ASSESSMENT AND IMPROVEMENT OF NITROGEN CYCLING IN SWAT

A Dissertation

by

ELIZABETH BROOKE HANEY

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Chair of Committee,	Raghavan Srinivasan
Committee Members,	Scott Allen Senseman
	Jay Angerer
	Jaehak Jeong
Head of Department,	Kathleen Kavanagh

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ABSTRACT

The Soil and Water Assessment Tool (SWAT) has been successfully used to predict alterations in streamflow, evapotranspiration and soil water. Previous research suggests that while the hydrologic balance in each watershed is accurately simulated with SWAT, the SWAT model over- or under-predicts crop yield relative to fertilizer inputs. The SWAT model previously contained three N simulation submodels: (1) basic; (2) N routines derived from the CENTURY model (SWAT-C); and (3) a one-pool C and N model (SWAT-One). We used the measurement of microbial activity coupled with the measurement of water-extractable N and C to add a flush of N after rainfall events to create a fourth N cycling option in SWAT (SWAT-flush). SWAT-flush was compared to soil-biological properties and the natural difference vegetative index on a wheat field in Temple, TX, to examine the sensitivity of SWAT-flush to field conditions and found it improved over basic SWAT.

Crop yields from a long-term experiment in Lahoma, OK, managed by Oklahoma State University were compared to wheat yield predicted by the four sub-models. Weather data obtained from the Lahoma research station were used to analyze the impact of precipitation and temperature on simulated and actual yields. Nitrogen use efficiency was analyzed as well as gains in yield relative to fertilizer applications for simulated and actual yields.

Actual crop yields were not significantly different from year to year nor for fertilizer treatments above 22.4 kg N ha^{-1}. Field crop response to fertilizer additions from year to year was highly variable. SWAT-C simulated average yields were closer than other N sub-models to average actual yield. Annually there was a stronger correlation between SWAT-flush and actual yields than the other submodels. None of the N-cycling routines could accurately predict annual variability in yield at any fertilizer rate. I found that SWAT-C and SWAT-flush are the most viable choices for accurately simulating long-term average wheat yields, although annual variability in yield prediction should be taken into consideration. Further research is needed to determine the effectiveness of SWAT-C and SWAT-flush in determining average and annual yield in various farming regions and with numerous agronomic crops.

DEDICATION

I dedicate this dissertation work to my family and friends, especially my two precious daughters, Maggie and Mollie. You two are the light in my life and bring me an immense joy I never even knew was possible. I could not have done this work without my admirable, fantastic and spirited husband of 15 years. You are my soul mate. I love you all beyond measure.

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Thanks to my family and friends who have helped and encouraged me along the way. Thank you to my Mom, Margaret, and Dedrae for listening to me for countless hours, for feeding me and my family, providing encouragement, and fooling me into thinking I am smart and brave.

I would like to thank my committee chair, Dr. Srinivasan, and my committee members, Dr. Senseman, Dr. Angerer, Dr. Jeong, Dr. Arnold, and Dr. White, for their guidance and support throughout the course of this research. Thank you also Dr. Haney for your direction and support.

Most importantly, thank you God. You are the Way and the Light.

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Contributors

This work was supervised by a dissertation committee consisting of Professors Raghavan Srinivasan [advisor] and Jay Angerer of the Department of Ecosystem Science and Management, Professor Jaehak Jeong, and Adjunct Professors Jeffery Arnold and Michael White of the Department of Biological and Agricultural Engineering.

Portions of data in Chapters 1 and 2 were provided by Dr. Richard Haney of the United States Department of Agriculture, Agriculture Research Services. The field data analyzed for Chapters 2 and 3 were provided by Professor William R. Raun of the Department of Plant and Soil Sciences at Oklahoma State University.

All other work conducted for the thesis (or) dissertation was completed by the student independently.

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CHAPTER I

INTRODUCTION AND LITERATURE REVIEW

Globally, through the production and use of N fertilizer, we have altered the Earth's N cycle affecting issues that range from global climate change to oceanic hypoxic zones. Nitrogen use in the world is so significant that the Haber-Bosch synthesis of ammonia from atmospheric N is responsible for nearly 2% of global energy consumption (European Commission, 2013). The production of N fertilizer has allowed for a drastic increase in yields, providing food for a growing human population that doubled to 6 billion in 50 years (Steffen et al., 2007).

As of 2011, when the latest National Land Cover Dataset (NLCD) was made, 1,252,997 km^2 of land in the conterminous US was classified as cropland (USGS, 2011). In many parts of the United States, N and P inputs to these agricultural lands are said to the be the primary nonpoint sources of pollution, including the Upper Mississippi River Basin (Jha et al., 2013). For lawmakers, environmental decision makers and scientists to identify and mitigate nonpoint source additions of N and P, one must be able to accurately predict N cycling in the environment and, in turn, accurately predict crop yield in response to mitigation efforts.

The Soil and Water Assessment Tool (SWAT) is a watershed scale model that was developed to predict the impact of land management practices on water, sediment and agricultural chemical yields in large complex watersheds with varying soils, land use, and management conditions over extended periods of time (Arnold et al., 2012).

The origins of the SWAT model trace back to the Chemicals, Runoff, and Erosion from Agricultural Management Systems (CREAMS) model, the Groundwater Loading Effects on Agricultural Management Systems (GLEAMS) model, and the Erosion Productivity Impact Calculator (EPIC) model, which were created by the USDA-ARS (Gassman et al., 2007). SWAT incorporates specific information about weather, soil properties, topography, vegetation, and land management practices occurring in the watershed (Neitsch et al., 2009), making it particularly suitable for assessing the effect of agricultural practices on crop production.

The minimum data required to run SWAT are commonly available from government agencies. The physical processes associated with land use, hydrology (water balance), erosion, plant growth, nutrient fate and cycling, carbon balance, flood routing, etc. are directly modeled by SWAT using this input data. Simulation of very large basins or a variety of management strategies under fluctuating climatic conditions can be performed without excessive investment of time or money because SWAT is computationally efficient. SWAT enables users to study long-term impacts, such as anthropogenic changes to the landscape and nutrient cycling that may beneficially or adversely affect an ecosystem. For example, SWAT has been used to model climate change and nutrient loading in the United States, Germany, the Czech Republic, and Canada (Jha et al., 2013; Kyrsanova et al., 2005; Martinkov et al., 2011; Shrestha et al., 2011; Ye and Grimm, 2013). The impact of climate change on crop growth and yield has recently been studied using SWAT in the Black Sea, Iran, India, China, and regions of the United States (Bar et al., 2014; Bhuvaneswari et al., 2013; Vaghefi et al., 2013;

Vaghefi et al., 2014; Wang et al., 2011; Xie et al., 2008). The SWAT model allows for crop growth simulation under nutrient limited scenarios, accounts for variations in soil properties, and allows flexibility in user inputs such as planting and harvest dates, and conservation practices. For example, the Conservation Effects Assessment Project (CEAP), which the SWAT model supports, has been utilized to determine the environmental impact of conservation practices in major watersheds throughout the conterminous US.

While SWAT has been successfully used to predict watershed processes, it was not clear how effective or accurate SWAT is at predicting crop growth or N cycling in the soil. Many N mineralization models, including EPIC, on which the N-cycling in SWAT is based, are founded on the PAPRAN (Production of arid Pastures limited by RAinfall and Nitrogen) model (Lauenroth et al., 1983; Neitsch et al., 2009, Matthews and Stephens, 2002; Seligman and van Keulen, 1981; Williams et al., 1995). The PAPRAN model was developed for high input agricultural systems and was not structured for no-till or conservation tillage systems where residue is not incorporated into the system (Matthews and Stephens, 2002). The PAPRAN model considers two sources of mineralization, fresh organic N associated with crop residue and microbial biomass and the stable organic N associated with the soil humic fraction. In general, these mineralization processes consider the C:N ratio of the soil, temperature, soil water content and sometimes soil C:P ratios. Mineralization is estimated as a function of organic N weight, soil water, and temperature.

Three major forms of N in soils are organic N associated with humus and the microbial biomass, mineral forms of N held by soil colloids, and N in solution. Nitrogen is added to the soil by fertilizer, rain, manure, residue, mineralization by the microbial biomass and fixation by bacteria. It is removed from the soil by leaching, plant uptake, volatilization, denitrification, and erosion. The main N pools represented in various models can consist of any combination of fresh or residue pools and stable and active organic nitrogen pools which feed into the inorganic nitrogen fraction. The SWAT model consists of three organic N pools (active, stable and residue or fresh) and two inorganic N pools (NO_3^- and NH_4^+). The amount of N initially placed in each pool can be based on theoretical soil C and N relationships rather than requiring confirmatory data. These theoretical associations consist of general relationships, which may or may not be reflective of soil and management conditions.

Organic N numbers are assigned assuming that the C:N ratio for humic materials is 14:1. The concentration of humic organic nitrogen is determined based on the SOC values for the soil from soil survey data. Then, the SWAT model determines the amount of organic nitrogen in the soil that should be designated to the active and stable nitrogen pools by assigning 20% of the organic N to the active pool and 80% of the organic N to the stable pool (Neitsch et al., 2009). After initialization, the residue pool is determined based on simulated management practices. The N resulting from decomposition and mineralization of the residue during simulation is added to the active organic and plant-available pools, respectively. Decomposition and mineralization in SWAT are dependent upon the decay rate of the plant, the C:N ratio of the residue in the soil layer, and soil temperature and water factors. SWAT arbitrarily assumes that 20% of the residue decomposed will be added to the active or humic N pool and the remaining 80% is considered mineralized and added to the NO_3^- pool.

In the field, immobilization and mineralization are controlled by microbial activity in the soil. Bacteria decompose organic material to obtain energy. Plant residue is broken into glucose to be used for protein synthesis, which requires N. If the residue containing the glucose contains enough N to meet the demand for protein synthesis the bacteria will use N from the organic material, resulting in mineralization of N. If there is not enough N to meet bacterial demand, the bacteria will use inorganic N from soil solution to meet the needs for protein synthesis, resulting in immobilization. If the N content of organic matter exceeds the needs for bacterial demand, mineralization occurs. The decomposition and mineralization routines in SWAT do not account for the effect of the fungal and bacterial population in the soil which controls these processes and is estimated to account for 250 to 900 kg C/ha depending upon the soil (Doran, 1987). We must attempt to replicate the influence the microbial biomass has on N cycling since it is the main driver of N cycling and soil fertility, ultimately influencing crop yield.

Nitrification and volatilization involve the conversion of NH_4^+ to either NO_3^- or NH_3, respectively. SWAT simulates both processes simultaneously then partitions the values between the two processes (Nietsch et al., 2009). The nitrification process in SWAT depends solely on the soil water and temperature factors. While temperature and moisture are critical forcing factors on the nitrification process, SWAT does not account for soil microbial activity, the pH of the soil, nor the water-extractable C or N content of the soil, which is the food source for the microbial population. Volatilization simulation in SWAT is dependent upon soil temperature and depth and includes a default cation exchange factor. In the field, volatilization is also strongly pH dependent and is affected by wind conditions and soil clay content and type. Currently, wind is not simulated in SWAT.

In recent years the technological base has increased to where we now have the power to observe microbiological processes in the soil, such as mineralization, on more localized physical and temporal scales. Microbes exist in soil in great abundance and their composition, adaptability, and structure are a result of the environment they inhabit. Microbes have adapted to the temperature, moisture levels, soil structure, crop and management inputs, as well as soil nutrient content. Since soil microbes are driven by their need to reproduce and by their need for acquiring C, N, and P in a ratio of 100: 10: 1 (C: N: P), it is safe to assume that soil microbes are a dependable indicator of N-cycling in the soil (Franzluebbers et al., 1996). It is well established that C is drives the soil nutrient-microbial recycling system (Paul and Juma, 1981; Tate, 1955; Bengtston et al., 2003) and the consistent need for C and N sets the stage for a standardized, universal measurement of soil microbial activity. Since soil microbes take in oxygen and release CO_2, we can couple this mechanism to their activity. It follows that soil microbial activity is a response to the level of soil quality/fertility in which they find themselves.

In addition to the usual standard components of mineralization and immobilization processes accounted for in modeling (C:N ratio, soil water and temperature), we can now also assess a real-time snapshot of the active microbial population using a measurement of microbial respiration. The measurement of microbial activity, coupled with the measurement of their food source, water-extractable N and C, which are broken down by soil microbes and released to the soil in plant available inorganic N forms, provide the initial N values and the mineralization rate necessary to model N cycle.

Haney et al. (2012) found that soil microbial activity measured as the flush of 1-d CO_2 following rewetting of dried soil was significantly correlated to water-extractable organic C (WEOC) and water-extractable organic N (WEON). Short-term C respiration from soil after drying and rewetting is also highly correlated with soil microbial biomass C and 24-d N mineralization (Haney et al., 2012). The laboratory drying and rewetting (D/R) process mimics the natural processes in the field that occur with rainfall events, the extent of which depends upon climatic and soil conditions. The mineralization of C and N following drying/rewetting can be used to quantify the portion of the soil microbial biomass that is most responsive to rainfall events, which can have a strong impact on nutrient availability (Franzluebbers et al., 2000). Specifically, every time it rains and the soil gets wet to a certain degree of field capacity, microbes activate, reproduce, eat long-chain organic molecules containing C, N and P, and in the process, convert organic N to plant available N. Given that soil microbes drive N mineralization, 1-day CO_2 evolution after D/R may be used to simulate the soil's ability to supply N (Haney and Haney, 2010). It is important to simulate a complete D/R cycle in order to mimic the natural D/R in the field. During a succession of drying and rewetting events in the lab, a uniform pattern of CO_2 evolution was exhibited, simulation which occurred under field conditions (Birch, 1958). Birch (1959) postulated that the common feature between the evolution of CO_2 and N mineralization after drying/rewetting soil was microbial death and subsequent mineralization. These studies suggest that physical alteration of the soil was not a primary factor for the mineralization of C and N. Much of the mineralization of C and N after rewetting dried soil is likely due to the death of heat susceptible microbes, death from water induced osmotic shock, and further renewal of the microbial population, and consumption of the organic C and N source.

Schimel and Bennett (2004) make a compelling case for rethinking our approach to estimating N mineralization by also considering the contribution of N from the water-soluble organic N pool. The model considers the basic C:N relationship that exists in organic matter and simulated the WEON pool as being accessed directly by the microbes and in proportion to microbially active C (MAC). For example, if microbes release 25% of the C through respiration, 25% of the WEON pool will be released as well.

Soil moisture is a determining factor in microbial activity and the corresponding release of nutrients. By using the field capacity of the soil as a gauge for microbial activity we are accounting for the spatial variability in the physical attributes of the soil. The movement of water in soil is dependent on the combined effects of porosity, gravity, mass flow, and capillary action. Soil porosity is influenced by texture, structure (e.g., degree of aggregation), and organic-matter content. For example, coarse-textured soils have larger pores than fine-grained soils, which allow for more water flow. Organic matter greatly increases the water-holding capacity of a soil. Capillary action is the natural movement of water using adhesion (attraction to solids) and cohesion forces (attraction between water molecules) and is counterbalanced by the effects of gravity and air pockets. Haney et al. (2008) indicated that microbial activity studies that involve D/R soils use gravimetric water content, soil matric potential, or percentage of water-filled pore space (WFPS) to achieve sufficient moisture content for peak microbial activity. Furthermore, Haney et al. (2008) indicate that a range of 30 to 70% WFPS is sufficient for peak microbial activity, which represents roughly 50% of field capacity (Haney et al., 2004).

The specific objectives of this study are to (1) develop a model to incorporate the flush of N after rainfall events into the SWAT model utilizing field soil-test data and examine its ability to detect variations in soil and plant conditions compared to the basic SWAT model; (2) determine if soil organic C can be used as a proxy for actual soil test data in SWAT with the addition of the N flush after rainfall events (SWAT-flush); (3) examine controlling factors determining actual and simulated winter wheat yields from a long-term wheat study; and (4) assess the ability of various N cycling sub-routines within SWAT to predict yield at a long-term fertilizer study in Oklahoma.

CHAPTER II

SPATIAL ANALYSIS AND MODELING OF N AT THE FIELD SCALE USING THE N FLUSH AFTER RAINFALL EVENTS IN SWAT*

Introduction

All the major components of environmental modeling have spatial distributions and these distributions affect biogeochemical processes. A geographic information system (GIS) is a valuable tool in describing the spatial characteristics of the environment, while environmental modeling simulates the environmental processes affected by the spatial distribution (Rao et al., 2000). Models can be used on a large scale to shape policy, like the Conservation Effects Assessment Program (CEAP) Hydrologic Unit Model for the United States/Soil Water Assessment Tool (HUMUS/SWAT) model. The HUMUS system improves on existing technologies for making national and regional water resource assessment considering both current and projected management conditions. The HUMUS system is conducted at the watershed scale using a Geographic Information System (GIS) to collect, manage, analyze and display the spatial and temporal inputs and outputs, and relational databases for managing the non-spatial data (Arnold et al., 2010). Other models, such as CENTURY, were developed to analyze long-term changes in N and C in soil in various ecosystems

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on a farm or regional scale (Metherell et al., 1993). On a field, farm or small watershed scale, the Agricultural Policy/Environmental Extender Model (APEX) simulates N dynamics with varying land management strategies, such as different nutrient management practices, tillage operations, and alternative cropping systems.

Many nitrogen mineralization models, including the Environmental Policy Integrated Climate Model (EPIC), on which the N cycling in SWAT is based on, are based on the PAPRAN (Production of Arid Pastures limited by RAinfall and Nitrogen) model (Lauenroth et al., 1983; Neitsch et al., 2009; Matthews and Stephens, 2002; Seligman and van Keulen, 1981; Williams, 1995). The PAPRAN model considers two sources of mineralization, fresh organic N associated with crop residue and microbial biomass and the stable organic N associated with the soil humic fraction. In general, these mineralization processes consider the C:N ratio of the soil, temperature, soil water content and sometimes soil C:P ratios. Mineralization is estimated as a function of organic N weight, soil water, and temperature. The incorporated PAPRAN model does not account for the contribution of the microbial population to the plant available N pool, resulting in an under-estimation of yield and possible over- or under-estimation of N runoff from natural systems and agricultural landscapes that are not conventionally tilled. We must accurately assess the microbial biomass and their activity since they are the main drivers of N cycling and soil fertility in general (Figure 1).

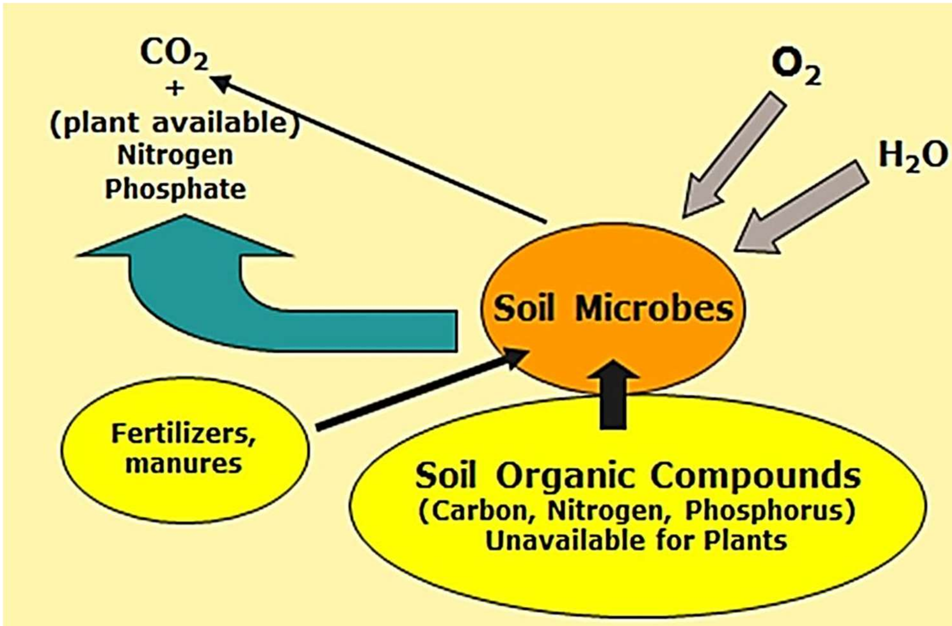

Figure 1. Soil microbes acting on soil organic matter to release N.

Over the years our technological capabilities have increased and now we can observe microbiological processes in the soil on more localized physical and temporal scales. Microbes exist in soil in great abundance and their composition, adaptability, and structure are a result of the environment they inhabit. Microbes have adapted to temperature and moisture levels, soil structure, crop and management inputs, as well as soil nutrient content. Since soil microbes are driven by their need to reproduce and by their need for acquiring C, N, and P in a ratio of 100: 10: 1 (C: N: P), it is safe to assume that soil microbes are a dependable indicator of N cycling in the soil (Franzluebbers et al., 1996). It is well established that C is the driver of the soil nutrient-microbial recycling system (Paul and Juma, 1981; Tate, 1995; Bengtston et al., 2003). The consistent need for C and N sets the stage for a standardized, universal measurement of soil microbial activity. Since soil microbes take in oxygen and release CO_2, we can couple this mechanism to their activity. It follows that soil microbial activity is a response to the level of soil quality/fertility in which they find themselves and we can now also assess a real-time snapshot of the active microbial population using a measurement of microbial respiration.

