (Table 2.1).

In order to explain the large differences in simulated and observed tile drainage, we first ran the calibrated model to simulate maize production at the water quality study site using the 1997 climate and rainfall data that were used to calibrate the model for cotton at a study site adjacent to the water quality study. The model had accurately simulated maize production in 1991 and 1992, and tile drainage and nitrate leaching in the winter of 1992 to 1993 under winter rye cover in CT treatments at the water quality study site (Abrahamson et al., in review). Total rainfall for the calibration period from 1 Jan 1992 through 13 Apr 1993 was 1905 mm, and the total rainfall for the current study in 1997 and 1998 was 2095 mm, a difference of 190 mm over fourteen and a half months (Fig. 2.2). Based on the rainfall amount and pattern in each period, it did not seem that differences in soil water recharge or water use during the cropping season in 1992 and 1993 versus 1997 and 1998 would have been different at the same study site. Maize production was accurately simulated using 1997 climate and rainfall data relative to expected values for maize biomass and yield and very similar to observed biomass and yield from the 1992 simulation. The trend and relative volume of simulated drainage were the same for the simulations of maize and cotton production during 1997 as they were for the calibrated model in 1992. This indicated that the model was performing in the same manner relative to simulated tile drainage in 1997 as it had for the cotton calibration period in 1997 and for the maize simulation in 1992. The antecedent moisture contents in the model calibration scenario in 1992 compared to the 1997 evaluation scenario at the beginning of the data collection period were nearly the same (Fig. 2.3). Measured rainfall events and rainfall intensity were also very similar in the calibration period and the current study period (data not shown). Total observed runoff was 138 mm for CT and 91 mm for NT treatments in the current study, and total simulated runoff was 38 mm for both CT and NT model simulations. However, a difference of 100 mm or less of runoff from each simulated and observed treatment did not account for differences of greater 500 mm between total observed and total simulated tile drainage in each treatment during the evaluation period.

We next considered differences between simulated and observed crop water use that could have affected simulated versus measured tile drainage. Total simulated cotton biomass was 7944 kg ha^{-1} for the CT treatment and 7279 kg ha^{-1} for the NT treatment. Total cotton biomass production is generally greater than 20,000 kg ha^{-1} in the southeastern U.S. (Carns and Mauney, 1968; Endale et al., 2002; Reddy et al., 2004; Schomberg and Endale, 2004). However, the results of simulated cotton production were similar to the results obtained for cotton production during the calibration of the model (Fig. 2.4) when the differences between observed and simulated water use during the period of peak water use were less than 0.3 mm d^{-1} based on calculations of rainfall minus observed and simulated soil moisture in a 60 cm soil profile (Abrahamson et al., in review). The difference between total simulated cotton biomass in the calibration scenario and total simulated cotton biomass for the current study was 1000 kg ha^{-1}. Although cotton was use can be as high 6 to 9 mm d^{-1} during the critical water use period of the growing season (Bednarz et al., 2002), a difference of 1000 kg ha^{-1} of biomass would result in a difference of less than 15 mm of water use during the cotton growing season based on the average amount of water required to produce 5000 kg of shoot biomass (Hanks, 1983).

The calculation of the simulated water balance revealed that simulated ⊿ *SW50_125* for the evaluation period was 40 mm or less for both the CT and NT treatments. Omitting this term from the calculations for the observed water balance assuming that observed ⊿ *SW50_125* was also small, calculated *Deep Drainage* was equal to 656 mm for the CT treatments. Observed *Tile Drainage* + calculated *Deep Drainage* was 885 mm for the CT treatment based on a 1.25 m soil profile. Simulated

Tile Drainage + *Deep Drainage* was 1333 mm for the CT treatment in a 1.25 m soil profile. The calculated value for *Deep Drainage* in the observed water balance was 487 mm for the NT treatment. Observed *Tile Drainage* + calculated *Deep Drainage* was 936 mm, and the simulated total was 1360 mm for the NT treatment. The simulated values of *ET* were less than the calculated values by 282 mm for the CT treatments and 313 mm for the NT treatments during the evaluation period (Table 2.2). If the simulated and calculated values of *ET* had been the same, the differences between total simulated drainage and total calculated drainage would have been 167 mm for the CT treatments and 112 mm for the NT treatments, within 16% and 15% respectively of measured drainage for each treatment.

The differences in the observed and simulated water balance for the cotton growing season revealed that calculated and simulated *ET* were different by 53 mm and 72 mm for the CT and NT treatments respectively while simulated and observed tile drainage were different by 219 mm and 181 mm respectively (Table 2.3). This would result in a difference in water use of less than 0.5 mm d^{-1} during the cotton growing season. The calculated and simulated values for *Tile Drainage* + *Deep Drainage* were different by 6 mm for the CT treatments and 22 mm for the NT treatments. In this case, the large values of simulated tile drainage compared to the observed values of tile drainage were likely due to the simulated upward flux of drainage by the model. This was due to the low K_s rate of the soil beneath the drains and the water table leakage rate at the bottom of this layer which created a perched water table in the model. The K_s of the soil layer beneath the tile drains is 0.2 cm h^{-1} and the water table leakage rate at the bottom of the layer is 0.0035 cm h^{-1} as calibrated for the earlier study. However, it is also not clear from the model documentation what the boundary condition is at the bottom of the user-designated soil profile in the model when the pressure head is negative at this depth.

Although a perched water table in the model could account for most of the simulated tile drainage during the cotton growing season, the simulated flux of *Deep Drainage* was small and positive for the entire evaluation period (Table 2.2). However, measured tile drainage during the winter rye growing season from Nov 1997 to May 1998 was 91 mm for the CT treatments and 262 mm for the NT treatments. Simulated tile drainage was 822 mm and 852 mm for the CT and the NT treatments. Simulated *ET* was under estimated by 192 mm for the CT treatments and 205 mm for the NT treatments compared to calculated *ET*, and total simulated and observed runoff were different by 35 mm for the CT treatments and 7 mm for the NT treatments. The differences in simulated and calculated *ET* and simulated and observed runoff did not explain all of the differences in total simulated and total measured tile drainage for the winter rye growing season. The calculated observed water balance for the period revealed that calculated *Deep Drainage* was 450 mm for the CT treatment and 303 mm for the NT treatment. The simulated value of *Deep Drainage* was 156 mm in the CT treatments and 155 mm in the NT treatments for the winter rye period. The total of observed *Tile Drainage* + calculated *Deep Drainage* was 545 mm for the CT treatments and 570 mm for the NT treatments. The simulated value of *Tile Drainage* + *Deep Drainage* was 979 mm for the CT treatments and 1007 mm for the NT treatments during the winter rye growing season (data not shown). This indicated that more water was captured by the tile drains in a 1.25 m soil profile during the winter rye period in the model while less water was captured by the drains in the field study and stored in the soil profile with less available water for deep seepage. The differences in simulated and calculated *ET* were likely due to the fact that we used the Quikplant submodel in the RZWQM to simulate winter rye growth. This model bases plant growth and development on a limited number of parameters such as maximum N uptake and maximum root depth supplied by the user (Ahuja et al., 2000). In contrast, the full plant production submodel in the RZWQM requires many phenological and physiological parameters that are not available or that are not well established for winter cover crops such as annual winter rye. However, the full production plant model under predicted *ET* and over predicted tile drainage during the cotton growing season, and therefore, may not have simulated winter rye growth more accurately than the Quikplant model did. The model accurately simulated tile drainage and leached nitrate during the winter rye growing season in 1992 to 1993 for the calibration study, therefore, we looked at other reasons for the large over predictions of tile drainage by the model during the winter rye growing season in the current study.

Annual winter rye is highly tolerant of aluminum toxicity (Foy, 1988; Rife et al., 1999; Pinto_Carnide and Guesdes-Pinto, 2000), which is a common characteristic in Cecil subsoils. Unlike cotton roots, which do not extend to depths much greater than 30 cm to 60 cm due to sensitivity to subsoil acidity (EFU Manual, 2004, http://www.back-to-basics.net/efu/efu.html; Sumner, 1994), winter rye roots can extend to depths greater than 180 cm (Frye et al., 1985; Sarrantonio, 1992), and can accumulate up to 150 kg N ha^{-1} in one growing season (Hoyt and Mikelsen, 1991; Shennan, 1992; Ditsch et al., 1993). The maximum root depth parameter that we used for winter rye in the model calibration study was 1.25 m, which is also the depth of the soil profile in the model. We used a value of 95 kg N ha^{-1} for maximum N uptake for winter rye based on the total measured N concentration of 93 kg ha^{-1} in above-ground rye biomass after the first crop was harvested in Apr 1992 at the water quality study site (McCracken et al., 1995). The authors in that study found that nitrate leaching losses were 3.3 kg ha^{-1} and significantly lower under the winter rye treatments than leaching losses under the fallow treatments. They attributed the lower leaching losses in winter rye cover treatments to greater soil water and nitrogen use by the rye crop as opposed to fallow treatments. The total observed leached nitrate in tile drains for the current study at the water quality plots was 1.4 kg ha^{-1} for the CT treatments and 1.3 kg ha^{-1} for the NT treatments while simulated leached nitrate in tile drains was 31.4 kg ha^{-1} for the CT treatments and 38.8 kg ha^{-1} for the NT treatments. As with observed and simulated drainage, the differences between simulated and observed values were large but the cumulative patterns were similar (Fig. 2.5). The regression analyses of the log transformed observed and simulated leached nitrate data showed little or no linear relationship between observed and simulated values (Table 2.1), and there was no effect of simulated tillage on simulated leached nitrate. Total simulated leached nitrate in *Deep Drainage* for the entire evaluation period was –1.4 kg ha^{-1} for the CT treatments and 6.9 kg ha^{-1} for the NT treatments. However, during the winter rye growing season, the model simulated 20 kg ha^{-1} of leached nitrate in *Deep Drainage* for the CT treatments and 21 kg ha^{-1} for the NT treatments. Simulated leached nitrate in tile drains during the winter rye period was 2.7 kg ha^{-1} in the CT treatments and 3.5 kg ha^{-1} in the NT treatments. This revealed that the winter rye crop at the study site took up more nitrate compared to simulated uptake because there was less observed leached nitrate in tile drains compared to simulated leached nitrate in tile drains and more simulated leached nitrate in simulated *Deep Drainage* during the winter growing season.