The measurement of microbial activity, coupled with the measurement of their food source, water-extractable N and C, which are broken down by soil microbes and released to the soil in plant available inorganic N forms, provide the initial N values and the mineralization rate necessary to modify N cycling routines. Using soil test data and spatial analysis N mineralization values are determined based on the relationships between water-extractable N and C as well as microbial activity.

The objective of this study was to: (1) quantify spatial variation of water-extractable organic and inorganic N, soil inorganic N, and microbial activity using updated soil-testing methods; (2) develop a field scale model to determine N mineralization for integration into the SWAT model; (3) use GIS to collect and analyze spatial and temporal inputs and outputs; and (4) predict wheat yield based on objectives 1, 2, and 3.

Materials and Methods

Research was conducted at a research field at the United States Department of Agriculture, Agricultural Research Service (USDA/ARS) Facility in Temple, Bell County, TX (31° 09' 09 ", -97° 24' 28", elevation: 205 m) in the Texas Blackland Prairies ecoregion. The climate is humid subtropical with a mean annual temperature of 19ºC and mean annual precipitation of 886 mm. Rainfall occurs year-round with hot summers and moderate seasonality. The field where the study was conducted consists of 33.6 ha that has been in consecutive cover/cash crop rotation for 5 years. Cash crop rotations consist of wheat and sorghum. Cover crops consist of a mixture of legumes and forbs. Soils consist of Austin Silty Clay 1 to 5% slopes and Houston Black Clay 1 to 3% slopes (Figure 2). At the time of sampling, the entire field had been planted in cover crops consisting of a mixture of legumes and forbs. The cover crop had not fully emerged, leaving sizable portions of the field that were either bare or covered with residue. The last three crops grown on the field were wheat in winter of 2011 and sorghum in the summers of 2012 and 2013.

All GIS analyses were conducted using ArcGIS 10.0. (ESRI, 2011). Information extraction and spatial analyses were performed using ArcGIS 10.0. Daily weather data were obtained from the weather station located at the USDA-ARS, Grassland, Soil and Water Research Laboratory in Temple, TX (www.ars.usda.gov/Research/docs.htm?docid=9697). Data include maximum and minimum air temperature, and total precipitation. Daily weather data were utilized to perform model runs on a daily time step to determine yield from the field of study from 1980 to 2004. The model was validated using weather data from 2011 and 2012. Weather data are used in the model to predict the daily fluxes of N as well as plant growth for yield simulation.

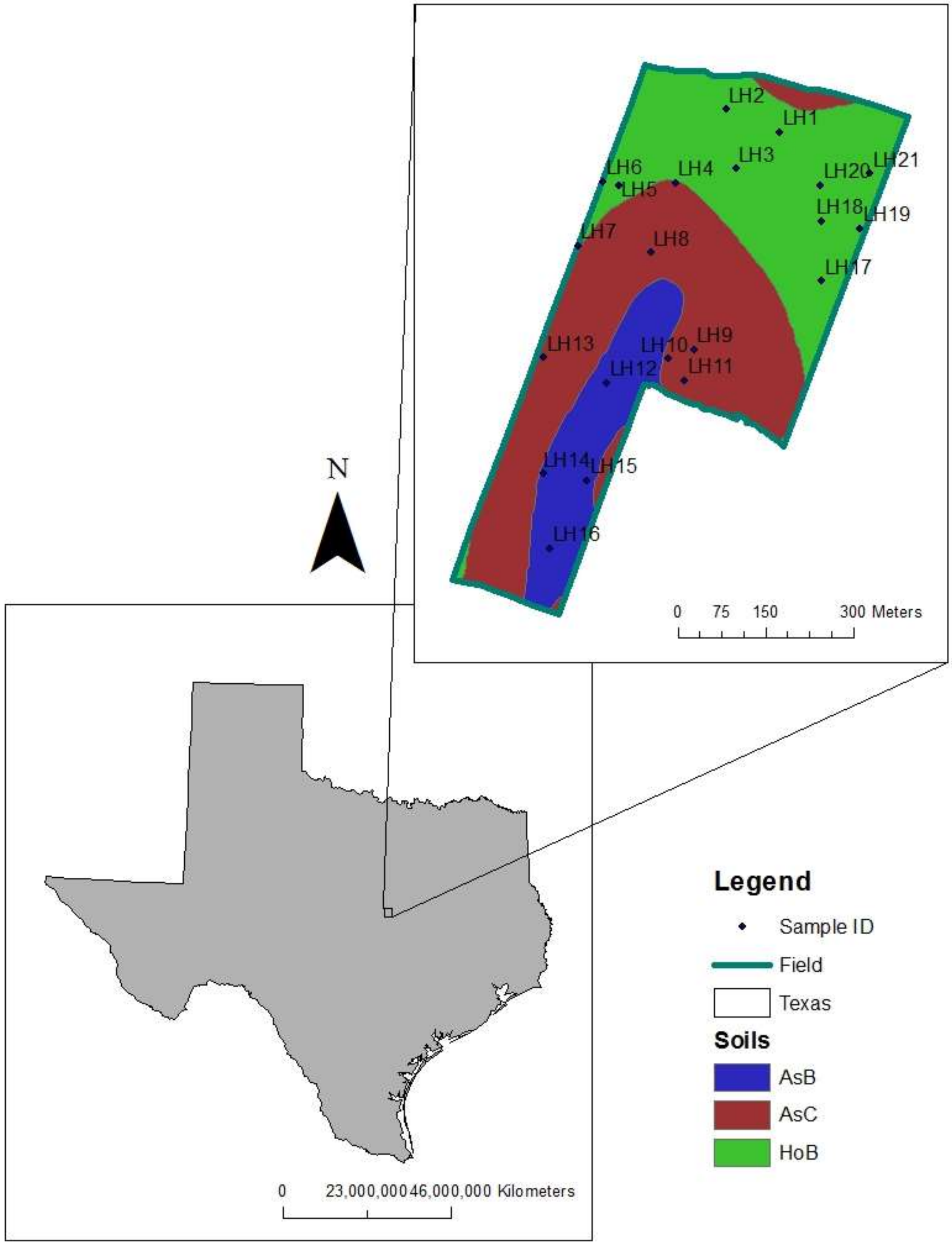

Figure 2. Soils within field of study.

The digital elevation model used for analyses is from the National Aeronautics and Space Administration (NASA) Shuttle Radar Topography Mission (SRTM) and was obtained from United States Geological Survey (USGS) Earth Explorer (earthexplorer.usgs.gov). Elevation models were arranged into tiles covering a degree latitude and longitude with an arcsecond or 30 m resolution. The data used are void filled using primarily Advanced Spaceborne Thermal Emission and Reflection Radiometer Global Digital Elevation Model version 2 (ASTER GDEM2) and secondly the USGS National Elevation Dataset. The SRTM digital elevation model (DEM) was used to develop 2 m elevation contours for determining soil samples locations. Contours were constructed using the Contour toolset in ArcGIS 10, ArcToolbox.

Soil sample points at least 100 m apart were randomly chosen based on 2m elevation contours as the constraining feature class (create random points) resulting in 21 points for the entire field. Soil samples from the top 15 cm of the upper soil profile were obtained at each sample point. The top 15 cm of soil were chosen since the majority of N cycling occurs at this depth. Each soil sample was dried at 50° C, ground to pass a 2-mm sieve and weighed into two 50-ml centrifuge tubes (4 g each) and one 50-ml plastic beakers (40 g each) that was perforated to allow water to be lifted by the soil. Soil samples are naturally able to reach field capacity through capillary action (Haney and Haney, 2010). One 4-g sample was extracted with 40 ml of DI water and the other with H3A extractant (Haney et al, 2010). The samples were shaken for 10 minutes, centrifuged for 5 min, and filtered through Whatman 2V (185 mm, 8 µm) filter paper. The water and H3A extracts were analyzed on a Seal Analytical rapid flow analyzer for

NO_3-N and NH_4-N. The water extract was also analyzed on a Teledyne-Tekmar Apollo 9000 C: N analyzer for water-extractable organic C and total water-extractable N (WEN). Water-extractable organic N (WEON) was determined from the difference of total water-extractable N and water-extractable NO_3-N and NH_4-N.

One-day CO_2 evolution was determined using the Solvita Gel System (Haney et al., 2008). The Solvita Gel System quantifies the relative differences in CO_2 respiration after drying and rewetting using a pH-sensitive gel paddle and digital color reader that incorporates diode array detection technology that selects the intensity of red, blue, and green emission. Samples were weighed (40 g) and wetted to field capacity using capillary action. Wetted samples were placed into 237 ml jars with lids accompanied by a Solvita gel paddle. The samples were incubated at 25°C for 1 day. After 1 day, the paddles were removed and placed in the Solvita digital reader for analysis of CO_2 concentration. The resulting data were used for the spatial analysis of N values throughout the field for ultimate use in the N cycling model.

Satellite imagery was obtained from the National Agriculture Imagery Program (NAIP) through the Texas Natural Resource Information System (TNRIS, www.tnris.org). The 1-m digital ortho rectified image was taken on June 28, 2012, during the summer growing season. Imagery during the winter wheat growing season was unavailable at the resolution necessary to perform analysis on the field of study; however, mixed cover crops were growing on the entire field at the time the imagery was obtained. The NAIP imagery contains 4 bands (red, green, blue and infrared). The aerial photograph was utilized to delineate the field, which was ground referenced by walking the delineated line while running the ArcGIS mobile application on an iPhone 5S. In addition, the aerial photo taken in 2012 was used to calculate the Normalized Difference Vegetation Index (NDVI) in ArcGIS 10.0. The final NDVI image was used to assess the validity of the output of the model simulations. The aerial photo was used to calculate the Normalized Difference Vegetation Index (NDVI) (Rouse et al., 1973) in ArcGIS 10.0 as follows:

$$NDVI = ((IR - R) / (IR + R)) * 100 + 100$$

where IR is the infrared band and R is the red band. The output values range from 0 to 200, with 200 indicating the greenest and most healthy vegetation and 0 representing dead vegetation or bare soil. The NDVI is preferred for vegetation monitoring as it naturally compensates for changing illumination conditions, surface slope, aspect, and other extraneous factors (Lillesand et al., 2004). The final NDVI image was used to validate the output of the model simulations.

Descriptive statistical analyses, correlations and regressions were performed using SigmaPlot Version 12.5 for Windows (Systat Software, Inc., 2012) and CurveExpert Profession v2.0.4 (Hyams, 2013). Kriging was used in ArcGIS 10.0 (ESRI, 2011) for spatial interpolation of values at unsampled locations based on sample data and their spatial structure determined using Moran's I analysis. Pearson product-moment correlation coefficients were determined between soil yield results using the modified N model, yield results from the SWAT model and NDVI using PASSaGE 2 (Rosenberg and Anderson, 2011). Because spatial autocorrelation in the model output variables affects does not meet the assumptions of classical tests of significance of correlation and regression coefficients, the statistical significance of these relationships was determined by Dutilleul's modified t-test (Legendre et al., 2002) which accounts for the effects of spatial autocorrelation. Dutilleul's modified t-tests were conducted using PASSaGE 2 (Rosenberg and Anderson, 2011).

Model Theory

The basic model structure was developed using the measured water-extractable organic C (WEOC) and N (WEON), and 1-d CO_2 analysis, as well as scientific knowledge regarding the interactions between soil microbes and water-extractable C and N in the soil. The interactions between the biology of the soil and the inorganic components of the soil are predictable and can be easily modeled using the soil test data that were obtained.

Haney et al. (2012) found that soil microbial activity measured as the flush of 1-d CO_2 following rewetting of dried soil was significantly correlated to WEOC and WEON. Figure 3 depicts the relationships between 1-d CO_2, WEOC, and WEON values for various soils throughout the contiguous United States (data from USDA-ARS). Short-term C respiration from soil after drying and rewetting is also highly correlated with soil microbial biomass C and 24-d N mineralization (Haney et al., 2012). The laboratory drying and rewetting (D/R) process mimics the natural processes in the field that occur with rainfall events, the extent of which depends upon climatic and soil conditions. The mineralization of C and N following drying/rewetting can be used to quantify the portion of the soil microbial biomass that is most responsive to rainfall events, which can have a strong impact on nutrient availability (Franzluebbers et al., 2000). Specifically, every time it rains and the soil gets wet to a certain degree of field capacity, microbes activate, reproduce, degrade long-chain organic molecules containing C, N and P, and in the process, convert organic N to plant available N. The pulse of C, N, and P can be 10 to 100 times the background level of turnover following rainfall after a dry period (Franzluebbers et al., 2000). Given that soil microbes drive N mineralization, 1-day CO_2 evolution after D/R may be used to simulate the soil's ability to supply N (Haney and Haney, 2010).

In the model, we used 1-d CO_2 values and WEOC concentrations to determine the microbially active C (MAC) pool using the following equation:

$$MAC = 1\text{-}d\ CO_2 / WEOC$$

where WEOC is the measurable pool of water-extractable organic C that is the food source for microbial activity measured as 1-d CO_2. The quantity of available substrate (C and N) available for mineralization is measured using the MAC ratio.

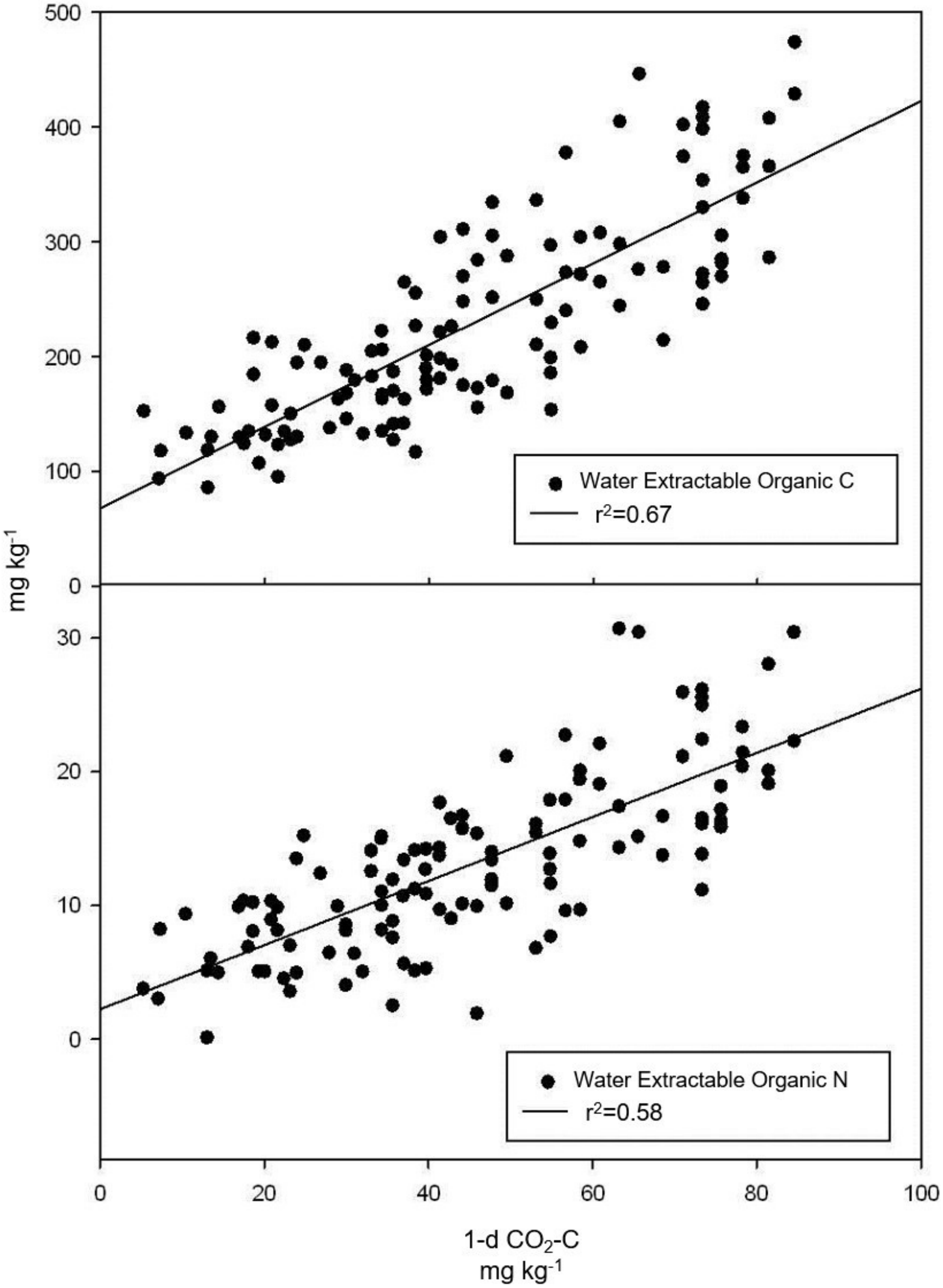

Figure 3. Relationships between 1-d CO_2-C and water-extractable N and C.

Schimel and Bennett (2004) suggest we rethink our approach to estimating N mineralization by also considering the contribution of N from the water-soluble organic N pool. The model considers the basic C:N relationship that exists in organic matter and simulated the WEON pool as being accessed directly by the microbes and in proportion to MAC. For example, if microbes release 25% of the C through respiration, 25% of the WEON pool will be released as well. The portion of N that is released from the WEON is therefore calculated as follows:

$$MAC\_WEON = WEON \times MAC$$

Because the release of N is triggered by rainfall in nature, in the model, rainfall events trigger the release of MAC_WEON as follows:

```
If (precipday >= 13 .and. sol_st(k,j) <= .25 * sol_sumfc(j)
        .and. k <= 2) then
      sol_weon(k,j) = sol_wen(k,j) - sol_win(k,j)
      sol_macweon(k,j) = sol_weon(k,j) * (sol_oneday(k,j) /
        sol_weoc(k,j))
End If
```

where *precipday* is the amount of rainfall accumulated on each day (mm), *sol_st(k,j)* is the soil moisture for the layer based on the percent of field capacity in the field, where *k* is the layer identifier and *j* is the field or hydrologic resource unit identifier. *sol_sumfc(j)* is the field capacity of the soil in the field. *sol_weon(k,j)* is the WEON for the soil layer in the field, *sol_wen(k,j)* is the total water-extractable N in the field, *sol_win(k,j)* is the water-extractable inorganic N in the field. *sol_macweon(k,j)* is the combination of Eqs. 6 and 7. The computed MAC_WEON is then added to the nitrate pool for the soil layer in the field (sol_no3(k,j)) using the following equation:

$$sol\_no3(k,j) = sol\_no3(k,j) + sol\_macweon(k,j)$$

The precipitation trigger was set equal to 13 mm, which is just enough to wet the soil and activate the microbes based on soil physical properties. In the field, significant pulses of NO_x emissions from rewetted dried soils have been seen from soils receiving as little as 12 mm rainfall (Franzluebbers et al., 2000) indicating that 13 mm is an appropriate rainfall level to observe a N flush. The soil moisture trigger is associated with a percent of field capacity to limit the N mineralization events. For example, if an appreciable rainfall event occurs on day 125 of the year and again on day 126 the soil will not have had sufficient time to complete a D/R cycle between those days and we do not want to simulate an additional release of N on day 126. It is important to simulate a complete D/R cycle to mimic the natural D/R in the field. During a succession of drying and rewetting events in the lab, a uniform pattern of CO_2 evolution was exhibited, which also occurred under field conditions (Birch, 1958). Birch (1959) postulated that the common feature between the evolution of CO_2 and N mineralization after drying/rewetting soil was microbial death and subsequent mineralization. These studies suggest that physical alteration of the soil was not a primary factor for the mineralization of C and N. Most of the mineralization of C and N after rewetting dried soil is likely due to the death of heat susceptible microbes, death from water induced osmotic shock, and further renewal of the microbial population, and consumption of the organic C and N source.

Nitrogen mineralization is not triggered unless the soil water is less than 25% of field capacity. By using the field capacity of the soil as a gauge we are accounting for the spatial variability in the physical attributes of the soil. The movement of water in soil is dependent on the combined effects of porosity, gravity, mass flow, and capillary action. Soil porosity is influenced by texture, structure (e.g., degree of aggregation), and organic-matter content. For example, coarse-textured soils have larger pores than fine-grained soils, which allow for more water flow. Organic matter greatly increases the water-holding capacity of a soil. Capillary action is the natural movement of water using adhesion (attraction to solids) and cohesion forces (attraction between water molecules) and is counterbalanced by the effects of gravity and air pockets. Haney and Haney (2010) indicate that microbial activity studies that involve D/R soils use gravimetric water content, soil matric potential, or percentage of water-filled pore space (WFPS) to achieve sufficient moisture content for peak microbial activity. Furthermore, Haney et al. (2008) indicate that a range of 30 to 70% WFPS is sufficient for peak microbial activity, which represents roughly 50% of field capacity (Haney et al., 2004). We used a value of 25% after calibrating the simulations with known fertilizer to known yield values from our study area.