Winter rye cover crops can reduce the potential for nitrate leaching by absorbing and storing N in plant tissue during winter months during soil water recharge, and by reducing percolation through transpiration (Bellocchi et al., 2002, Weinert et al., 2002). In those studies the authors found that over wintering cover crops such as winter rye lowered soil mineral N by 155 kg ha^{-1}. Similar results were found for winter rye cover cropping practices following continuous maize rotation in a mid-Atlantic coastal plains study (Staver and Brinsfield, 1998). Total measured winter rye biomass at the water quality study site in April 1998 was greater than total measured winter rye biomass in 1993 by 1.8 t ha^{-1} in the CT treatments and 2.0 t ha^{-1} in the NT treatments (McCracken et al., 1995; Endale, unpublished data). Although rainfall was greater for the 1997 to 1998 winter rye growing season by 128 mm, greater total winter rye biomass production in Apr 1998, and the reduction of leached nitrate by the winter rye crop in 1993 compared to fallow treatments suggest that measured tile drainage and leaching losses may have been reduced by greater water and nitrogen uptake due to continuous winter cover crop management practices since 1991 at the study site. Given the growth habits of winter rye cited in recent similar studies, and the values of measured winter rye biomass at the water quality study site in 1998, it is reasonable to assume that the winter rye crop has begun to take up more water and soil nitrogen since the first winter rye cover crops were planted in Nov 1991 and Nov 1992, followed by winter wheat from 1994 through 1996, and winter rye in 1997. The winter rye roots may have also begun to grow deeper into the soil based on similar studies of rooting depths of winter rye cover crops previously cited. In addition, based on a study of maize followed by a winter rye cover crop in Minnesota, USA, winter rye biomass production decreased when rainfall and temperatures were below normal for the growing season in two of three years. However, biomass N concentration increased (Strock et al., 2004). During the three-year period in that study, maximum annual biomass production was 3 t ha^{-1}, and average annual production was 1.5 t ha^{-1}. The authors found that winter rye cover cropping reduced subsurface drainage by 11%, and reduced leached nitrate in subsurface drainage by 13% over the three-year period even with below average rainfall and temperature conditions in two of the years.

The differences between the observed values of tile drainage and leached nitrate in 1992 and 1993 compared to the observed values in 1997 and 1998, and the large differences in simulated and observed values in 1997 and 1998 appear to be due to the over and under estimation of some of the simulated water balance components by the model. However, based upon our evaluation of the differences in total rye biomass in 1993 and 1998, the amount of nitrate and water lost to total drainage in 1998 compared to 1993, and the studies cited above in winter rye cover crop management practices similar to our study, it is likely that there is less soil water and soil nitrogen available for drainage and nitrate leaching now than there was in 1992 and 1993 at the water quality study site. Although the Quikplant submodel that we used for winter rye growth in the RZWQM did not simulate water use by the winter rye cover crop accurately, the ability of a model to simulate these types of changes in crop water and nitrogen use by a winter cover crop would provide a valuable tool for modelers and researchers to evaluate the effects of agricultural management practices such as annual cover cropping practices on surface and ground water quality.

SUMMARY

The RZWQM accurately simulated tile drainage and leached nitrate during the calibration study from 1991 through 1993 at the water quality study site while in maize production with a winter rye cover crop under conventional till management practices. The model did not accurately simulate the volume of tile drainage and leached nitrate for the evaluation period in the current study after the study site was converted to cotton production with a winter rye cover crop under conventional and no tillage management practices in 1997 and 1998. However, total drainage was reasonably well simulated during the cotton growing season based on our analyses of the simulated and observed

water balances for the period. The differences in simulated and observed tile drainage and leached nitrate for the evaluation period appeared to be due to 1) the under estimation of simulated ET for the cotton and winter rye crops and, 2) the differences in the amount of soil water and soil nitrogen available for tile drainage and nitrate leaching at the study site compared to the period when the model was calibrated. The over estimation of tile drainage was also due to the fact that the bottom boundary of the soil profile as it was designed in the model for the calibration scenarios did not work well for the evaluation period in the current study. The model simulated a perched water table that partitioned water between tile drainage, runoff, ET, and soil water storage based on a 1.25 m soil profile. In the current study, less water was available at the depth of the tile drains and drained to below 1.25 m in the soil profile at the study site compared to the calibration period in 1992 and 1993.

The lack of significant differences due to tillage for simulated tile drainage and leached nitrate may have been due to the fact that the model was only calibrated for conventional tillage and was not calibrated for no tillage management practices. Although there were no significant differences in simulated tile drainage and simulated leached nitrate between tillage treatments, a longer simulation period over several years might reveal more differences due to tillage based on apparent differences in simulated PET, ET, and runoff that occurred during the evaluation period in this study.

Model simulations of cover crop development for annual winter cover crop management practices could be improved by processes that allow soil water and nitrogen uptake to vary as biomass changes and increases from one growing season to the next, similar to that of perennial plants. The model simulates crop growth based on fixed plant parameters such as maximum nitrogen uptake and maximum root depth. The model cannot exceed these values in order for crop development to respond within a wider range of perturbations in soil water and nitrogen under various climatic conditions, which seem to occur in annual winter rye from one growing season to the next. A simulated crop production process that could respond in this way would be a valuable tool for simulating the effect of cover crop management practices on agricultural production worldwide.