The model was initialized using the initial inorganic N, WEN, WEOC, and 1-d CO_2 values obtained from the soil analysis of the 21 fields. Weather data for 1980 to 2004 and slope and elevation values for each soil sample were used as input parameters. We treated each soil sample site as its own hydrologic resource unit for simulation purposes. For each soil sample and the corresponding soil values, we conducted simulations of wheat yield by varying fertilizer rates (67.2, 44.8, 33.6, 22.4, and 0 kg N ha^{-1}). In addition, one sample dataset was chosen to simulate a fertilizer response curve for 9 different fertilizer rates (335.6, 223.9, 167.9, 111.9, 67.2, 44.8, 33.6, 22.4, and 0 kg N ha^{-1}). The model was partially validated using 2 simulations, one for wheat in 2011 and the other for sorghum in 2012. The actual field received no fertilizer, so fertilization was not conducted during the simulations.

Modified model results were compared to the traditional SWAT model simulations using the same parameters described above. The SWAT model currently does not have parameters for WEOC, WEON, or 1-d CO_2 results; however, initial soil-test N and P values were utilized. A complete description of the theory and equations used in the SWAT model can be found at swat.tamu.edu.

Results

Soil Data

The mean initial inorganic N and P concentrations were 3.95 mg kg^{-1} and 3.96 mg kg^{-1}, respectively. Total WEN (organic plus inorganic N) ranged from 16.00 to 26.09 mg kg^{-1}, with a mean value of 20.99 mg kg^{-1}. Water-extractable inorganic N values were similar to H3A extractable N values with a mean N concentration of 4.11 mg kg^{-1}, with all values ranging between 1.11 and 6.72 mg kg^{-1}. One-day CO_2 values ranges from 12.27 to 34.26 mg kg^{-1} with a mean value of 22.34 mg kg^{-1}. Water-extractable organic C values range from 208.91 mg kg^{-1} to 343.65 mg kg^{-1} with a mean concentration of 246.01 mg kg^{-1}. The mean, standard deviation, standard error, minimum, maximum and median values are reported in Table 1. Water-extractable organic N was determined by subtracting water-extractable inorganic N from WEN.

Table 1. Soil-test analyses results.

Soil Attribute*	Mean mg kg^{-1}	Std. Dev	Std. Error	Max mg kg^{-1}	Min mg kg^{-1}	Median mg kg^{-1}
Initial inorganic N	3.95	1.31	0.29	7.03	1.06	3.79
Phosphate	3.96	1.04	0.23	5.65	1.80	4.07
Water-extractable N	20.99	2.76	0.60	26.09	16.00	21.12
Water-extractable inorganic N	4.11	1.37	0.30	6.72	1.11	3.92
One-day CO_2-C	22.34	5.72	1.25	34.26	12.27	21.66
Water-extractable organic C	246.01	27.65	6.03	343.65	208.91	242.86

To visualize the spatial variability of the soil test data, kriging was performed. The data were first assessed for normality using histograms and Normal Quantile-Quantile Plots were used to determine their suitability for spatial interpolation. The results indicate that the data were mostly normal, excepting water-extractable organic carbon, which appeared more normal after a log transformation. The data were also analyzed for normality using the Shapiro-Wilk test for normality. Results from 1-day CO_2 analysis were normal according to the Shapiro-Wilk test (W-Statistic = 0.986, p = 0.987, Passed). Water-extractable total N and inorganic N data were also normal according to the Shapiro-Wilk test (W-Statistic = 0.954, p = 0.412, Passed and W-Statistic = 0.975, p = 0.846, Passed, respectively). Water-extractable organic C data were also normal according to the Shapiro-Wilk test, when one extreme outlier was taken out of consideration (W-Statistic = 0.971, p = 0.780, Passed). A test that passes indicates that the data matches the pattern expected if the data was drawn from a population with a normal distribution. Interpolation results are best when the data are normally distributed for kriging and co-kriging. Wang et al. (2013) found that N values interpolated by ordinary kriging perform well. The drawback to ordinary kriging is that it causes smoothing effects and has some difficulty dealing with co-variables. The authors further indicated that ordinary kriging has advantages over other interpolation methods when the study region is relatively flat and uniform, like our field in this study. Kriging is a form of linear least squares estimation and assumes a constant but unknown mean. Kriging weights the surrounding measured values as a measure of distance for prediction of an unmeasured location. The general formula is as follows:

$$Z(s_o) = \sum_{i=1}^{N} \lambda_i Z(s_i)$$

where $Z(s_i)$ is the measure value at the i^{th} location, λ_i is an unknown weight for the measured value at the i^{th} location, s_o is the prediction location, and *N* is the number of measured values. The weights are dependent upon the distance between measured points and the prediction location, as well as the overall spatial arrangement of the measured points. For kriging to be valid, spatial autocorrelation must exist. In ordinary kriging, the weight depends on a fitted model to the measured points, the distance to the prediction location, and the spatial relationships among the measured values (ESRI, 2011).

Kriging was used in ArcGIS for spatial interpolation of values at unsampled locations based on sample data and their spatial structure analyzed using semivariogram analysis. Semivariogram analysis was performed for WEN, 1-d CO_2, and WEOC using ArcGIS 10.0 (ESRI, 2011). Nugget variance, range, structure variance and sill were used to evaluate spatial structure. The nugget is the variance at lag distance zero and is caused by measurement error or variation at scales smaller than the sampling unit. The sill is the lag distance that defines the range of spatial continuity. Beyond the range, the values are considered spatially unrelated. The difference between the sill and the nugget contains the spatial variance. The range of the model varied from 213 to 504 m, beyond which no spatial autocorrelation exists. The strength of the spatial structure at the sampling scale is determined using the following equation:

% strength of spatial structure = (Sill-nugget)/sill

Using this relationship, we determined that the strength of the spatial structure for WEN is 100%, because the nugget value is 0. The strength of the spatial structures for 1-d CO_2 and WEOC are less than zero and 21% indicating that the spatial autocorrelation was not strong. It is possible that a different model would be more suited for analyzing the spatial structure of 1-d CO_2 and WEOC or additional samples are needed.

Ordinary kriging based on the variogram analysis provided estimates of WEN, 1-d CO_2 and WEOC (Figures 4 through 6) values for the 15-cm depth increment at location which had not been sampled. This enables us to develop a map of these values across the study area. When the kriged maps are compared visually with the DEM and aerial photograph of the area, it is apparent the soil values vary with the elevation of the field. WEOC values appear to decrease in a northerly direction, corresponding to a decrease in elevation. WEN and 1-d CO_2 values appear to increase at the lower elevation in the northern section of the field and decrease in an outwardly direction from the lowest elevation. An anomalous high WEOC value was present at the lower elevation, which was removed for kriging purposed because it skewed the normality of the data. It is possible that the WEOC values are higher in this location, but that this area was not adequately sampled. It makes sense that WEN and 1-d CO_2 values would increase with a dip in the elevation as the soil health would be greater in this location due to increased available moisture.

Model Simulation Results

Initial validation results using actual yield and weather data for 2011 and 2012 indicate that the yield results from the modified N model were 2.4 and 3.8 Mg ha^{-1}, respectively, while actual yield results were 3.0 and 3.5 Mg ha^{-1}. These results are closer to the actual values than the yield predicted with the SWAT model, which were 1.5 and 0.8 Mg ha^{-1} for 2011 and 2012, respectively. More actual yield data are needed to determine the validity of these results.

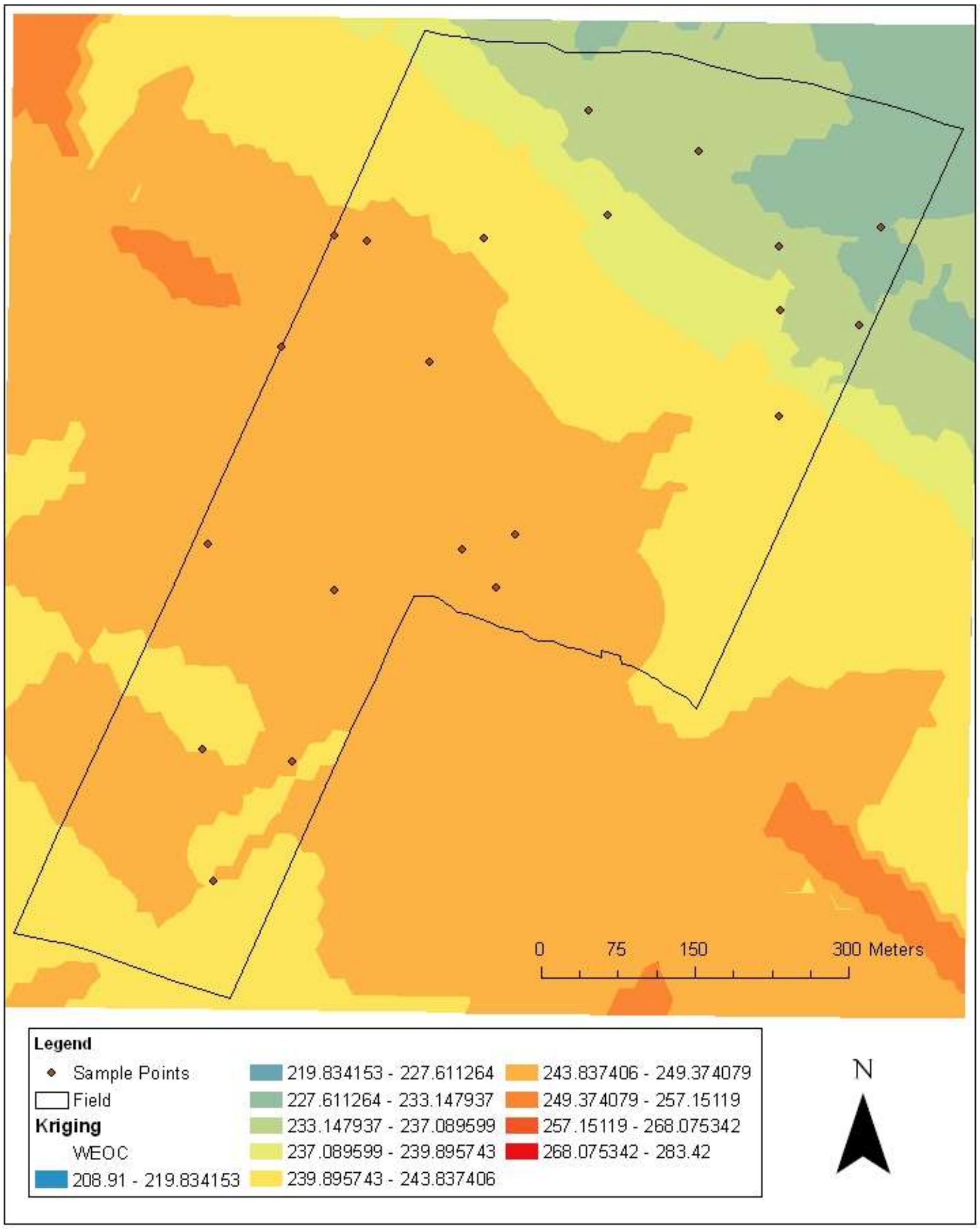

Figure 4. Kriging results for water-extractable organic C (WEOC, mg kg^{-1}) throughout the study area.

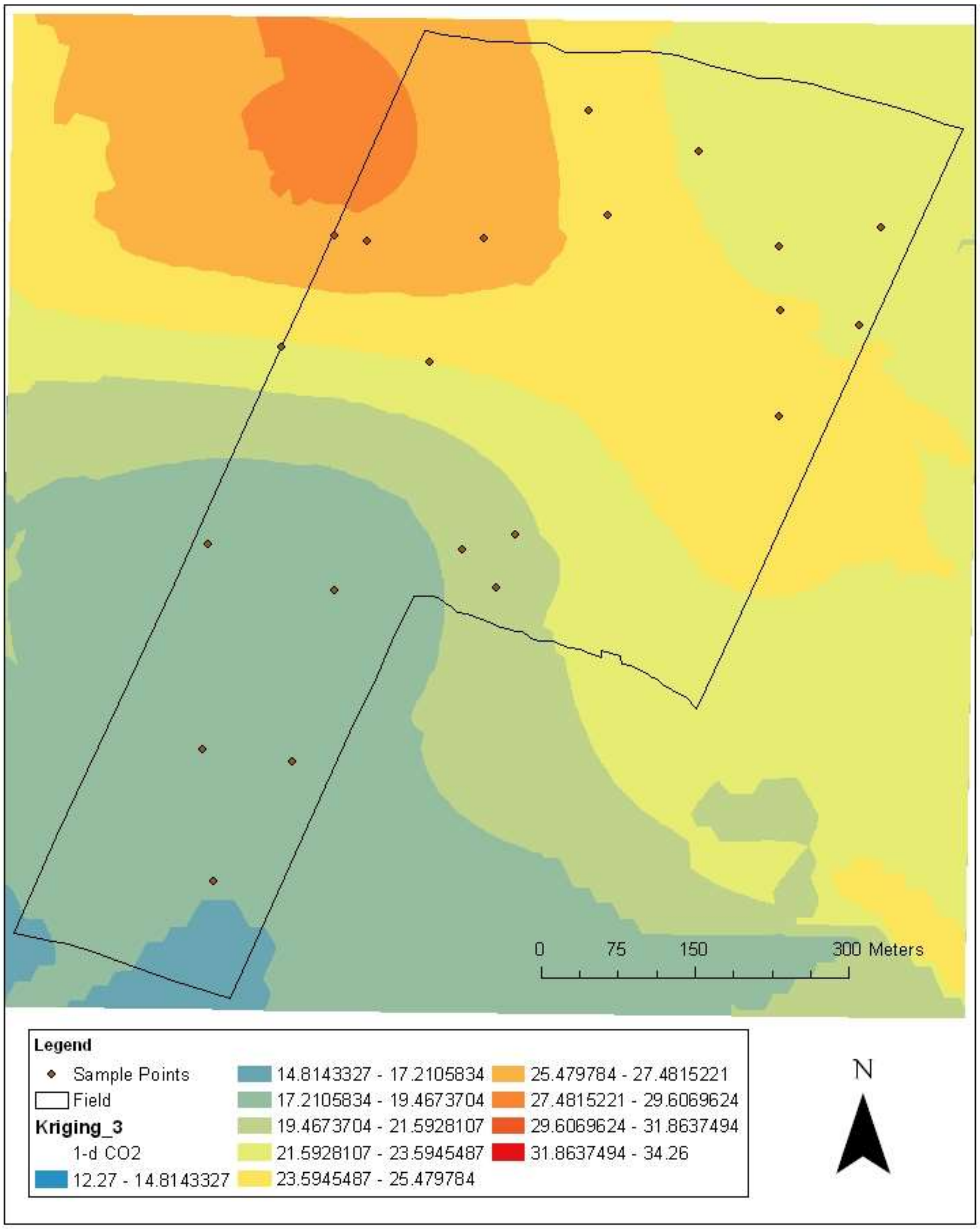

Figure 5. Kriging results for 1-d CO_2 (mg kg^{-1}) analysis throughout the study area.

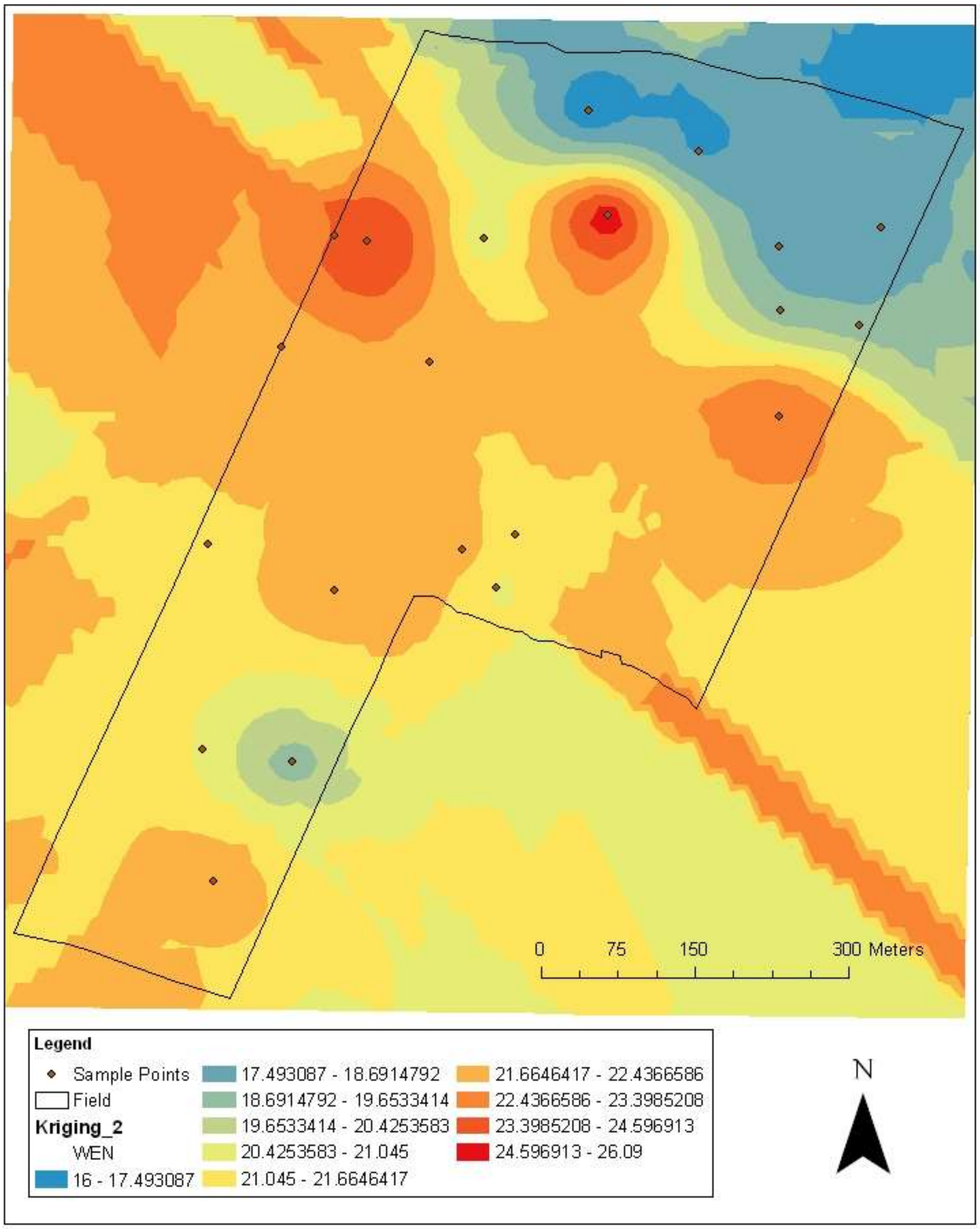

Figure 6. Kriging results for water-extractable N (WEN, mg kg^{-1}) throughout the study area.

End users of the SWAT model report they receive little to no yield results when no fertilizer is applied during simulation. I found that over 27 years of simulation wheat yield ranged from 0.05 to 3.4 Mg ha^{-1}, with one sample site consistently having higher yields than the others. It is unclear why this site had increased yield over the other sites. The median yield value is near 1.3 Mg ha^{-1}, which is low considering the natural fertility of the soil. Fertilizer has not been applied to the field in many years and wheat yields average around 2.0 Mg ha^{-1}. Yield results from wheat rotations with no fertilizer using the modified model ranged from about 1.0 to almost 6.0 Mg ha^{-1} with an average value around 2.0 Mg ha^{-1}. The modified N routine increased the range of predicted yield and the median yield. In fact, the range in yield values for all fertilizer treatments increased when using the modified model as compared to the SWAT model. Yield results for each of the 27 years simulated are strongly correlated to N fertilizer input when using the SWAT model ($r^2 = 0.80$), and show only a weak correlation when using the modified N model ($r^2 = 0.38$). Multiple linear regression analysis indicates that a linear combination of precipitation, fertilizer application, and N mineralization from the water soluble organic C and N pool contributes to predicting yield ($p < 0.05$). The relationship can be explained by the following equation:

*Yield = 30.604 + (0.139 x Precipitation) + (0.175 * fertilizer N) + (0.290 * N mineralized)*

Use of the multiple linear regression greatly improves the strength of the correlation between yield and determining process values ($r^2 = 0.77$, Table 2).

We used the CurveExpert software to fit yield results for varying fertilizer rates from 0 to 335.6 kg N ha^{-1}, which resulted in a best-fit model using a Rational Model (Figures 7 and 8). The Rational Model follows the equation:

$$y = \frac{a + bx}{1 + cx + dx^2}$$

The SWAT model yield results had a stronger correlation with fertilizer application (r^2 = 0.93) than the modified N model (r^2 = 0.79) when using the Rational Model.

Table 2. Multiple linear regression results for yield, precipitation, N mineralization, and fertilizer application values from the new N model simulation.

	Coefficient	Std. Error	t	p
Constant	30.60	0.51	59.17	<0.001
Precipitation	0.14	0.01	10.92	<0.001
Fertilizer N	0.18	0.01	25.09	<0.001
N Mineralization	0.29	0.00	64.39	<0.001

Analysis of Variance:

	DF	SS	MS	F	p
Regression	3.00	336369.46	112123.15	2880.38	<0.001
Residual	2621.00	102026.40	38.93		
Total	2624.00	438395.86	167.07		

	SSIncr	SSMarg
Precipitation	10186.58	4644.46
Fertilizer N	64808.62	24502.27
N Mineralization	161374.27	161374.27

	p
Precipitation	<0.001
Fertilizer N	<0.001
N Mineralization	<0.001

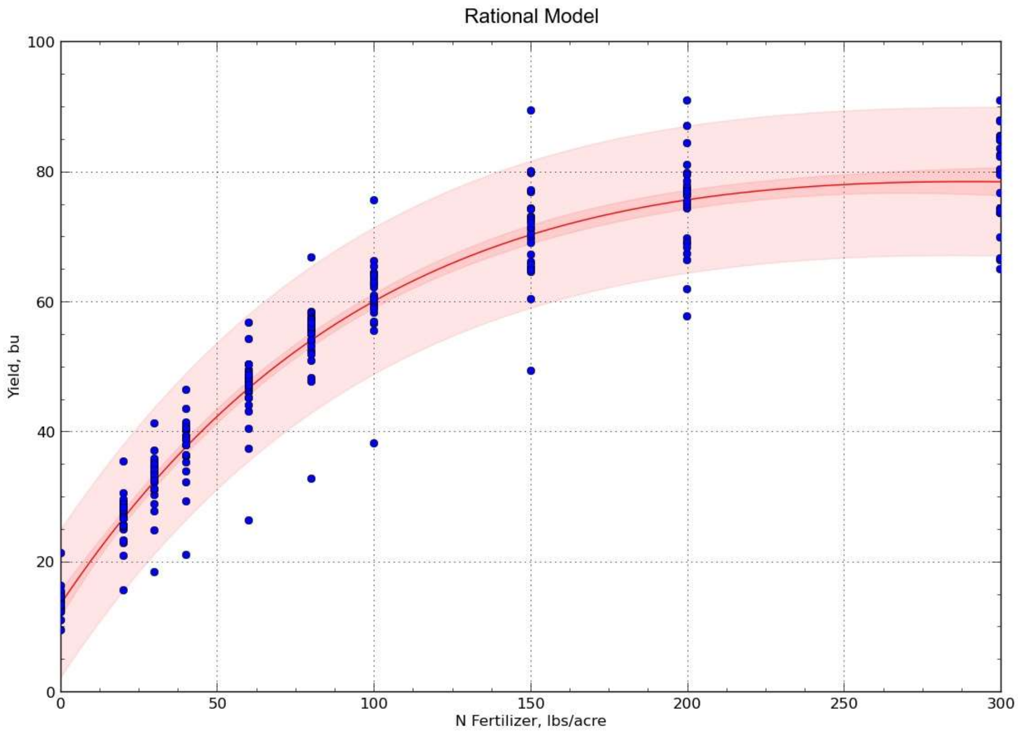

Figure 7. Rational Model describing the relationship of yield simulation values using the SWAT model with increasing fertilizer application (r^2 = 0.93).

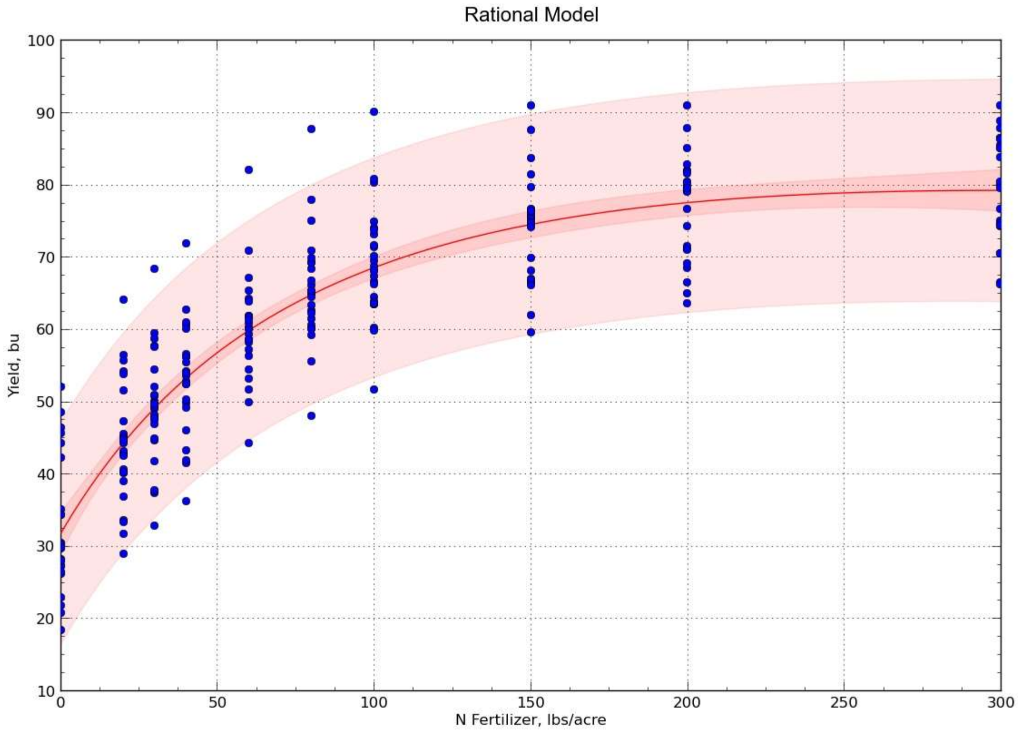

Figure 8. Relationship between increasing fertilizer application and yield simulated using the modified N model (r^2 = 0.79).

The yield values obtained varied temporally when using either the SWAT or the modified N model (Figure 9). Yearly yield values and variability were consistantly higher from the modified N model than from the SWAT model. The yield values obtained from the modified N model were also consistantly higher for each soil sample as would be expected with the additon of N mineralization resulting from microbial activity (Figure 10). The spatial relationships between yield values from the SWAT model and the modified N model are depicted in the xyz contour plot in Figure 11. SWAT simulated yield values indicate that the yield is greater in the southern portion of the field, while simulated yield values using the modified N model are greater in the northern portion of the field. Analysis using Moran's I for spatial autocorrelation detected significant spatial variability in yield from both models. For the yield data resulting from both the modified and the SWAT model simulations, given the z-score of 85.3 and 85.2, there is less than 1% likelihood that the resulting clustered patterns could be the result of random chance.

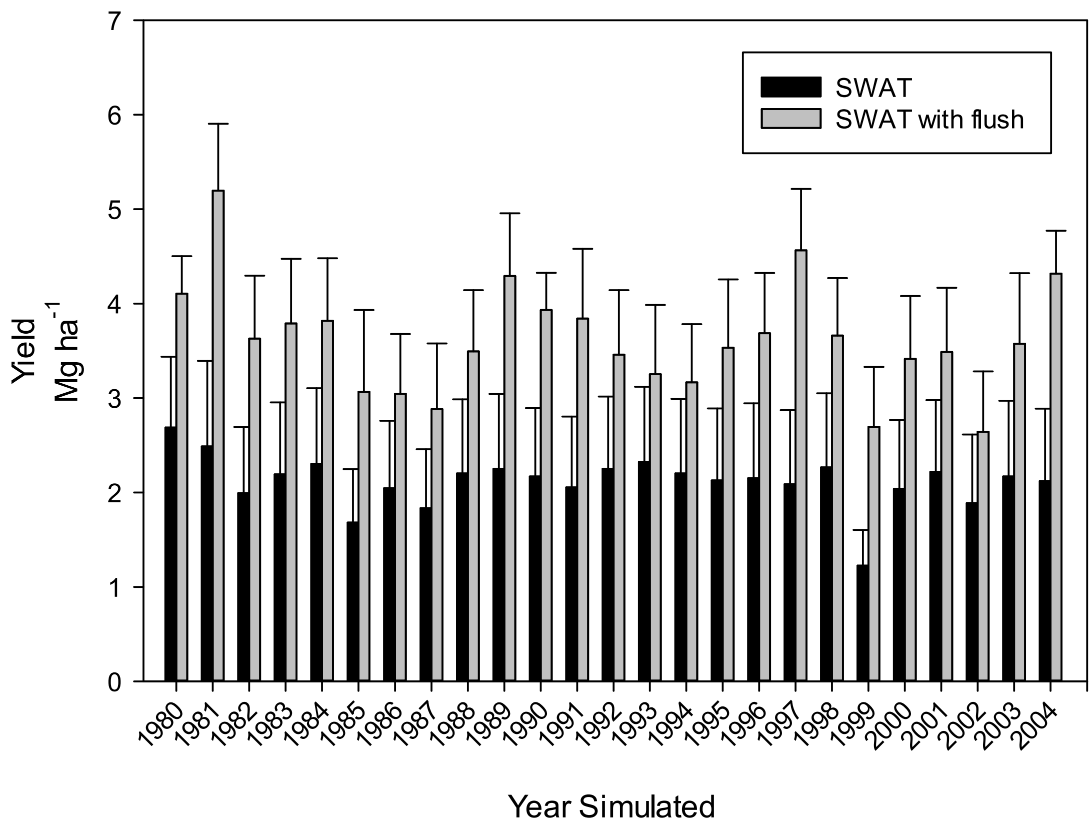

Figure 9. Wheat yield results by year averaged over all fertilizer treatment simulations using SWAT with the added flush of N and unmodified SWAT.

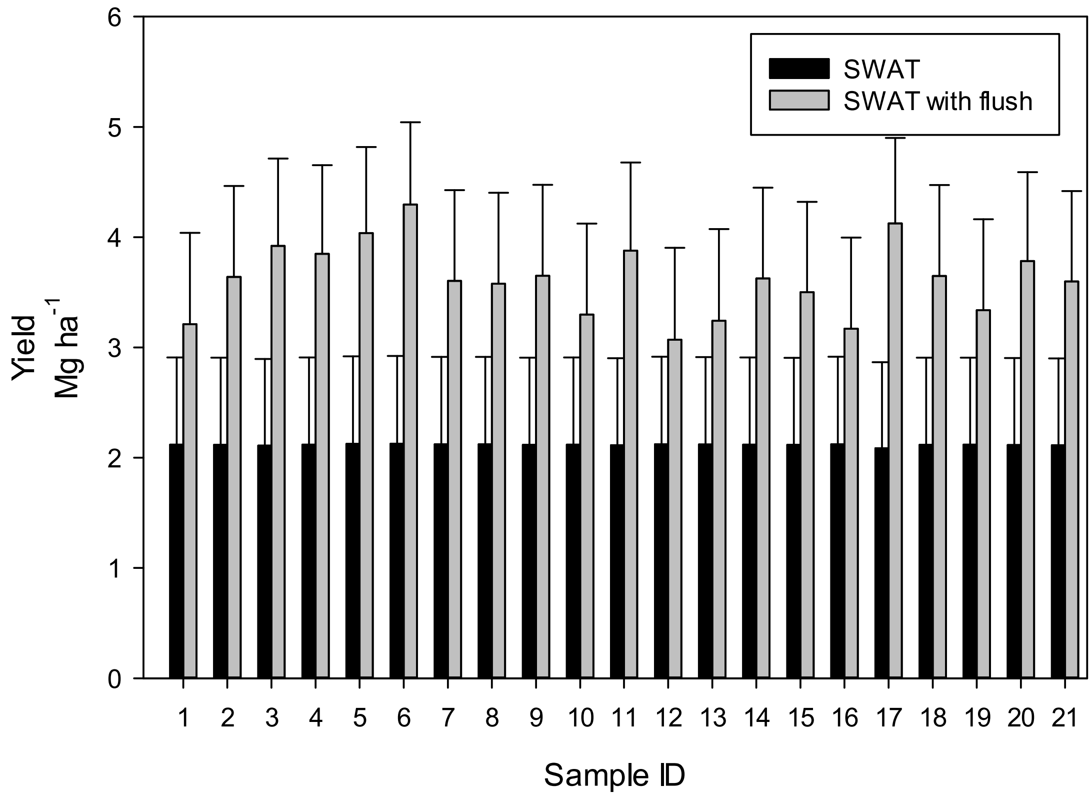

Figure 10. Average wheat yield results from 27 years of simulations by soil sample using SWAT with the added flush of N and unmodified SWAT.

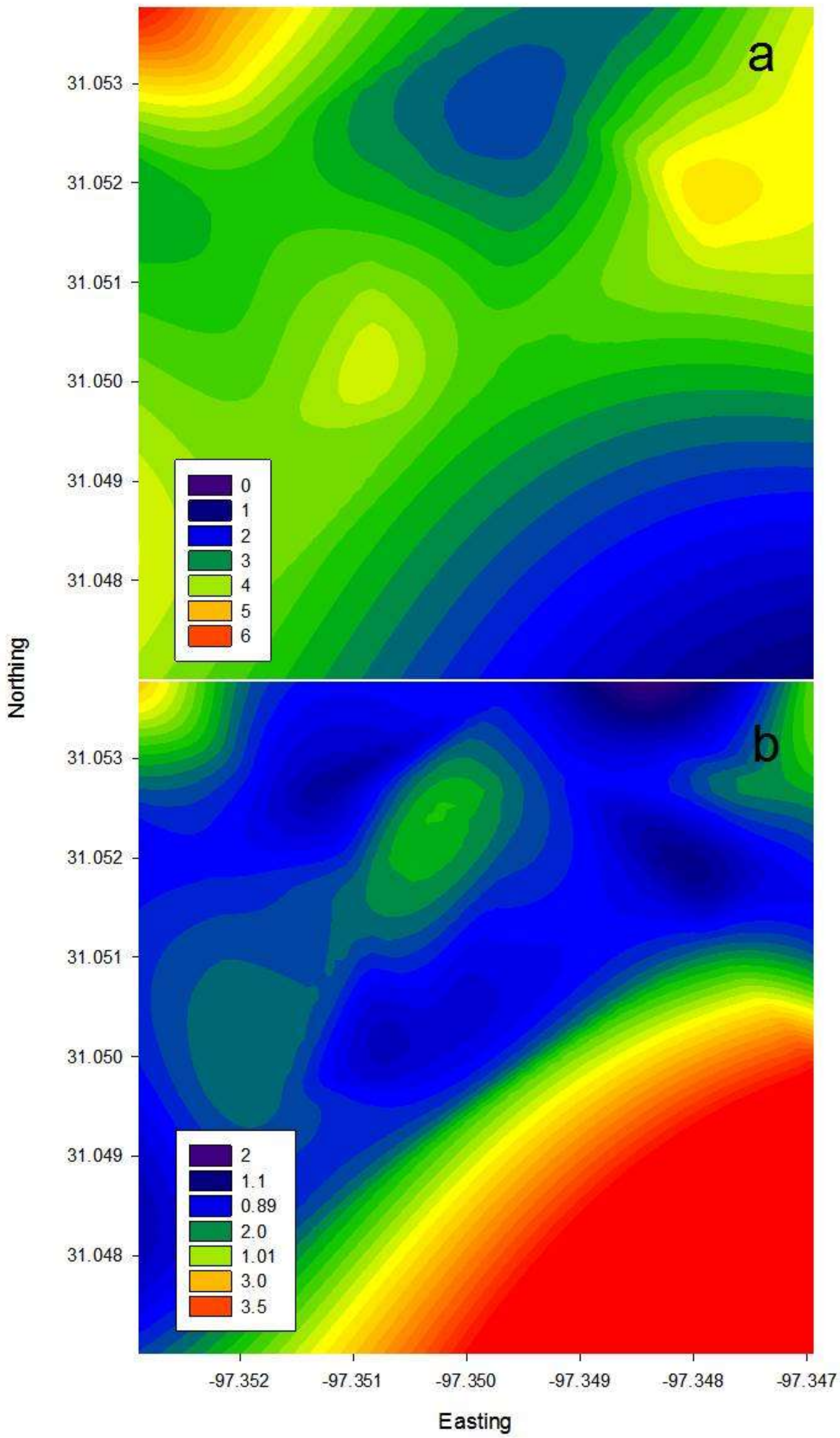

Figure 11. Wheat yield values (kg/ha) using the modified N model (a) and the SWAT model (b).

Because we do not have actual yearly yield data for all 27 years of simulation available for validation, NDVI is being used as a proxy for average yield data for the years 1980 through 2004 to determine if the modified model is predicting yield accurately. NDVI greenness factors were compared to kriged yield results from both models. If the model is predicting yield properly, the yield should correspond to greenness in the field. The greenness is an indicator of soil health and viability of plant growth. It follows that if the models are properly simulating N cycling in the soil, the yield should correspond to the greenness index from the NDVI. The NDVI data for the field indicate that plant growth is greatest in the northern portion of the field at the lower elevations. The simulation model yield results using the modified N model appear to correspond with the NDVI greenness factor, while the results from the SWAT model do not (Figure 12). The modified t-test for correlation (Table 3) indicate that both the modified N and SWAT model yield results are correlated with NDVI values ($P < 0.005$), however, the modified model has a significantly stronger correlation ($P < 0.001$).

Table 3. Modified t-test for correlation between yield results and Normalized Difference Vegetation Index values.

Variable 1	Variable 2	Covariance	P(Cov)	Correlation	Corrected P (Cor)	Effective Sample Size
Modified N routine	SWAT	-4.04	0.00005	-0.51	0.00002	62.7
Modified N routine	NDVI value	3.81	0.00014	0.38	0.00009	100.3
SWAT	NDVI value	-3.21	0.00135	-0.32	0.00115	103.1

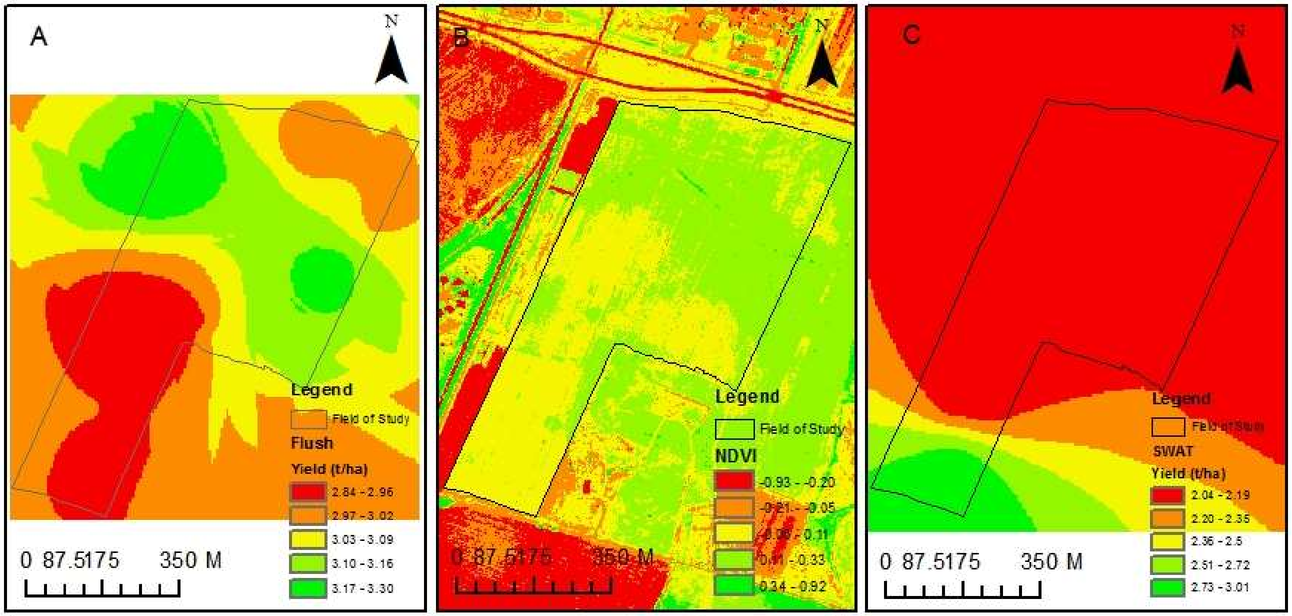

Figure 12. Kriged yield results from the modified N model (A) and the SWAT model (C) as compared to Normalized Difference Vegetation Index analysis (B) derived from an aerial photograph of the area.