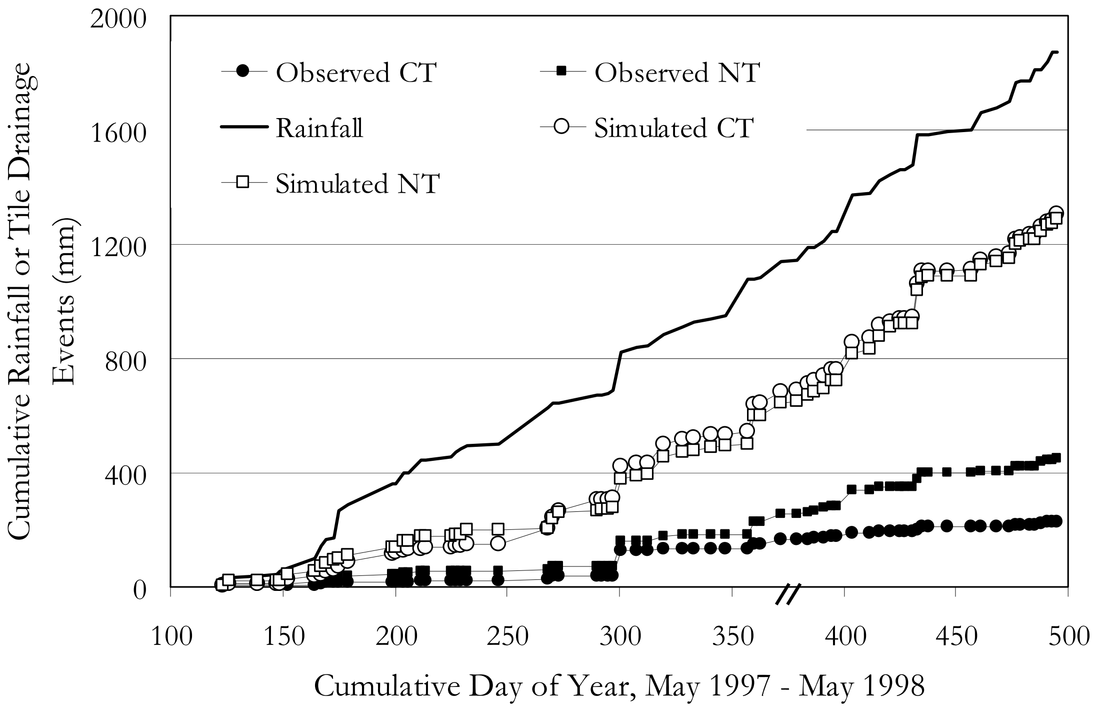


Fig. 2.1. Cumulative rainfall and simulated and observed tile drainage for the evaluation period.

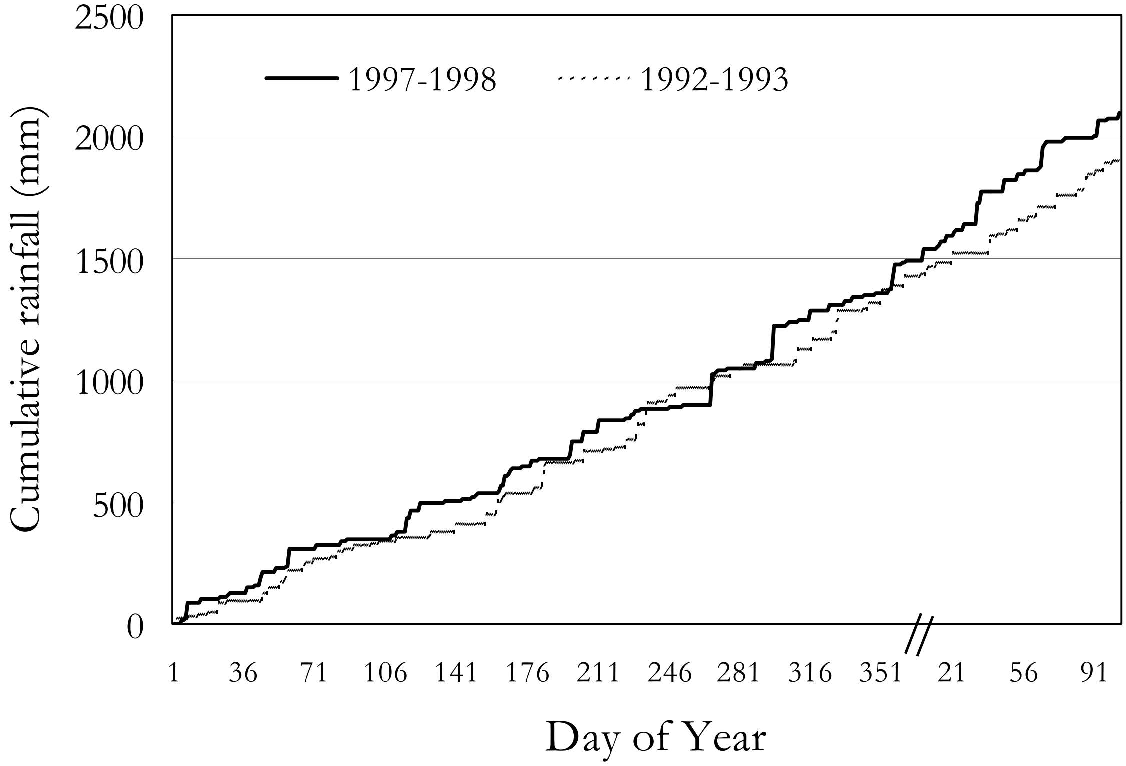


Fig. 2.2. Cumulative rainfall showing similar pattern and amount of rainfall for model calibration period for tile drainage in maize production 1 Jan 1992 through 13 Apr 1993, and for the current test of the model in cotton production during the same period from 1997 to 1998.

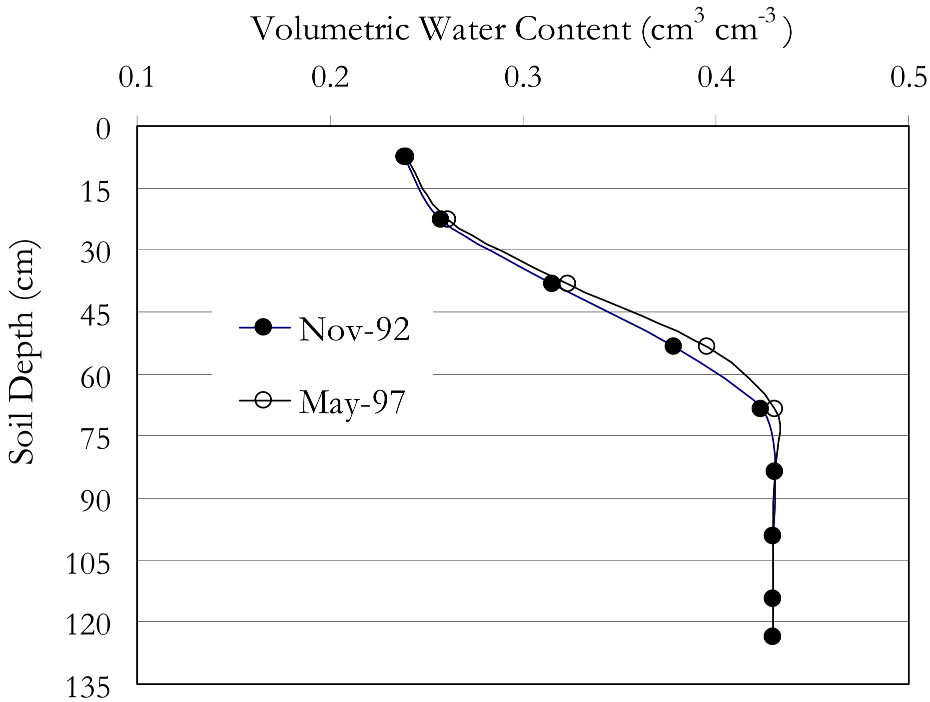
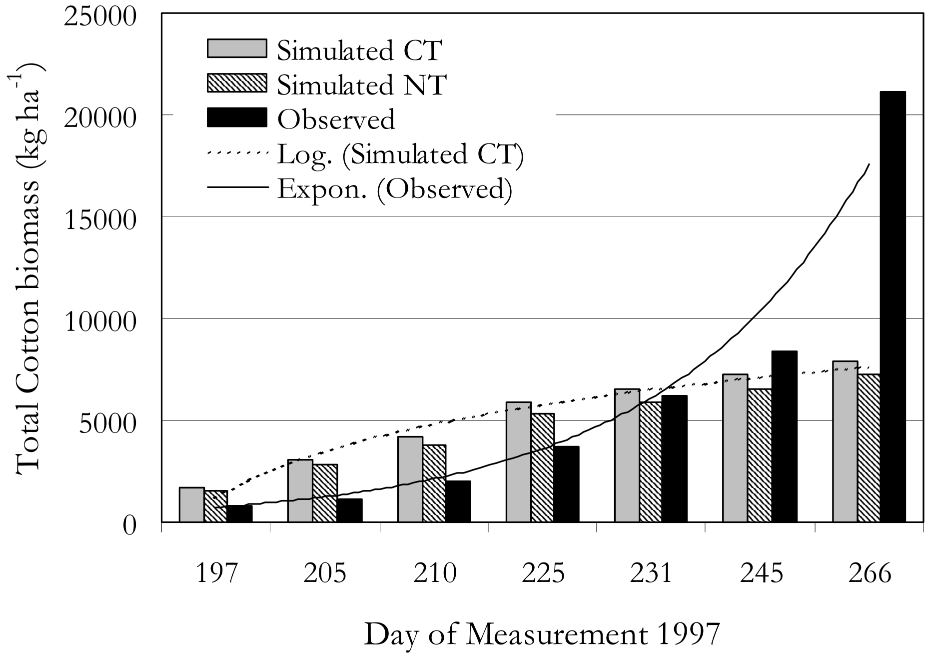


Fig. 2.3. Initial volumetric soil water content for the calibration simulation in Nov 1992 and for the current evaluation study in May 1997.