Discussion

Soil properties are heterogeneous in nature and consist of continuous variables that change over spatial and temporal ranges. Early models describing the processes of N cycling use simple chemically and spatially lumped models (Manzoni and Porporato, 2009). Some biogeochemical models use a discrete representation of soil layers with different chemical and physical features or a continuous description of nutrient dynamics along the soil profile. What these models fail to do; however, is explicitly describe the spatial dynamics of water, organic matter or nutrients at a horizontally continuous spatial scale over a daily variable time step. The purpose of this study was to develop a N model that can capture the spatially explicit scale of N cycling over a large temporal range.

The continuous nature of the soil properties being used in the N cycling model (WEOC, WEON, and 1-day CO_2) allow for spatial interpolation over the field of interest. Because 1-day CO_2 analysis is a measure of microbial activity and microbial biomass is the driver of soil C and N cycling (Manzoni and Porporato, 2009) we would expect to see a strong correlation between the soil properties of interest throughout the field. Because the variables are spatially autocorrelated a normal linear regression analysis is inappropriate to examine the relationships between them. Semivariogram analysis of the spatially interpolated soil test results was used examine the spatial structure of the driving factors for N mineralization. The analysis results indicate that the spatial structures of 1-d CO_2 and WEOC values were weak as compared to the spatial structure for WEN. It's possible that a stronger spatial structure may have been obtained by modifying the kriging and semivariogram models used to evaluate the spatial structures of 1-d CO_2 and WEOC. Additional soil samples may also have been necessary to accurately capture the spatial variability of these parameters. In addition, the ordinary kriging method used did not account for the possible anisotropic nature of the soil values. Visual assessment of the kriging results indicates that at least some of the spatial variability was related to elevation changes from the north to south; however, this variation was not accounted for in the semivariogram analysis. Topography could potentially impact water-extractable soil C values and microbial activity as assessed using 1-d CO_2 analysis, which can regulate N cycling. Further spatial statistical analyses should include co-kriging analysis with elevation and possibly with vegetation parameters derived from NDVI analysis. Correlation analysis may be useful in further understanding the relationships between soil properties, elevation, and vegetation parameters.

Statistical evaluation indicates that the modified N model is useful in detecting the natural N mineralization power of the soil. Initial validation results using actual yield and weather data for 2011 and 2012 indicate that the yields were a little high for the zero fertilizer application simulations so some adjustment to the model is needed. The modified N model does appear to account for spatial variation in soil properties and temporal variation in climate factors. More data are needed over a wider spatial range (regional or larger) to determine how well the modified N model behaves under various climatic and soil conditions.

Conclusions

The objective of this study was to quantify the spatial variation of soil biogeochemical factors that affect N cycling in the soil and use these data to develop a field scale model to determine N mineralization for integration into the SWAT model. Due to the spatial nature of soil factors, it was essential to use a GIS to collect and analyze spatial and temporal inputs and outputs.

Statistical results showing a strong correlation between yield and fertilizer inputs resulting from simulation with the SWAT model is problematic and indicates that the SWAT model is not properly accounting for the natural N cycling processes in the soil. The relationship between yield, rainfall, N mineralization, and fertilizer when using the modified N model is a definite improvement over the current N routines in SWAT as yield is more closely reflecting the complexity of the processes involved in plant growth, when all other aspects are held equal. When the Rational Model is used to describe the relationship between fertilization rate and yield, yield values increased accordingly with fertilizer application, eventually leveling off as fertilizer use exceeded needs of the plant. This relationship is expected as the benefits of fertilizer application will cease as plant nutrient stress is completely eliminated by excess available nutrients.

Results from the simulations indicate that yearly yield values and the variability of these yield values were consistantly greater from the modified N model than from the SWAT model. The yield values obtained from the modified N model were also consistantly higher for each soil sample as would be expected with the additon of N mineralization resulting from microbial activity. The spatial variability in yield results by sample increased with the modified N model as compared to the SWAT model.

In SWAT, soil properties are determined using the soil characteristics obtained from soil survey data. SWAT model output was not sensitive to the changes in the default soil properties associated with the soil series descriptions or elevation changes. In addition, because the N model in SWAT is based on the very large pools of soil organic C and N, which are 40 times larger than the active pool of N and C that the microbes utilize to cycle N, it is less sensitive to spatial variation of N mineralization. For example, spatial analyses of soil properties indicate that healthier soil is located at the north end of the field, which corresponds to the lower elevations within the study area. The SWAT model predicts that this area has the lowest yield, when in the field, it has the highest yield. This is because yields predicted by the SWAT model are almost solely based on fertilizer input and exclude the natural N pools that we are accounting for in the modified model.

The yield data resulting from the modified model simulation were sensitive to soil changes as well as elevation changes. The modified N model naturally considers the spatial variability of soils over geographic areas because as the C:N ratio of a soil varies, the MAC_WEON calculation will vary accordingly. In addition, the MAC_WEON calculation used in the modified N model reflects the variation in soil health spatially by into account the viability of the microbial population. Temporal and climatic variability is accounted for by including the precipitation trigger in the SWAT simulated plant growth cycle. The equations used to model the complex biogeochemical N cycling relationships are elegant in their simplicity, yet capture the spatial complexity associated with their processes.

Future studies will need to include long-term yield data for varying soils, crops and management practices in varying climates. Research may also include variations in the approach to data attainment and management for larger projects at the watershed scale. Data acquisition may be challenging for large scale projects as it will not be practical to soil test large areas. Satellite imagery may play a critical role in further development for large-scale simulations. In addition to the impracticality of large-scale soil sampling, only a few laboratories throughout the United States offer the soil tests that the modified N model is based upon. It will be important to test the use of default values for soil test results and may be necessary to find a proxy for soil test data, possibly using NDVI analysis.

The modified N model incorporated into SWAT may be useful to regulators to help with the simulation of new conservation practices that include the effect of lower fertilizer inputs on nutrient runoff and pollution. Not only did this study result in an improved N model, it also succeeded in demonstrating the use of spatial analyses to determine the validity of model input data and output results.

CHAPTER III

SWAT AND SWAT-FLUSH SIMULATED VS. ACTUAL WHEAT YIELD IN LONG-TERM TRIALS

Introduction

Through the production and use of nitrogen (N) fertilizer, we have altered the Earth's N cycle affecting issues that range from global climate change to oceanic hypoxic zones. Nitrogen use in the world is so significant that the Haber-Bosch synthesis of ammonia from atmospheric N is responsible for nearly 2% of global energy consumption (European Commission, 2013). As of 2011, when the latest National Land Cover Dataset (NLCD) was made, 1,253,000 km^2 of land in the conterminous US was classified as cropland (USGS, 2011). In many parts of the United States, N and phosphorus (P) inputs to these agricultural lands are considered to be the primary nonpoint sources of pollution, including the Upper Mississippi River Basin (Jha et al., 2013). For lawmakers, environmental decision makers and scientists to identify and mitigate nonpoint source nutrient pollution, we must be able to accurately predict N cycling in in response to fertilization and resulting crop yields at both the field and watershed scales.

The Soil and Water Assessment Tool (SWAT) is an environmental process-based model that performs at a daily time step and has been used to predict crop yield at various temporal and spatial scales (Arnold et al., 2012). SWAT utilizes information about weather, soil properties, topography, vegetation, and land management practices occurring in the watershed (Neitsch et al., 2009), making it suitable for assessing the effect of management practices on agricultural production. In SWAT, crop yield is predicted by simulating complex processes including the hydrologic, soil and water nutrient, and plant-growth cycles.

The origins of the SWAT model trace back to the Chemicals, Runoff, and Erosion from Agricultural Management Systems (CREAMS) model, the Groundwater Loading Effects on Agricultural Management Systems (GLEAMS) model, and EPIC model, which were created by the USDA-ARS (Gassman et al., 2007). The SWAT model allows for crop growth simulation under nutrient limited scenarios and accounts for variations in soil properties. The many and varied uses of SWAT are discussed in detail in Gassman et al. (2007) and range from N and P loss studies to large-scale watershed hydrologic assessments throughout the world. Nitrogen cycling in SWAT originates from the Environmental Policy Integrated Climate Model (EPIC), which is based on the PAPRAN (Production of Arid Pastures limited by RAinfall and Nitrogen) model (Lauenroth et al., 1983, Neitsch et al., 2009, Matthews and Stephens, 2002, Seligman and van Keulen, 1981, Williams, 1995). The N cycling model in SWAT has been supplemented with a fast-acting microbial flush of N that mimics crop green up after rainfall events (SWAT-flush, Haney et al., 2016).

Haney et al. (2012) found that soil microbial activity measured as the flush of CO_2 in 24 hr. (1-d CO_2) following rewetting of dried soil was significantly correlated to water-extractable organic C (WEOC) and water-extractable organic N (WEON). Short-term C respiration from soil after drying and rewetting is also highly correlated with soil microbial biomass C and 24-d N mineralization (Haney et al., 2012). The laboratory drying and rewetting (D/R) process mimics the natural processes in the field that occur with rainfall events, the extent of which depends upon climatic and soil conditions. The mineralization of C and N following drying/rewetting (D/R) has been used to quantify the portion of the soil microbial biomass that is most responsive to rainfall events, which can have a strong impact on nutrient availability (Franzluebbers et al., 2000). Specifically, every time it rains and soil moisture increases, microbes activate, reproduce, eat long-chain organic molecules containing C, N and P, and in the process, convert organic N to plant available N. Given that soil microbes drive N mineralization, 1-day CO_2 evolution after D/R may be used to simulate the soil's ability to supply N (Haney and Haney, 2010). It is important to simulate a complete D/R cycle to mimic the natural D/R in the field. During a succession of drying and rewetting events in the lab, a uniform pattern of CO_2 evolution was exhibited, simulation which occurred under field conditions (Birch, 1958). Birch (1959) postulated that the common feature between the evolution of CO_2 and N mineralization after (D/R) soil was microbial death and subsequent mineralization. Much of the mineralization of C and N after rewetting dried soil is likely due to the death of heat susceptible microbes, death from water induced osmotic shock, and further renewal of the microbial population, and consumption of the organic C and N source.

The SWAT N subroutine with the flush of N contains the same pools as the basic SWAT N model, with added pulses of NO_3^- after a significant rainfall event on a sufficiently dry soil. Previously, the modified N model was tested at the field level using actual soil-test data measured against the satellite derived Normalized Difference Vegetative Index (NDVI). Haney et al. (2016) found that when using the modified N model, SWAT was better able to predict spatial variations in NDVI in the field as well as soil properties indicative of soil health (soil organic N and C, for example). The modified N model uses WEOC, total water-extractable N (WEN), WEON, and o1-d CO_2 to replicate N flushes after rainfall events (Haney et al., 2012).

In this study, we compared wheat yields predicted by SWAT-flush to yields from long-term wheat studies in Oklahoma. The objectives of this paper are to determine if SOC can be used as a proxy for actual soil test data in SWAT-flush and to examine the controlling factors determining actual and simulated winter wheat yields.

Materials and Methods

We previously conducted research using biogeochemical soil-test data at the field scale to simulate the N flush that occurs in soil after D/R with the SWAT model (Haney et al. 2016). This replicated flush (SWAT-flush) represents the increase in microbial activity and subsequent release of N that occurs after a rainfall event as described in Birch (1958, 1959), Franzluebbers et al. (2000), Haney and Haney (2010), and Haney et al. (2004, 2012). The amount of NO_3^- (mg kg^{-1}) released after a rainfall event was based on the water soluble organic C and N (WSOC and WSON, mg kg^{-1}) and microbial activity determined using 1-day CO_2 (mg C/kg soil) evolution, as follows:

$$Flush\ of\ NO_3^- = WSON \times (1\ day\ CO_2 \div WSOC)$$

The flush of N was reproduced in the top 10 mm of soil to mimic rapid changes in soil moisture, temperature and N cycling at the soil surface. After a rainfall event greater than 26 mm occurs on sufficiently dry soil (based on soil matric potential), a flush of N is added to the NO_3^- pool. All the remaining N processes were unaltered from the basic SWAT N cycling model. Haney et al. (2016) found that wheat yields predicted by SWAT-flush were more spatially correlated with NDVI than the original SWAT model, indicating better representation of actual field growing conditions. SWAT-flush performed significantly better than SWAT at low levels of fertilizer application. In addition, wheat yields predicted when using the SWAT-flush were more spatially representative of tested field and soil conditions than when simulated using the basic SWAT model.

As opposed to the SWAT-flush simulations at field level studies (Haney et al. 2016), actual WSOC, WSON, and 1-day CO_2 values were not available for this study. To use the SWAT-flush subroutines, SOC values were used as a proxy to set initial model values for WSOC, WSON, and 1-day CO_2. The link between SOC and 1-d CO_2, WSOC and WSON in soils from Idaho, Georgia, Maine, Mississippi, Oklahoma, Texas and Wyoming under various management conditions has been described by Haney et al. (2012). Analyses results from 116 soil samples from throughout the US were used to develop regression equations between SOC, WSOC, WSON, and 1-day CO_2. Sixty-six of the samples were from the North American Proficiency Testing Program (NAPT) without location specific information and the remaining are from samples obtained in Oklahoma, Texas, Idaho, Georgia, and Wyoming. The soils have a wide range of SOC and total N values. The soils studied also vary in texture, pH and come from areas under various management scenarios. Soil organic C and total N (TN) values for the NAPT soils are provided with the samples upon procurement, while the remaining SOC and TN values were determined on 2-g subsamples using dry combustion (Elementar; Hanau, Germany).

Each soil sample was dried at 50° C, ground to pass a 2-mm sieve and weighed into two 50-ml centrifuge tubes (4 g each) and one 50-ml plastic beaker (40 g each) that was perforated to allow water to be lifted by the soil. Soil samples are naturally able to reach field capacity through capillary action (Haney and Haney, 2010). One 4-g sample was extracted with 40 ml of DI water and the other with H3A extractant (Haney et al., 2010). The water and H3A extracts were analyzed on a Seal Analytical rapid flow analyzer for NO_3-N and NH_4-N. The water extract was analyzed on a Teledyne-Tekmar Apollo 9000 C: N analyzer for WSOC and water-extractable N (WEN). Water-extractable organic N (WSON) was determined from the difference of total WEN and water-extractable NO_3-N and NH_4-N. One-day CO_2 evolution was determined using the Solvita Gel System (Haney et al., 2008). Soil data were analyzed using linear regression analysis to determine the relationships between the various soil properties using SigmaPlot Version 12.5 for Windows (Systat, 2012).

Soil organic C (SOC) was correlated with WSOC ($r^2 = 0.57$) in the soils tested. The weak correlation was expected since the WSOC pool is roughly 80 times smaller than the total SOC pool (% Organic Matter) in the soil. The percent of SOC reflects the total amount of C present in the soil, while WSOC reflects the quality of organic C and is the readily available energy source for soil microbes (Haney et al., 2012). WSOC was significantly correlated with soil respiration and WSON (r^2 = 0.76 and r^2 = 0.84, respectively). These data correspond to previous research showing that microbial activity, as measured using 1-day CO_2, is correlated to WSOC and WSON (Haney et al., 2012). The WSON pool can be easily broken down by soil microbes and released to the soil in inorganic N forms that are plant available (Haney et al., 2008, 2012). The results suggest that SOC values may be used to estimate 1-d CO_2, WSOC and WSON in SWAT-flush. Regression lines were passed through the origin for use in SWAT-flush to prevent the occurrence of negative C and N values (Figure 13). The resulting regression equations were incorporated in to the SWAT-flush code. SOC values for the Grant silt loam were included in the soil input file in SWAT and converted to WSON, 1-d CO_2 and WSOC during the model run.

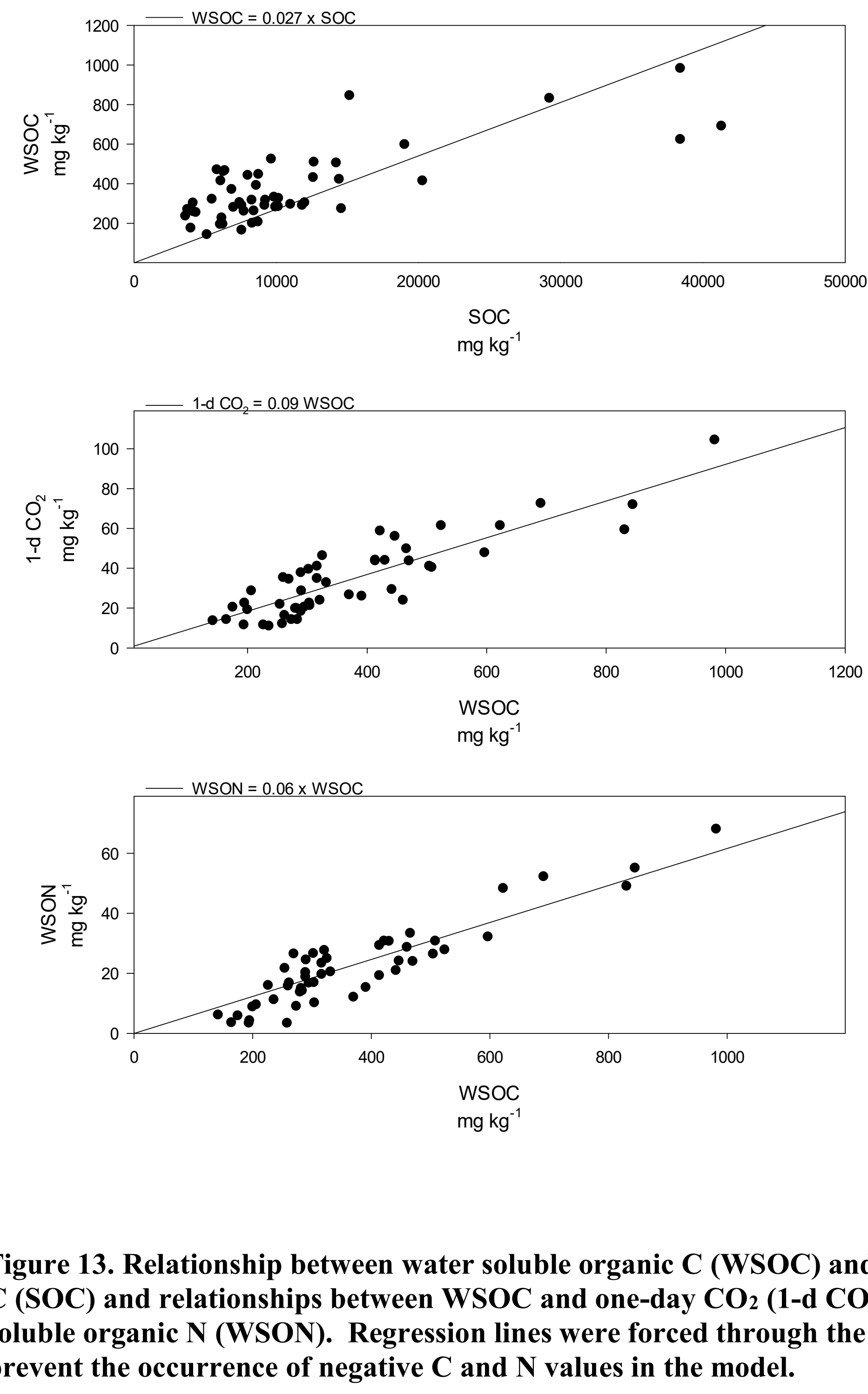

Figure 13. Relationship between water soluble organic C (WSOC) and Soil Organic C (SOC) and relationships between WSOC and one-day CO_2 (1-d CO_2) and water soluble organic N (WSON). Regression lines were forced through the origin to prevent the occurrence of negative C and N values in the model.

Yield from simulations using SWAT-flush were compared to yield data obtained from long-term wheat yield experiments managed by Oklahoma State University (OSU, http://nue.okstate.edu/Long_Term_Experiments/E502.htm). The research station is located at the North Central Agricultural Research Station near Lahoma, OK (36.42° N, 97.87° W) in Garfield county (Raun et al, 2000). Average annual rainfall in at the experiment site is approximately 800 mm (Schroder et al., 2011) and the mean annual temperature is 15.6 °C (Raun et al., 1998). The pH of the soil averages 5.7 in the top 30 cm (Raun et al., 1998). Experiment 502 was established in 1970 to study the response of wheat grain yield to varying rates of long-term N, P, and K fertilizer application. The randomized complete block (4 replications) designed experiment is conducted on continuous winter wheat grown on a Grant silt loam (fine-silty, mixed, thermic Udic Argiustoll). OSU applied Urea N (46-0-0) pre-plant at rates of 0, 22.4, 44.8, 67.3, 89.7, 112.1 kg N ha^{-1} and triple superphosphate (0-46-0) at the rates of 9.9, 19.7, 29.6, 39.5 kg P/ha between early August and early October annually. Planting was conducted between late September to late October and harvest followed between early June to early July depending upon weather conditions.