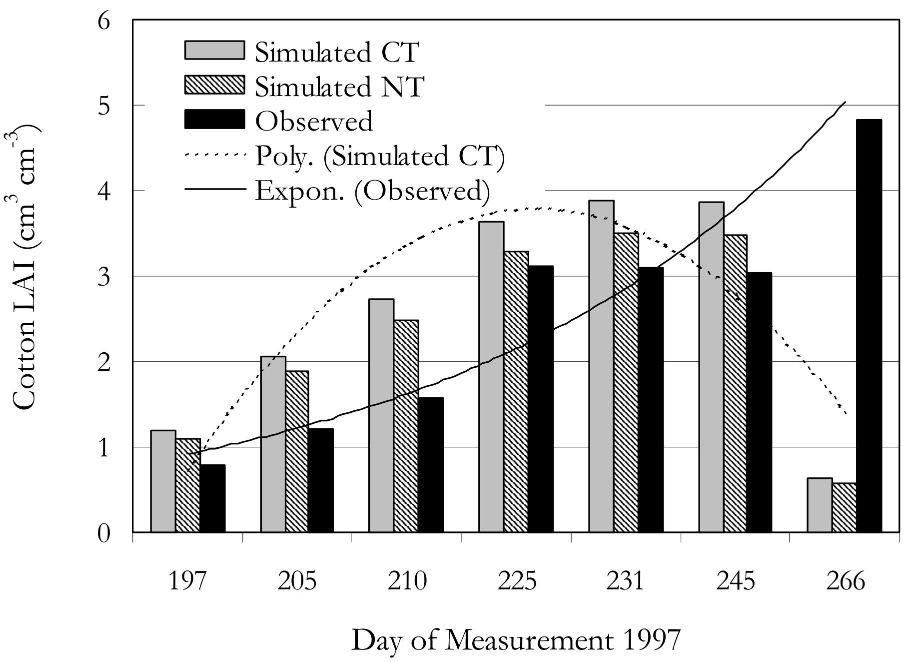


Fig. 2.4. a) Observed and simulated biomass development and, b) observed and simulated leaf area index for cotton in 1997. Observed data is from the field site that was used for calibration and simulated data is for the current study at the water quality site.

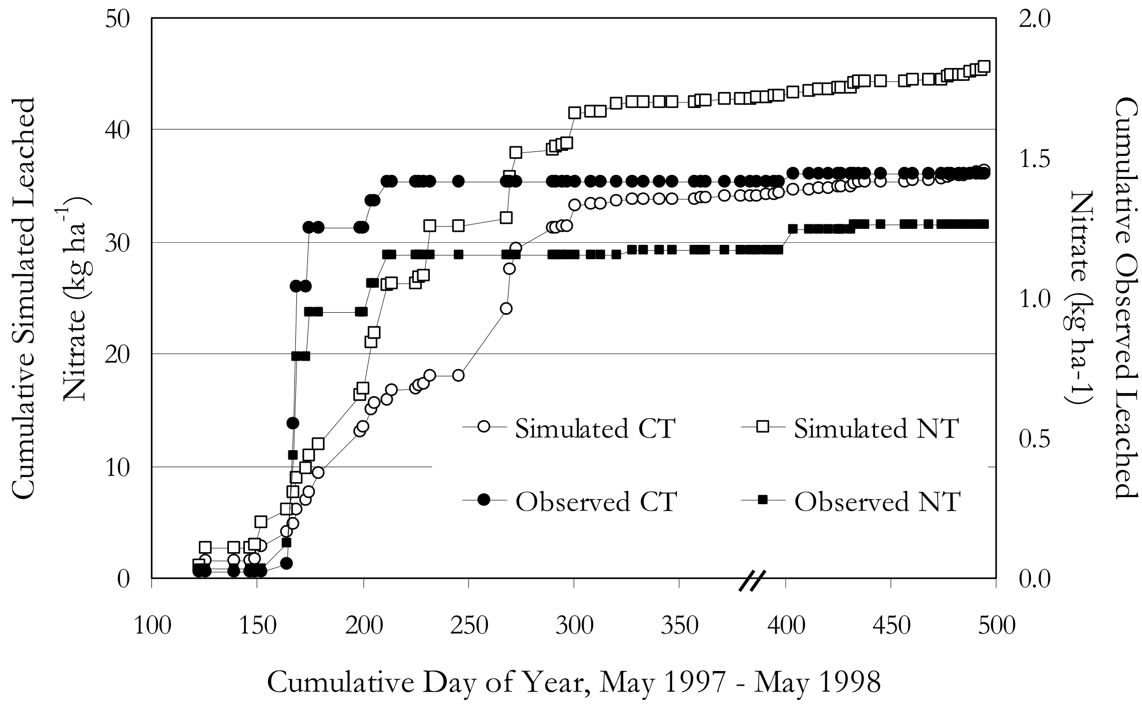


Fig. 2.5. Cumulative simulated leached nitrate on the left-hand axis and cumulative observed leached nitrate on the right-hand axis to show the correlation for the evaluation period.

Table 2.1 Statistics for measured and simulated CT and NT treatments for a) tile drainage and b) leached nitrate based on regression analyses for the evaluation period. Leached nitrate is log transformed for regression analysis.

(a)	Tile Drainage					
Treatment	Observed	Simulated	RMSE	r	Intercept	Slope
	--------- mm ---------					
CT	229	1303	8.4	0.65	-1.8 †	0.27 *
NT	448	1291	7.6	0.85	-2.4 **	0.48*

(b)	Leached Nitrate					
Treatment	Observed	Simulated	RMSE	r	Intercept	Slope
	-------- kg ha^{-1} --------					
CT	1.4	31.4	1.4	0.34	-2.2**	0.63†
NT	1.3	38.8	1.0	0.58	-2.5**	0.61†

RMSE, root mean square error; r, correlation coefficient; intercept and slope.

† Not significantly different from 0 at $p < 0.05$.

** Significantly different from 0 at $p < 0.05$.

* Significantly different from 1 at $p < 0.05$.

Table 2.2. Observed and simulated water balances for the evaluation period.

3 May 1997 to 9 May 1998						
	CT		NT		Observed minus Predicted	
Rainfall = 1805 mm	Obs	Pred	Obs	Pred	CT	NT
Component	------------- mm -------------				--- mm ---	
ET	861	579	861	548	282	313
Runoff	138	38	91	38	101	54
ΔSW50	-79	-121	-83	-114	42	31
ΔSW50_125	-	-40	-	-38	-	-
Drainage (Tiles)	229	1303	448	1291	-1074	-842
Deep Drainage	-	30	-	69	-	-
Balance	656	16	487	11	640	476
Deep Drainage + Tile Drainage	885	1333	936	1360	-449	-425

Table 2.3. Observed and simulated water balances for the cotton growing season in 1997.