SWAT input files were developed using local weather and soils data in the Texas Best Management Practice Evaluation Tool (TBET, White et al., 2012). TBET serves as an interface for SWAT for evaluation of management practices effects on annual runoff, sediment, N and P losses from agricultural fields. The interface gave us a simplified way to develop SWAT input files for management conditions replicating those used in

Experiment 502. Weather data were obtained from the National Oceanic and Atmospheric Administration (NOAA) National Weather Service Cooperative Observer Program, Lahoma Research Station (USD00344950) weather station (Latitude: 36.3894, Longitude: -98.1061, Elevation: 388.6m).

Soils data were obtained from SSURGO (USDA-NRCS, 1995) and were used to determine the initial 1-d CO_2, WSOC and WSON values. The SSURGO database was developed by the USDA-NRCS and includes organic matter data for 18,000 soil series in the U.S. SSURGO data is available at a scale of 1:24,000 and can be used for county, farm and ranch and landowner planning. Zhang et al. (2014) found that SSURGO performed well at the county-scale when determining crop yields and Net Ecosystem Production (NEP). Further modifications to the SWAT-flush model from the Haney et al. (2016) study include the addition of a 15-cm layer to the top of soil profile where the N flush occurs (formerly just in top 10 cm) to more accurately simulate microbial activity in the soil.

Yield simulations using SWAT and SWAT-flush ran for 27 years (1985 to 2012), with 1985 and 1986 serving as warm up years. Management data included actual planting and harvest dates from 1985 to 2013. An average planting date of October 21 and harvest date of June 13 were used in the 6 cases where dates were unavailable. Urea and P application rates corresponded to the 12 combinations of N and P rates used in Experiment 502.

Simulated yield data were compared to average and yearly actual yield. The relationship between yield and annual, growing season and spring precipitation and temperature values were analyzed using linear regression, analysis of variance (ANOVA). Yield data were also analyzed using Percent Bias (PBIAS), which is calculated as:

$$PBIAS = \left[\frac{\sum_{t=1}^{T}(f_t - y_t)}{\sum_{t=1}^{T}(y_t)}\right] \times 100$$

where f_t is the simulated yield value at time t, and y_t is the actual yield at time t. PBIAS statistically measures the average tendency of simulated data to be greater or less than observed values (Srinivasan et al., 2010). Negative PBIAS values indicate model under-estimation, while positive values indicate model over--estimation bias (Gupta et al., 1999). PBIAS values less than 15% are considered acceptable.

Nitrogen Use Efficiency (NUE) was calculated by taking the average yield at the 22.4, 44.8, 67.3, 89.7 and 112.1 kg N ha^{-1} fertilizer application rates, subtracting the control (0 kg N ha^{-1}) yield and dividing by the fertilizer application rate. Average and yearly fertilizer response curves were generated for simulated and actual yields by subtracting the control yield from yield from each fertilizer treatment and plotting against fertilizer treatment.

Results and Discussion

Yields predicted by SWAT and SWAT-flush were highly correlated with actual average yields and with increasing fertilizer treatments. These data agree with Haney et al. (2016) who found that SWAT simulated yields are highly dependent upon fertilizer N, with unrealistically low yields at 0 kg N ha^{-1} applied and increasing yields at higher fertilizer rates. SWAT under-predicts yield at all fertilizer levels (PBIAS = -59). These data contradict research showing that SWAT tends to over-estimate yield when adequate fertilization is simulated with reported average PBIAS values of 8 for corn and soybean crops in the Upper Mississippi River Basin (Srinivasan et al., 2010). SWAT-flush yields are closer to the 1:1 relationship between actual and simulated yield than SWAT and most closely predicts average yield (PBIAS = -3, Figure 14). The correlation between simulated and actual average yield agrees with Mittelstet et al. (2015) who also found that average small grain and row crop yields simulated with SWAT over a 50-year period in western Oklahoma correlated with National Agricultural Statistics Service (NASS) average yield data.

The slope of the regressions in Figure 14 may be explained by erroneous estimates of NUE, which reflect on inaccurate modeling methods. SWAT and SWAT-flush appear to over-estimate NUE values at higher fertilizer rates, (20% simulated NUE versus 14% actual NUE at 112.1 kg N ha^{-1} applied) causing yields to increase unrealistically with additional N applied. All calculated NUE values were lower than reported NUE values, which range from 23% to 50% (average 33%) in winter wheat cropping systems (Raun et al., 1998, Raun and Johnson, 1999; Thomason et al., 2000). SWAT and SWAT-flush NUE values were not significantly different ($p = 0.05$) for any year simulated, indicating that estimated N uptake did not vary with annual temperature or precipitation values. In contrast, there is a statistically significant difference ($p < 0.001$) between annual field NUE values, as would be expected with varying annual growing conditions and stresses.

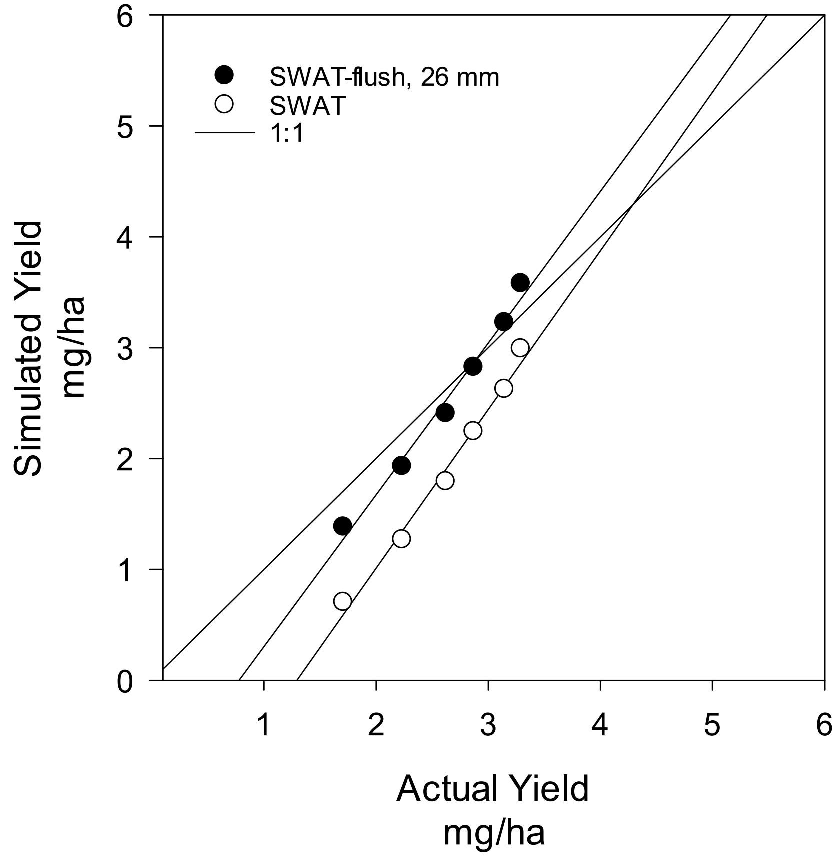

Figure 14. Relationship between actual wheat yields averaged over 26 years and yields predicted by SWAT and SWAT-flush. Simulated yields were all strongly correlated with actual yields ($r^2 = 0.99$); however, the regression between SWAT-flush and actual yields was closest to the 1:1 relationship.

Actual average yields from the 44.8, 67.3, 89.7, and 112.1 kg N ha^{-1} treatments were not significantly different from each other ($p = <0.001$, Figure 15). These data correspond with research by Arnall et al. (2009) that indicates wheat grain yields do not always vary with differing N application rates. Raun et al. (2010) also found that grain yield did not correlate with fertilizer treatments at the same research site as well as at other sites in Oklahoma and Nebraska. Similarly, in long-term corn and wheat N-fertilizer experiments from Iowa, Oklahoma, Nebraska, and Wisconsin, increased N fertilization did not result in increased yield over moderate N fertilization rates (Arnall et al., 2013). The data indicating that there is no significant difference between actual yields at higher fertilization rates (> 22.4 kg N ha^{-1}) is important when attempting to simulate yield with environmental models as we would expect N fertilization to greatly affect plant-growth processes. In fact, the differences in the mean yields from each fertilizer treatment simulated by SWAT and SWAT-flush are greater than would be expected by chance and there is a statistically significant difference ($p = <0.001$) indicating that these models are not accurately representing field conditions.

Because there was a significant difference in NUE values for the field data, but not a significant difference between yields from fertilizer treatments above 22.4 kg N ha^{-1}, we examined actual fertilizer response curves for each year during the study. Annual gains in yield and fertilizer response curves for actual and simulated yields were generated by subtracting the control (0 kg N ha^{-1}) yield from the fertilizer plot yields.

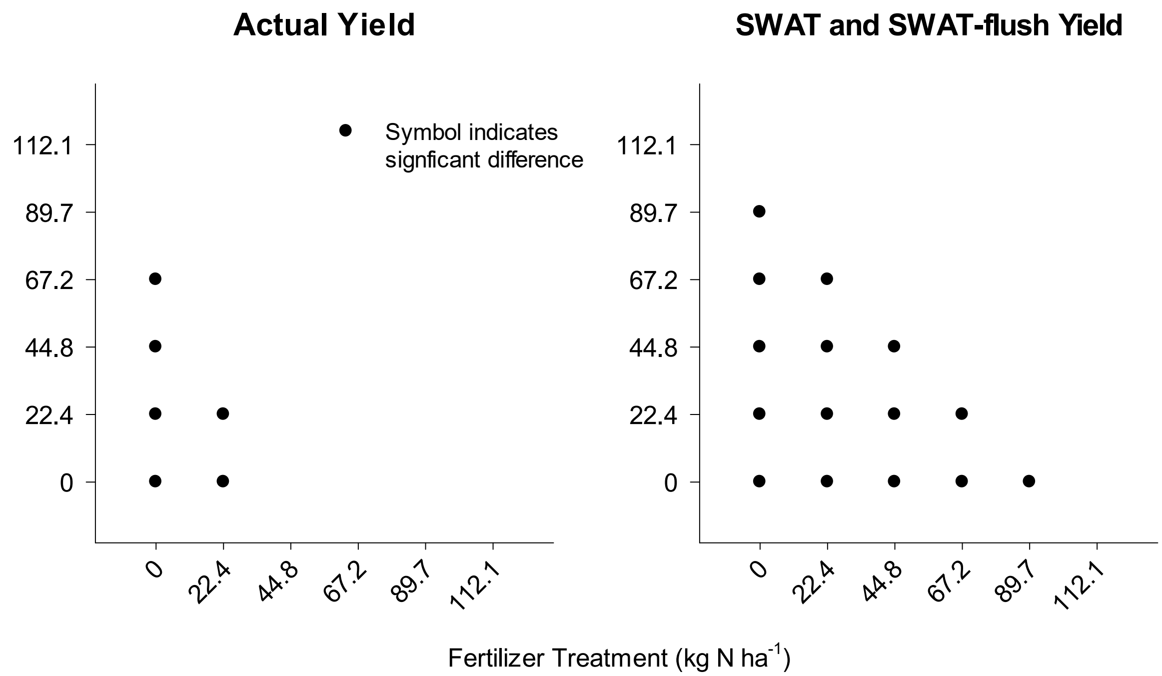

Figure 15. Analysis of variance of actual yields and yield simulated by SWAT and SWAT-flush by fertilizer treatment averaged over the period of study. The symbol indicates a significant difference between treatments.

While the annual fertilizer response curves were overall strongly correlated with the gain in yield, individual yearly fertilizer response curves were highly variable (Figures 16 and 17). In 1987, 1988, 1990, 1992, 1993, 2000, and 2001, actual yield decreased at the highest fertilization rate (112 kg N ha^{-1}) as compared to the 67.3 kg N ha^{-1} treatment. During several years (1987, 1991, 2001, 2002, 2006, and 2007) there was a loss in gain or negligible gain in yield with increasing fertilizer application rates. Similarly, the fertilizer response curves for simulated yields were highly variable (data not shown).

Most notably, in 2001 and 2012 there was no response to simulated fertilizer additions. Variability in gains in yield increase as the fertilizer rate increases for simulated and actual yield (Figure 18). The mean gain in actual yield was greatest for the 89.7 kg N ha^{-1} fertilizer treatment and actual gains were more variable than simulated gains in yield. These data agree with findings by Mohammed et al. (2013) which indicate that in wheat grain yield, the highest rates of N fertilization do not result in the highest yielding plots. Although we did find a correlation between the yearly increase in yield and increasing fertilizer application, the observed variation in fertilizer response from year to year at the experiment site indicate that on annual basis, yield response to N cannot be predicted. These data are supported by Raun et al. (2010) who indicate that N response and yield measurements were independent in long term studies in Oklahoma and Nebraska. While plant growth relative to fertilizer application is expected to vary with changing environmental conditions, we were surprised to find the drastic differences in response curves from year to year.

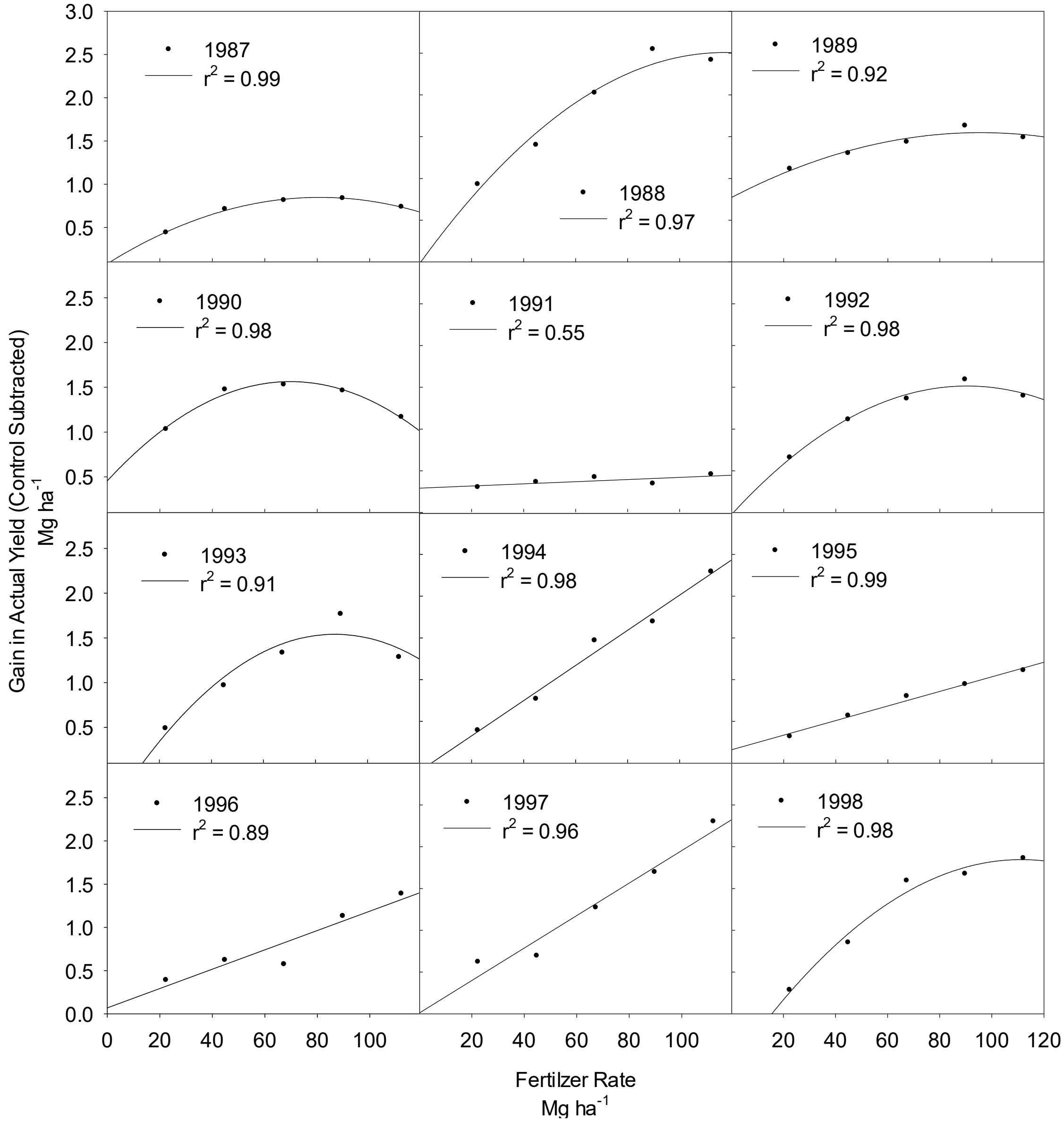

Figure 16. Yearly fertilizer response curves for the field experiment years 1987 through 1998.

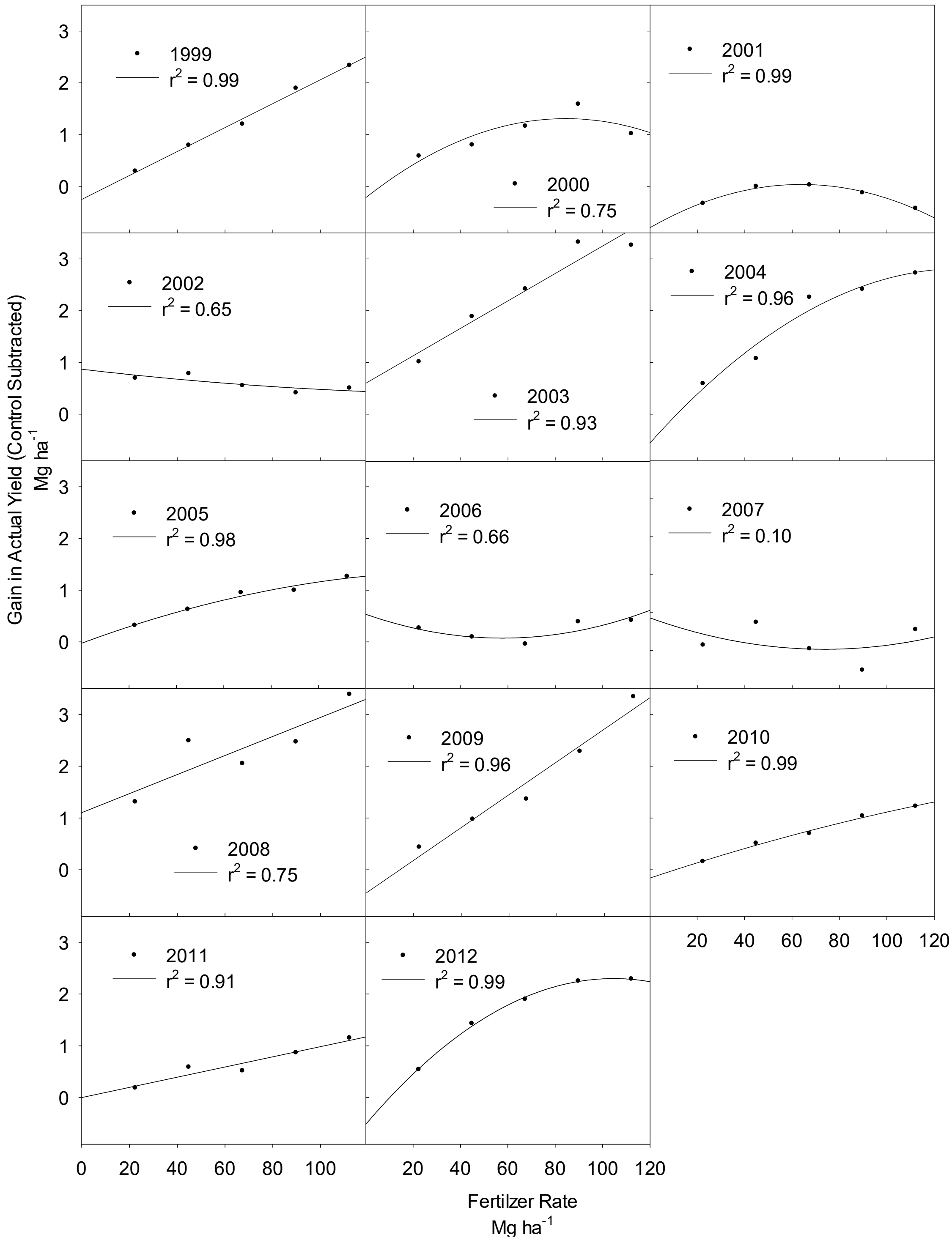

Figure 17. Yearly fertilizer response curves for the field experiment years 1999 through 2012.

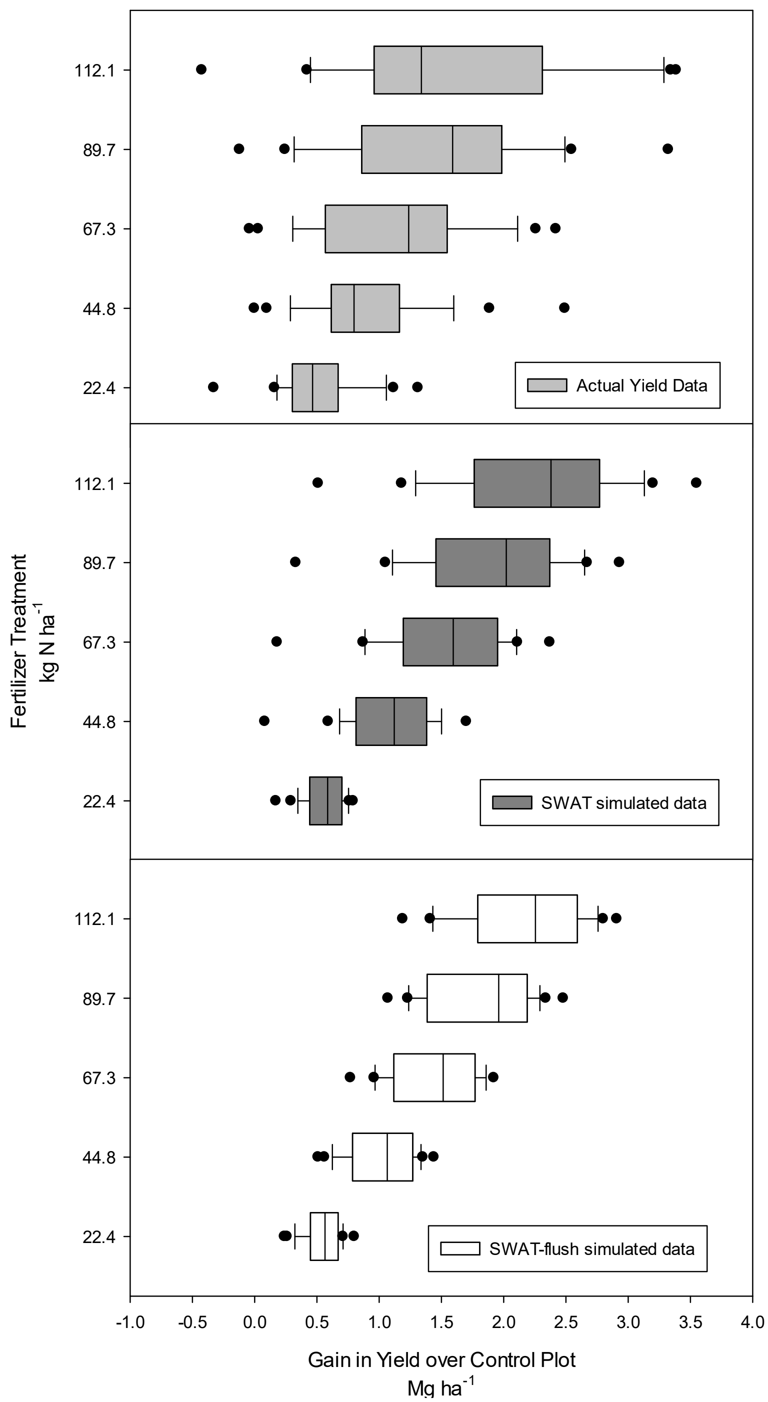

Figure 18. Variability in the gain in yield for fertilized plots over the control plot (0 kg N ha^{-1}) for actual, SWAT simulated, and SWAT-flush simulated yield data.

Only actual annual yields from 2003 and 2008 were significantly different from the remaining years in the study, as well as 1988 vs. 2001 and 2010, and 2010 vs. 2012 ($p =< 0.001$) also being significantly different from each other. In the years with high yields (especially 2003 and 2008) NUE values exceeded 100% indicating that gains in yield were not attributed to fertilizer application alone and N was obtained from mineralization or residual N in the soil. Similarly, there was no significant difference in SWAT simulated yields from year to year ($p = 0.145$). In contrast, SWAT-flush simulated yields had greater variability, with several years being significantly different from each other according to ANOVA analysis ($p =< 0.001$). These data contrast with results reported by Mittelstet et al. (2015) who indicate that while yields varied from year to year over a 50-year period, simulated yields were not significantly different. Ultimately, crop yield is dependent upon the aboveground biomass growth as regulated by temperature, N and water stress as well as a predetermined harvest index, which is the fraction of biomass removed as dry economic yield (i.e. the grain portion of wheat). Detecting inter-annual variability and the source of variability is important when simulating processes that may or may not control yield in the field and in the model. However; because the variability in actual yields was limited mainly to 2003 and 2008 and yields from each fertilizer treatment were not significantly different from each other, it may be difficult for us to determine the forcing factors affecting annual yield.

Simulated annual yields, averaged for all fertilizer treatments, do no correlate with actual annual yields averaged over all fertilizer treatments (SWAT, $r^2 = 0.01$; SWAT-flush, $r^2 = 0.10$; Figure 19). Actual annual yields for each fertilizer treatment also do not correlate with simulated yields for the corresponding fertilizer treatment (SWAT, $r^2 < 0.05$; SWAT-flush, $r^2 < 0.23$).

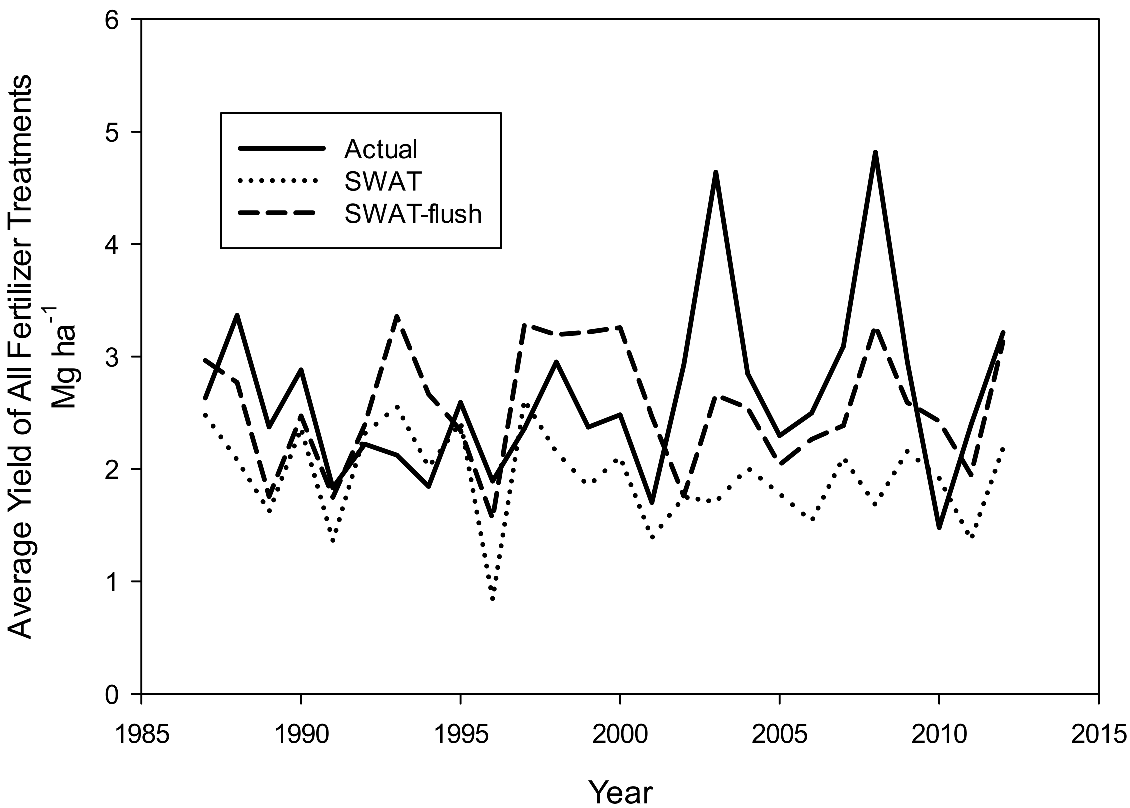

Figure 19. Average simulated and actual yields by year. There was no correlation between annual simulated and actual annual yields when yields were averaged across all fertilizer treatments (SWAT, r^2 = 0.01; SWAT-flush, r^2 = 0.10).

These data correspond to findings by Kiniry et al. (1995) and Srinivasan et al. (2010) who indicate that the EPIC plant growth model sometimes does not accurately replicate annual variations in crop yields well. Srinivasan et al. (2010) attribute the inability of SWAT to predict annual yields consistently to a lack of site specific soils and management data at the scale of their study; however, soils information, planting and harvesting dates, and tillage practices were well documented at the Lahoma, OK study site and closely followed in the SWAT management input files. Therefore, in this case the lack of management data was not the source of inter-annual discrepancies. The lack of a relationship between actual and simulated yield is supported a study by Wang et al. (2016), who found that the SWAT model did not simulate annual corn yield well when soil moisture values were not used in calibration.

Actual and simulated yields were not correlated with annual (r^2 <, 0.18), growing season (actual, $r^2 < 0.02$; SWAT, $r^2 < 0.24$; SWAT-flush, $r^2 < 0.28$) or spring (February to June) precipitation (actual, $r^2 < 0.03$; SWAT, $r^2 < 0.30$; SWAT-flush, $r^2 < 0.31$) for any fertilizer treatment. Actual and simulated yields tend to increase or peak the year following a wet year; however, that was not always the case (Figure 20). The two highest yielding years in the field, 2003 and 2008, followed years with higher than average total and growing season rainfalls; however, many years following higher than average rainfalls did not experience greater than average yields. Actual and simulated yields were also not correlated with total, growing season or spring average temperatures or any combination of rainfall and temperature independent variables ($r^2 < 0.02$) agreeing with data from Girma et al. (2007) who found that actual wheat yield for the same field study could not be predicted by fertilizer treatment or cumulative precipitation.

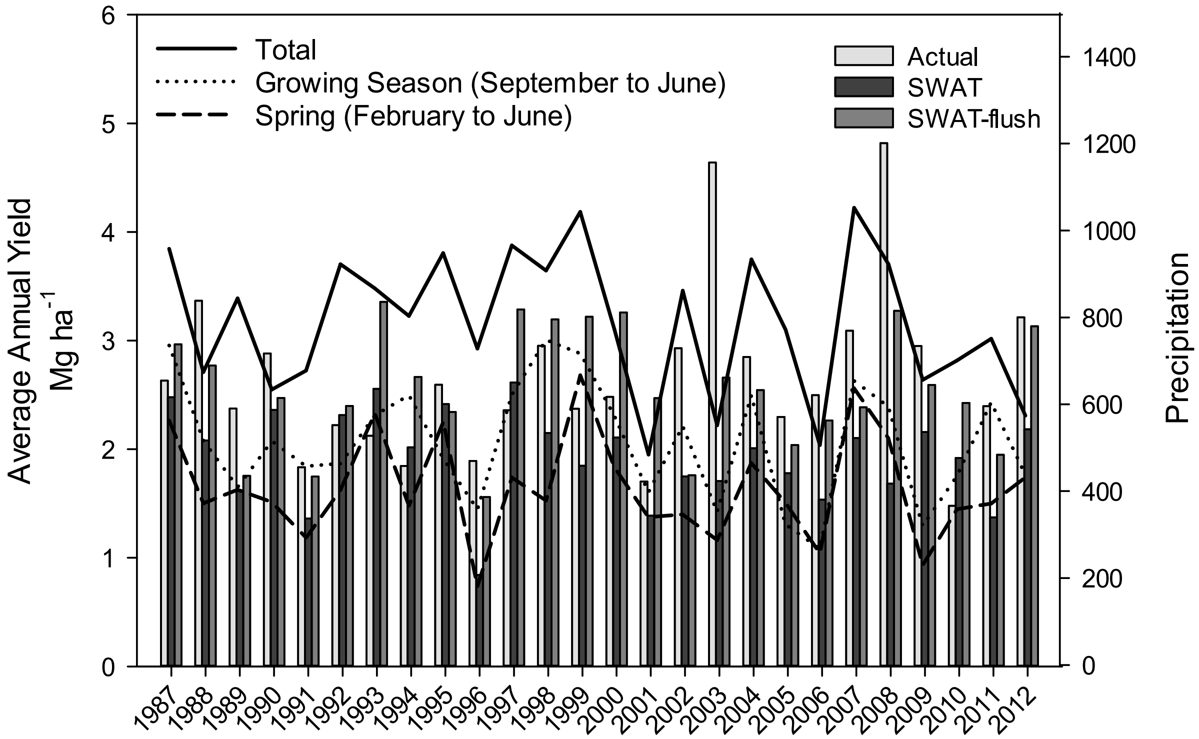

Figure 20. Average annual yields compared to growing season, spring, and total precipitation.

In SWAT, potential plant growth under ideal growing conditions is calculated daily. This growth is tempered by water, temperature or nutrient stress by comparing optimal and actual levels for each type of plant. Stress is calculated non-linearly between 0 and 1, with 0 being optimal temperature, moisture or nutrient levels and 1 being the highest stress level for each factor. Optimal biomass growth is multiplied by the highest stress factor for each day to determine actual growth. In our simulations temperature stress occurred more often than any other stressors; however, estimated yield was not correlated with cumulative temperature, water or phosphorus stress days. SWAT (r^2 = 0.78) and SWAT-flush (r^2 = 0.75) simulated yields could be best predicted with a linear combination of N fertilizer (kg N ha^{-1}), N mineralized (kg N ha^{-1}) and the number of N stress days.

Conclusions

There was no significant difference between actual yields at fertilization rates greater than 22.4 kg N ha^{-1} or a significant correlation between actual yields and precipitation or temperature. These data are important as the model assumptions, as well as agricultural producer expectations, are that N fertilization and weather greatly affect annual grain yield. This information should not only be alarming to the modeling community, but also to agricultural producers and economists, as our traditions may be based on falsely held beliefs. While gains in actual yields on a yearly basis were correlated with increasing fertilizer applications in most years, the response to fertilizer was highly variable from year to year. The data indicate that from year to year at this study site there was no predictable wheat yield or economic gain to be had from fertilizing at high rates, regardless of the commonly held misperception that the more N inputs, the greater the yield. While it may be true that an increase in yield will be observed by the application of 112.1 kg N ha^{-1} versus a control plot, the data in presented in this paper indicate that fertilization rates exceeding 44.8 kg N ha^{-1} have no significant effect on wheat yield. NUE values were considerably low in the field which may be a contributing factor to N nonpoint pollution. These data are noteworthy as agricultural producers are not only losing money by applying fertilizer at rates that do not significantly affect yield, but also that N losses from the over-application of fertilizer are potentially threatening our environment.

While actual and simulated yields over the 26-year study period were highly correlated, SWAT under-predicted yield. SWAT-flush yield estimations were improved over basic SWAT and average yields were closer to the 1:1 relationship between average predicted and actual yield. Neither model accurately predicted annual variability in yields. These data indicate that N modeling in SWAT may not be effective in simulating soil processes sensitive to changing environments, such as soil moisture and temperature resulting in erroneous yield prediction.

Further research needs to be conducted to increase the accuracy of annual yield prediction. In the model, basing annual yield on an arbitrary yield potential tempered by N, temperature, and moisture stress is problematic as is seen in the discrepancy between simulated yield and actual yields. Moreover, our ill-conceived concept of yield potential and N response is mirrored in the field as evidenced by low NUE values, lack of fertilizer response, and lack of correlation between environmental factors and yield. Clearly, there is a dearth of knowledge regarding the complex soil/plant/environmental interactions in the field that must be further considered and examined. In the meantime, SWAT-flush should be utilized to more closely predict wheat crop yields when averaged over a longer study period.

CHAPTER IV

COMPARISON OF WHEAT YIELD SIMULATED USING THREE N CYCLING OPTIONS IN SWAT

Introduction

The Soil and Water Assessment Tool (SWAT) model has been successfully used to predict streamflow, evapotranspiration and soil water. The crop growth model in SWAT was adapted from the EPIC model (Williams et al., 1995) and is similar in concept to the crop growth models in Agricultural Policy/Environmental Extender Model (APEX, Gassman et al., 2010), ALMANAC, and WEPP, which have undergone significant crop yield validation. SWAT crop yields have been validated for several grain crops (Gassman et al., 2010).

Preliminary data suggest that while the hydrologic balance in each watershed may be accurately simulated with SWAT, the SWAT model tends to over- or under-predict wheat yield responses to N-fertilizer application. For example, Haney et al. (2016) found that simulated wheat yield increased strongly with N-fertilizer additions (r^2=0.80), yields at higher N fertilizer rates were over-estimated and at lower N fertilizer rates were under-estimated. In addition, when N fertilizer was not applied during simulation, predicted yields were close to 0 Mg ha^{-1}. These results indicate that SWAT is not properly accounting for soil N cycling processes. Yield under-estimates at low fertilization rates could occur if modelled N - mineralization rates are under-estimated, causing under-prediction of plant N availability and over-estimates of N limitation.

Under-estimates of plant N availability can compound yield errors by suppressing yield responses to simulated soil water variation. Many current N cycle models, including SWAT, tend to neglect the contribution of the soil microbial population to the plant-available N pool, resulting in an under-estimation of yield and possible over- or under-estimation of N runoff from natural and agricultural landscapes.

The SWAT model now has three different N simulation options, SWAT-flush (Haney et al., under review), N routines derived from the CENTURY model (Zhang et al., 2013), and a one-pool C and N model option (Kemanian et al. 2011). SWAT-flush cycles N through three organic N pools (fresh residue, stable and active organic) and two inorganic N (NO_3^- and NH_4^+) pools with an added flush of N after significant rainfall events (greater than 26 mm). The variation of the CENTURY model is more complex than SWAT-flush, simulating microbial, slow and passive soil organic N, surface microbial N, above and below ground structural and metabolic N, and mineral N (Zhang et al., 2013). On the other hand, the one-pool C model merges C, N, and P soil organic matter (SOM) pools within each soil layer, as well as separate residue and manure pools in the topsoil and subsoil.

In this study, measured wheat yield from a long-term fertilizer study research plot in north-central OK, were compared to simulated wheat yield values from SWAT-flush, SWAT-C, and SWAT-One. The objective of this study is to assess the ability of various N cycling sub-routines within SWAT to predict yield at a long-term fertilizer study in Oklahoma.

Materials and Methods

SWAT-flush utilizes three organic N pools (fresh, stable and active organic) and two inorganic N pools (NO_3^- and NH_4^+) and an added flush of NO_3^- after rainfall events greater than 26 mm (Figure 21). The SWAT-flush model algorithms were derived from the PAPRAN (Production of Arid Pastures limited by RAinfall and Nitrogen) model (Seligman and van Keulen, 1981). Mineralization, decay, and immobilization equations are first order kinetics, which are based on the substrate amount, determined by a model "warm up" period of several years prior to the years of interest.

The sizes of the organic N pools are assigned assuming that the C:N ratio for humic materials is 14:1. The concentration of humic organic nitrogen is determined based on the soil organic C (SOC) values from soil data contained in SWAT input files. The soil data must be entered by the user and can either be obtained from soil sampling or publicly available data sets such as the Soil Survey Geographic Data Base (SSURGO, USDA-NRCS, 1995).