Cotton Growing Season -14 May 1997 to 3 Oct 1997						
	CT		NT		Observed minus Predicted	
Rainfall = 547 mm	Obs	Pred	Obs	Pred	CT	NT
Component	------------ mm -------------				---- mm ----	
ET	512	459	512	440	53	72
Runoff	20	0	9	0	20	9
ΔSW50	-74	-22	-80	-26	-52	-54
ΔSW50_125	-	-7.4		-8.5	-	-
Drainage (Tiles)	35	254	60	241	-219	-181
Deep Drainage	-	-159		-113	-	-
Balance	53	23	46	12	31	34
Deep Drainage + Tile Drainage	88	95	106	129	-6	-22

CHAPTER 4

CONCLUSIONS

This study 1) evaluated the Root Zone Water Quality Model (RZWQM) for simulating tile drainage and nitrate leaching from maize and cotton production systems under conventional and no tillage agricultural management practices in Cecil soils of the Georgia Piedmont, 2) tested the sensitivity of simulated tile drainage and nitrate leaching to macroporosity in maize and cotton production systems, and 3) compared observed and simulated cotton development relative to cotton water use in conventional tillage versus no tillage management systems. The model accurately simulated tile drainage and leached nitrate in maize production under conventional tillage management practices with a winter rye cover crop during the calibration period. There were no significant differences due to the effect of macroporosity on simulated tile drainage or leached nitrate. This agrees with the measured data collected at the study site from intact soil cores that showed preferential flow in the Cecil soils occured mainly in the soil mesopore region and through infilled macropores rather than through open, distinct, or well-defined macropores. When the model was parameterized for cotton growth and development, the model could not simulate the large increase in biomass during the last twenty-one days of reproduction. This can be attributed to the fact that the model will not allocate carbon for leaf and stem biomass past the simulated vegetative stage. Cotton is an indeterminate crop and continues leaf production as part of its fruiting structures for cotton boll development into the reproductive stage. However, the average differences between simulated and observed cotton water use were less than 0.15 mm d^{-1} based on development during the critical water use period from first square until peak bloom, and less than 0.3 mm d^{-1} during the critical peak bloom period. This indicates that the model accurately simulated water use during the calibration period, and could satisfy the objective to test the calibrated model with an independent dataset based upon a water balance analysis for simulation of tile drainage and leached nitrate in cotton production and winter rye cover cropping practices.

The RZWQM accurately simulated tile drainage and leached nitrate during the calibration study from 1991 through 1993 at the water quality study site while in maize production with a winter rye cover crop under conventional till management practices. The model did not accurately simulate the volume of tile drainage and leached nitrate for the evaluation period in the current study after the study site was converted to cotton production with a winter rye cover crop under conventional and no tillage management practices in 1997 and 1998. However, total drainage was reasonably well simulated during the cotton growing season based on our analyses of the simulated and observed water balances for the period. The differences in simulated and observed tile drainage and leached nitrate appeared to be due to 1) the under estimation of simulated ET for the cotton and winter rye crops and, 2) the differences in the amount of soil water and soil nitrogen available for tile drainage and nitrate leaching at the study site compared to the period when the model was calibrated due to continuous winter cover cropping practices that have been used at the study site since that time. The over estimation of tile drainage was also due to the fact that the bottom boundary of the soil profile as it was designed in the model for the calibration scenarios did not work well for the evaluation period in the current study. The model simulated a perched water table that partitioned water between tile drainage, runoff, ET, and soil water storage based on a 1.25 m soil profile. In the field study, less water was available at the depth of the tile drains and drained to below 1.25 m in the soil profile.

Model simulations of cover crop development for annual winter cover crop management practices could be improved by processes that allow soil water and nitrogen uptake to vary as biomass changes and increases from one growing season to the next, similar to that of perennial plants. The model simulates crop growth based on fixed plant parameters such as maximum nitrogen uptake and maximum root depth and cannot exceed these values in order for a crop to respond to various perturbations in soil water and nitrogen such as those that may occur in annual winter rye from one growing season to the next.

There were no differences due to tillage in simulated tile drainage or leached nitrate by the model. However, there were apparent differences in simulated ET and PET due to tillage treatments. This indicates that the model is responding to the effects of conventional tillage compared to no tillage management practices, and for longer simulation periods, the RZWQM may accurately explain the effects of tillage on processes such as tile drainage and leached nitrate in the southern Piedmont.

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APPENDIX A

A1. Physical properties of the 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 dia. 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	Macro-porosity
	--- cm ---	--- cm ---	cm h^{-1}	------- g cm^{-3} -------			--- cm ---	-------- % -------			------- cm -------		%
1	1-5	1-7	18	2.64	1.34	Ap	0-21	78	15	7	0-20	0.014	0.014
2	5-15	6-12	20	2.65	1.56			78	15	7		0.020	0.020
3	15-25	17-23	8	2.72	1.69	BA	21-26	43	20	37		0.020	0.020
4	25-35	27-33	18	2.72	1.43	Bt1	26-102	30	20	50	30-45	0.020	0.020
5	35-65	57-63	10	2.65	1.37			30	20	50		0.025	0.025
6	65-95	87-93	2.6	2.65	1.51			30	20	50	45-60	0.025	0.025
7	95-125	127-133	0.2	2.65	1.55	Bt2	102-131	34	25	41		0.025	0.025

A2. 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 Water Content						Brooks-Corey parameters	
	Depth	--------------- $cm^3\ cm^{-3}$ @ kPa ---------------					Ks	h_a	λ
Soil Layer No.	cm	Saturation	10	30	100	1500	$cm\ h^{-1}$	kPa	Fraction
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

A3. Initial soil temperatures and field capacity volumetric water content on 1 Jan 1996 used for model calibration.

	Depth	Soil Temperature	Water Content
Soil Layer No.	cm	ºC	$cm^3\ cm^{-3}$
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

A4. Soil nutrient parameters with units per gram of soil as used in model. Data compiled from Franzluebbers (personal communication, 2001) and Johnson et al. (1999).

	Depth	Total Organic C	Fast Residue	Humus			Aerobic heterotrophs	Autotrophs	An-aerobic heterotrophs	NO_3-N	NH_4-N
				Fast	Transition	Stable					
Soil Layer No.	cm	ug g^{-1}	---- ug C g^{-1} ----				---- # orgs g^{-1} ----			ug N g^{-1}	
1	5	6960	1044	1044	2088	2784	1083000	285000	285000	2.85	1.58
2	15	5800	725	725	2030	2320	632700	161500	161500	2.85	1.58
3	25	4060	406	406	1624	1624	383800	76000	76000	2.85	1.58
4	35	3480	261	261	1218	1740	273600	57000	57000	2.50	1.11
5	65	2900	145	145	870	1740	228000	47500	47500	2.50	1.00
6	95	2320	116	116	696	1392	182400	38000	38000	3.22	1.38
7	125	2320	116	116	696	1392	146300	28500	28500	3.22	1.38

A5. Management options for all crops used in model calibration.

	Planting Date				Fertilization
Crop	1991	1992	1997	Tillage operation(s)	(kg ha^{-1})
Maize	24 Apr	24 Apr	-	Moldboard Plow Tandem disk	168
Winter Rye	18 Oct	30 Oct		Row planter/coulter	-
Cotton	-	-	16 May	Moldboard Plow	66

A6. 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 et al., 2000), and were also used for calibrating maize and cotton for the current study. Values for ranges taken from model recommendations for maize.

Parameter	Definition	Value range	Units
μ_1	Maximum active nitrogen 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
-	Nitrogen sufficiency index – trigger for timed application of fertilizer	0 - 1	-
-	Luxurious nitrogen uptake factor – increases or reduces uptake	0 - 1	-

A7. 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

APPENDIX B

Tile drainage is implemented in the RZWQM by the Hooghoudt equation as applied by Skaggs (1978), with drain flux, q, defined as:

$$q = S_d (z', t) = 8 K_e d_e m + 4 K_e m 2 / L 2 \Delta z \; ; \; \omega > d$$

where $S_d (z', t)$ = flux or point sink term for tile drainage which is included in the point sink term, $S(z, t)$ along with the distributed sink due to root uptake, $S_r (z', t)$ for subtraction from the Richards equation, z' = depth of the drain, t = time (hr^{-1}), K_e = effective lateral hydraulic conductivity (cm hr^{-1}), Δz = soil depth increment at z', m = water table height above the drain, and ω is the distance from the water table to the bottom of the restricting layer. The effective lateral saturated hydraulic conductivity, K_e, is calculated as:

$$K_e = K_{sj} t_j + \sum K_{si} T_i / t_j + \sum T_i$$

where the subscript i represents the i^{th} soil horizon and j represents the horizon where the water table is currently located, K_{si} = saturated hydraulic conductivity in horizon i, T_i = thickness of layer i; and t_j = depth of the water table to the bottom of horizon j, where the water table is in horizon j.

To correct for the two-dimensional effects of tile drainage by estimating the flux at the center point between two parallel drains, an equivalent depth, d_e, is calculated according to Moody (1967) as:

$$d_e = d / 1 + d / L (8 / \pi \; \ln (d / r_e) - a)$$

for:

$$L / d > 3 \text{ where } \alpha = 3.55 - 1.6 \text{ x } d / L + 2 (d / L)^2$$

and:

$$d_e = L\pi \ / \ (8\ (\ln\ (L\ /\ r_e) - 1.15\ )$$

for L / d < 3

where d_e = equivalent depth from the drain to the bottom of the restrictive soil layer, d = distance from the drain to the bottom of the restrictive soil layer, L = distance between the drains, r_e = effective drain radius defined as the radius such that a completely open drain tube with radius r_e will offer the same resistance to inflow as a real tube with radius, r (Skaggs, 1978). All units are in cm.

APPENDIX C

C1. Parameters used for cotton in generic plant growth submodel. Physical parameters from Schomberg et al., (2004) and physiological parameters from Carns and Mauney, (1968).

Physical Parameters						
Root Depth	Stem diameter	Stem height	Above-ground biomass when height=1/2 max height	4-Leaf stage	Mature	LAI max
cm			g $plant^{-1}$			cm^3 cm^{-3}
100	60	112	23	10	244	5.0

Phenological / Physiological Parameters							
Air temperature for plant growth º C			Days spent transecting growth stage				
Max	Min	Optimum	Germ.	Emergence	4-Leaf	Vegetative	Reproductive
40	16	21	3	3	7	115	40