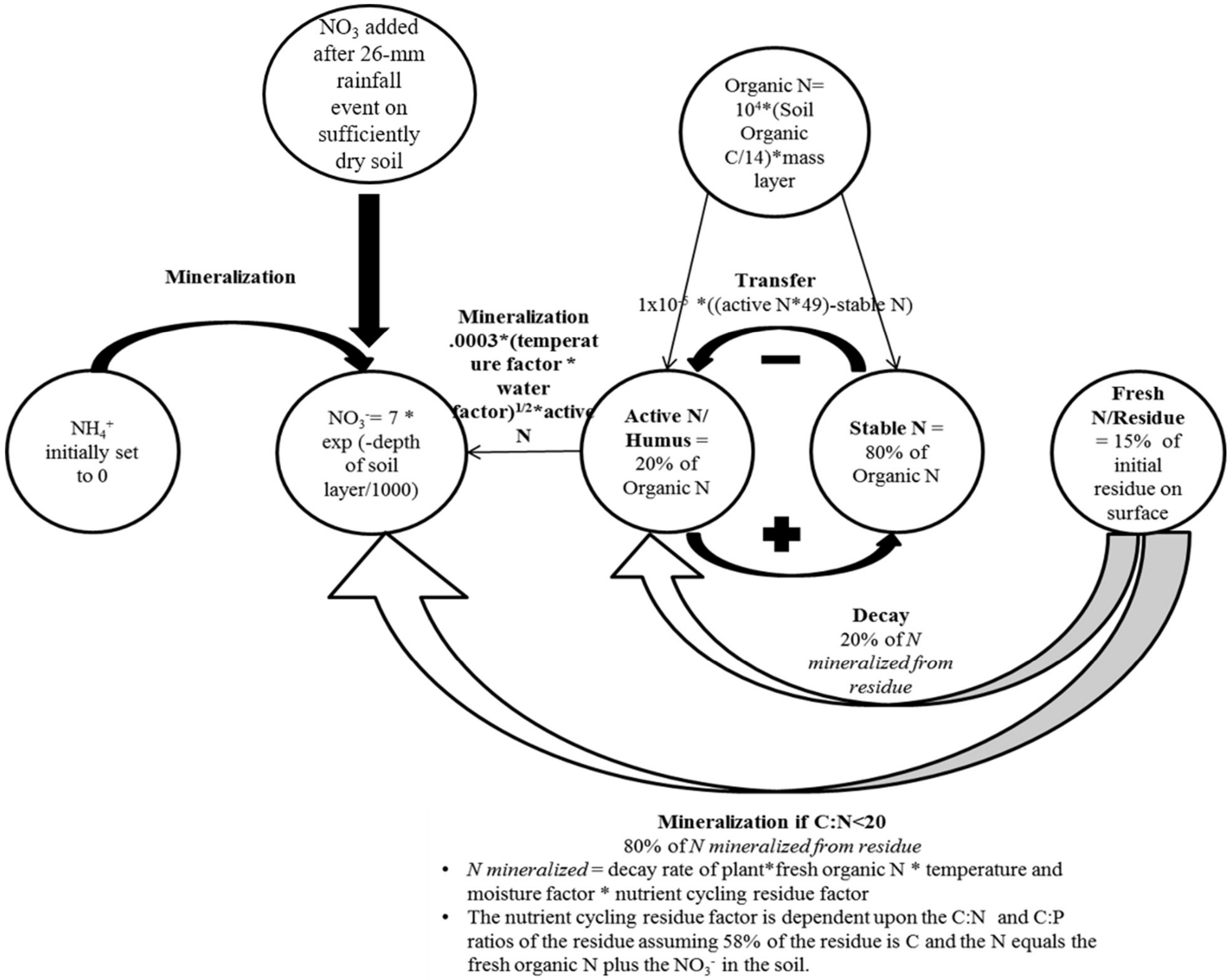

Figure 21. The N cycle as defined in the SWAT-flush model (Haney et al., 2016; Neitsch et al., 2009).

SWAT-flush then assigns 20% of the organic N to the active pool and 80% of the organic N to the stable pool (Neitsch et al., 2009). The initial residue (fresh) pool is assigned to the top 10 mm of the soil profile and is set to 15% of the initial amount of residue on the soil surface, and does not include root biomass. After initialization, the fresh pool is determined based on simulated management practices. The simulated N resulting from decomposition and mineralization of the fresh pool is partitioned as 20% to the active organic and 80% to the NO_3^- pool. Decomposition and mineralization in SWAT-flush depend on the residue decomposition rate, the C:N and C:P ratios of the residue in the soil layer, and soil temperature and water content. N cycling processes are calculated for each soil layer within the profile.

Initial NO_3^- concentration is an exponential function of soil depth. The NH_4^+ pool is initially set to zero and only contributes to the NO_3 pool when urea fertilizer is added to the soil. Nitrification and volatilization describe the conversion of NH_4^+ to either NO_3^- or NH_3, respectively. SWAT-flush simulates both processes simultaneously then partitions the calculated values between the two processes (Nietsch et al., 2009). The nitrification process in SWAT-flush depends solely on the soil water and temperature. While temperature and soil moisture are critical forcing factors on the nitrification process, SWAT-flush does not specifically account for soil microbial activity, soil pH, or the water-extractable soil C or N content, which form the C and N source for the microbial population. Volatilization simulation in SWAT-flush depends on soil temperature and depth and includes a default cation exchange factor. Volatilization is also strongly affected by soil pH, wind conditions, and soil clay content and type (Coyne, 1999).

SWAT-flush incorporates an addition of NO_3^- to the NO_3^- pool after a rainfall event was based on the water soluble organic C and N (WSOC and WSON) and microbial activity determined using 1-d CO_2 evolution.

$$Flush\ of\ NO_3^- = WSON \times (1 - d\ CO_2 \div WSOC)$$

The flush of N is added to the top 10 mm of soil to simulate rapid changes in soil moisture, temperature and N cycling at the soil surface. After a significant rainfall event (greater than 26 mm) occurs on sufficiently dry soil (based on soil matric potential), a flush of N is added to the NO_3^- pool.

The CENTURY-based N simulation option was first incorporated into the Environmental Policy Integrated Climate (EPIC) model (Williams, 1995), and was then incorporated into SWAT for testing at the watershed scale and referred to hereafter as SWAT-C (Zhang et al., 2013). The CENTURY option is a multi-pool model whose strength lies in the linkage between organic C and N dynamics. The CENTURY option in SWAT (SWAT-C) includes a residue pool consisting of lignin, non-lignin, and metabolic residue, each having its own decomposition rates (Figure 22). Residue dynamics occur at the surface of the soil and in the top 10-mm layer of soil. SOM is simulated as microbial, slow, and passive pools, each with their own turnover rates. The microbial pool occurs in all soil layers, while the slow and passive pools exist in all soil layers except the top 10 mm. Decomposition of residue and mineralization of SOM depends upon lignin content of the residue, soil temperature, texture and moisture, tillage effects, and O_2 content. Depth profiles of O_2 in SWAT-C differ from both those of CENTURY model and SWAT-flush. Residue composition and lignin content are calculated based on plant age. All mineralization and decomposition processes result in the simultaneous transformation of C and N and ultimate release of CO_2 (Zhang et al., 2013).

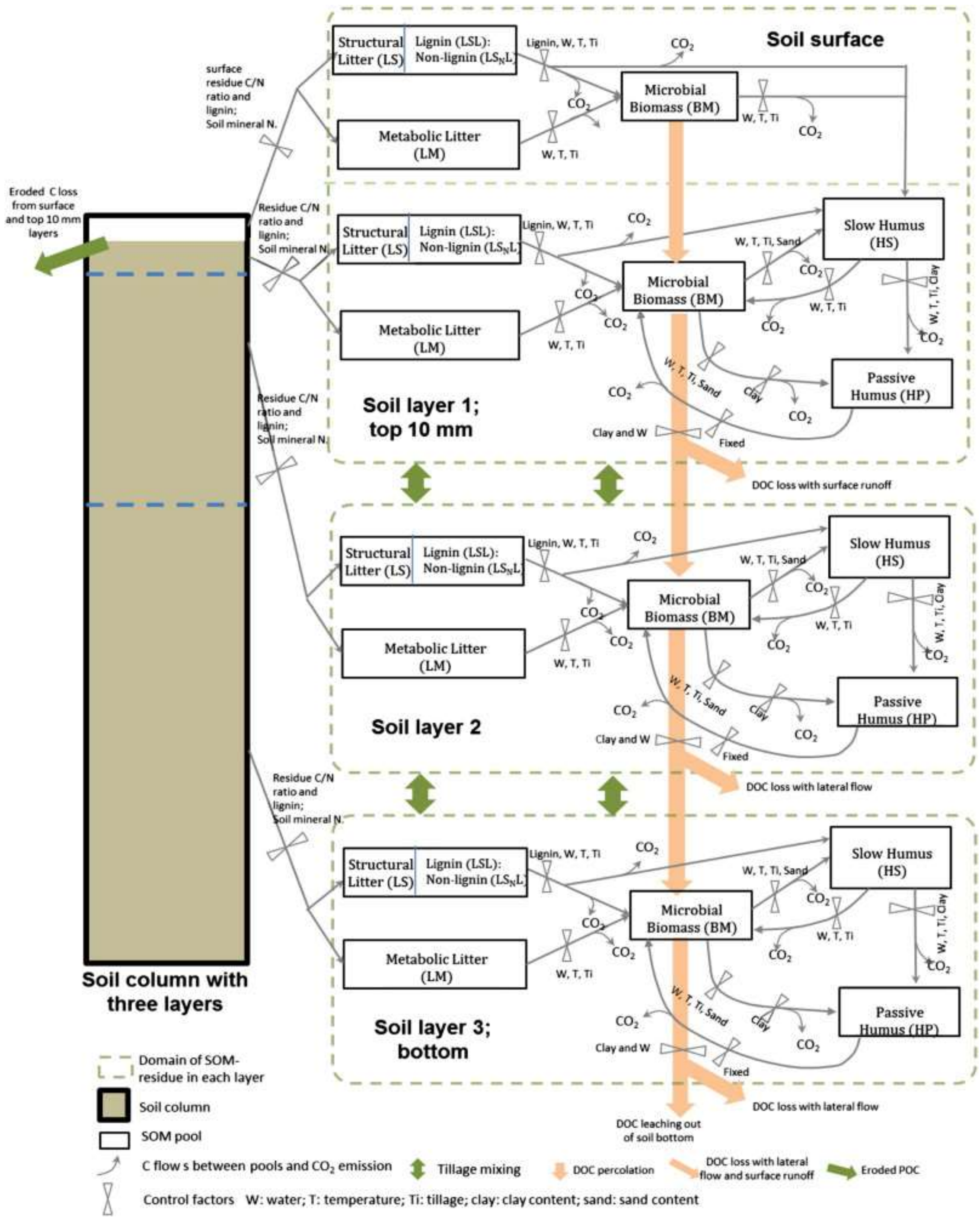

Figure 22. Carbon and N cycling in the SWAT-C subroutine in SWAT (Reprinted from Zhang, X., R.C. Izaurralde, J.G. Arnold, J.R. Williams, and R. Srinivasan, Modifying the Soil and Water Assessment Tool to simulate cropland carbon flux: Model development and initial evaluation, Page 812, 2013, with permission of Elsevier).

As with other models where N dynamics are based on first-order kinetics (basic SWAT), C and N flows in the SWAT-C are controlled by the size of the pools. It is therefore critical that the various organic pools are initialized and tracked correctly. It has been reported the CENTURY model successfully simulates daily CO_2 fluxes except during rewetting periods, which is when important N mineralization fluxes occur (Luo and Zhou, 2010). SWAT-C was tested by Zhang et al. (2013) by comparing simulated results to corn and soybean crop yields on lands across the U.S. Midwest. They found that SWAT-C performed well in its simulations of annual crop yield for sites where detailed management data was known. On the site where management data was not available or sparse, model performance was reduced. In general, Zhang et al. (2013) found that long-term average crop production (corn and soybean) was predicted well using SWAT-C.

The third N cycling option is SWAT-One, a one-pool C, N, and P model (Kemanian et al., 2011). SWAT-One simulates decomposition of a lumped C, N, and P soil organic matter (SOM) pool within each soil layer, as well as residue and manure pools in the topsoil and subsoil (Figure 23). Decomposition of residue and manure follows first order kinetics and results in either mineralization or immobilization depending upon the humification rate and C:N and C:P ratios of the residue, the manure and the SOM. Manure and residue C is either incorporated into the soil C pool or respired as CO_2, and their decomposition rates are functions of soil temperature and moisture. Maximum formation of humus from residue is 0.18 g/g, and the manure maximum humification rate is 1.6 times higher. N mineralized is transferred to the soil NH_4^+ pool. The C:N and C:P ratios of newly formed SOM vary throughout simulation depending upon available mineral N and residue or manure C:N ratios. If there is not enough organic N to supply the microbial N needed for decomposition with a continuously changing soil C:N ratio, mineral N is immobilized. SOM decomposes depending upon a tillage factor and soil moisture. Mineralized N from the SOM is transferred to the NH_4^+ pool and is always positive. Testing of the SWAT-One option has been minimal to date.

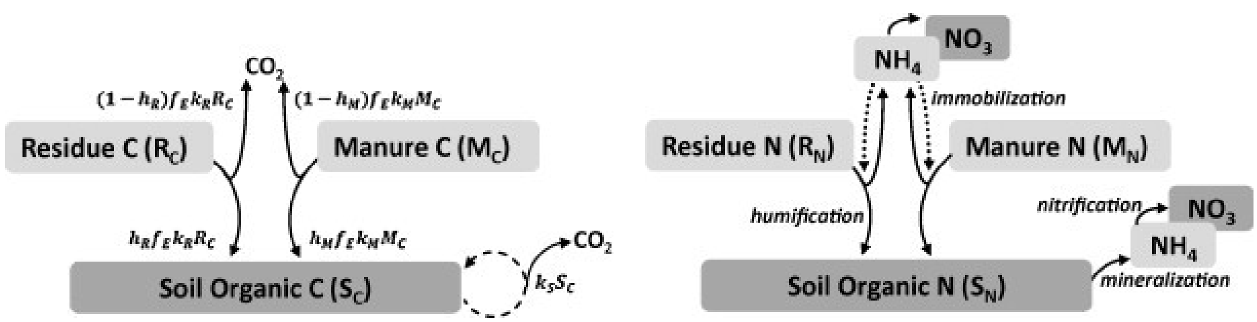

Figure 23. The one-pool C, N, and P submodel (SWAT-One) within SWAT ((Reprinted from Kemanian, A.R., S. Julich, V.S. Manoranjan, and J.R. Arnold, Integrating soil carbon cycling with that of nitrogen and phosphorus in the watershed model SWAT: Theory and model testing, Page 1915, 2011, with permission of Elsevier).

The various SWAT simulations were compared to data obtained from Oklahoma State University's long-term wheat yield study (Experiment 502) in Lahoma, OK. The Experiment 502 plot research is conducted (http://nue.okstate.edu/Long_Term_Experiments/E502.htm) at the North Central Agricultural Research Station near Lahoma, OK (36.42° N, 97.87° W) in Garfield county (Raun et al, 2000). The OSU study was established in 1970 to study the response of wheat grain yield to varying rates of long-term N, P, and K fertilizer application. The randomized complete block (4 replications) designed experiment is conducted on continuous winter wheat grown under conventional tillage on a Grant silt loam (fine-silty, mixed, thermic Udic Argiustoll). The soil has an average pH of 5.7 in the top 30 cm (Raun et al., 1998). Soil depth, texture, slope, albedo and SOC content were obtained from SSURGO (USDA-NRCS, 1995). Mean average temperature at the research site is 15.6 °C (Raun et al., 1998) with an average annual rainfall of approximately 800 mm (Schroder et al., 2011). Nitrogen was applied as Urea (46-0-0) at pre-plant rates of 0, 22.4, 44.8, 67.3, 89.7, 112.1 kg N ha^{-1} annually. Phosphorus was applied as triple superphosphate (0-46-0) at the rates of 9.9, 19.7, 29.6, 39.5 kg P/ha annually. Fertilizer application occurred between early August and early October and planting followed from late September to late October. The wheat seeding rate varied between 0.07 and 0.08 Mg ha^{-1}. Grain was harvested from early June to early July, depending upon weather conditions.

Yield simulations were performed by constructing a set of SWAT input files using local weather and soils data in the Texas Best Management Practice Evaluation Tool (TBET, White et al., 2012). Weather data were obtained from the National Oceanic and Atmospheric Administration (NOAA) National Weather Service Cooperative Observer Program, Lahoma Research Station (USD00344950) weather station (Latitude: 36.3894, Longitude: -98.1061, Elevation: 388.6m). Simulations were run for 28 years from 1981 to 2012, for which yield data and most actual planting and harvest dates were available. 1985 and 1986 served as warm up years, to allow initial fractions of SOC and other variables to stabilize prior to simulation of the period of study. When dates were unavailable, an average October 21 planting date and June 13 harvest date was used (6 cases where one was missing). Simulations included 12 combinations of N and P rates and forms that correspond with the fertilizer rates used in Experiment 502.

Simulations were performed with uncalibrated SWAT models. Previous research has indicated that the SWAT model can successfully predict crop yield without calibration (Srinivasan et al., 2010). In addition, we were interested in seeing the raw results from an uncalibrated model for comparison to actual field data. Yield data obtained from each N modeling option in SWAT (SWAT-flush, SWAT-C, and SWAT-One) were compared to historical yield data using linear regression analysis, descriptive statistical analyses, percent bias (PBIAS), Nash-Sutcliffe efficiency (NSE) and nitrogen use efficiency (NUE) analysis, Pearson Correlation Coefficients and Analysis of Variance (ANOVA, Systat, 2012).

Nitrogen Use Efficiency was calculated by taking the average yield at the 22, 45, 67, 90 and 112 kg N ha^{-1} fertilizer application rates, subtracting the control (0 kg N ha^{-1}) yield and dividing by the fertilizer application rate. NUE is chiefly regulated in all SWAT model N variations using attributes listed in the plant growth database (crop.dat). This database includes plant classification (i.e., warm-season annual), radiation-use efficiency, harvest index, maximum potential leaf area index (LAI), optimal and base temperature for plant growth, maximum rooting depth and canopy height, the fraction of N in the harvested portion of the biomass, and potential heat unit information at various stages of growth (Kiniry et al., 1995). The optimal N that should be in plant biomass on a given day is calculated by first determining the fraction of N in the plant as a function of growth stage under optimal growing conditions. Specifically, the fraction of N in a plant on a given day is determined based on the fraction of heat units accumulated on that day and the fraction of N at emergence, maturity, and midseason which were determined experimentally for winter wheat by The University of Saskatchewan (Kiniry et al., 1995). Optimal biomass N for the day is the product of the fraction of N in the plant on a given day and the biomass on the same day:

$$bio_{N,opt} = fr_N \cdot bio$$

where $bio_{N,opt}$ is the optimal mass of nitrogen stored in plant material for the current growth stage (kg N ha^{-1}), fr_N is the optimal fraction of nitrogen in the plant biomass for the current growth stage, and *bio* is the total plant biomass on a given day (kg ha^{-1}). Potential N uptake is subsequently determined using the following equation:

$$N_{up} = \text{Min}\begin{cases} bio_{N,opt} - bio_N \\ 4 \cdot fr_{N,3} \cdot \Delta bio \end{cases}$$

where N_{up} is the potential nitrogen uptake (kg N ha^{-1}), $bio_{N,opt}$ is the optimal mass of nitrogen stored in plant material for the current growth stage (kg N ha^{-1}), bio_N is the actual mass of nitrogen stored in plant material (kg N ha^{-1}), $fr_{N,3}$ is the normal fraction of nitrogen in the plant biomass at maturity, and Δbio is the potential increase in total plant biomass on a given day (Neitsch et al., 2009). Daily control of N uptake depends upon biomass growth each day and the amount of available N in the soil. The amount of available N is determined by initial N in the soil, fertilizer applications, leaching and surface N runoff.

The Nash-Sutcliffe efficiency (NSE) was calculated for simulated versus actual yields for each year, averaged over all fertilizer treatments, to determine how well the observed values versus simulated values fit the 1:1 regression line. NSE is calculated as follows:

$$NSE = 1 - \sum_{t=1}^{T} \frac{(y_t - f_t)^2}{\sum_{t=1}^{T} (y_t - \bar{y})^2}$$

where f_t is the simulated yield value at time t, y_t is the actual yield at time t, and $\bar{y}$ is the mean of the observed data values for the entire evaluation period. NSE values range from -∞ to 1 and the larger the NSE values, the better the model performance (Srinivasan et al., 2010). Percent bias (PBIAS) was used to statistically measure the average propensity of simulated data to be larger or smaller than observed values (Srinivasan et al., 2010). Percent bias is calculated as:

$$PBIAS = \left[\frac{\sum_{t=1}^{T} (f_t - y_t)}{\sum_{t=1}^{T} (y_t)} \right] \times 100$$

where f_t is the simulated yield value at time t, and y_t is the actual yield at time t. Smaller PBIAS values are desired. Negative PBIAS values indicate model under-estimation, while positive values indicate model over-estimation bias (Gupta et al., 1999). PBIAS values less than 15% are considered acceptable.

Results and Discussion

Actual and simulated yields averaged over 28 years were positively correlated with N fertilizer additions ($r^2 > 0.96$) except SWAT-One ($r^2 = 0.33$, Figure 24). When no fertilizer was applied, actual wheat yields averaged 1.71 Mg ha^{-1}. SWAT-C average simulated yield was 1.97 Mg ha^{-1} at 0 kg N ha^{-1} applied and was closest among the submodels to simulating actual yield at this fertilizer rate (PBIAS, 13%). SWAT-C most closely simulated the effect of fertilizer on average actual wheat yield over a 28-year period according to regression and PBIAS analysis (PBIAS, 2%; Table 4). SWAT flush had an improved average NSE value (NSE, -0.05) over SWAT-C (NSE, -0.52). SWAT-One over-estimated yield across simulated fertilizer application (PBIAS, 61%). SWAT-flush under-estimated yield below the 67.3 kg N ha^{-1} fertilizer treatment, but over-estimated at higher fertilization levels (PBIAS -19% at 0 kg N ha^{-1} and 9% at 112.1 kg N ha^{-1}). Srinivasan et al. (2010) found that PBIAS values of simulated yield varied from region to region depending upon the soil data used by SWAT to simulate soil processes. The data in this study; however, indicate that the PBIAS of simulated yield can also vary drastically depending upon the way that N cycling is treated in the model. The yield under-estimates from SWAT-flush at lower levels of N fertilization suggest that his submodel under-estimates plant N availability (or over-estimates N losses) and would lead to over-estimates of the N-fertilizer inputs needed to achieve a given yield.

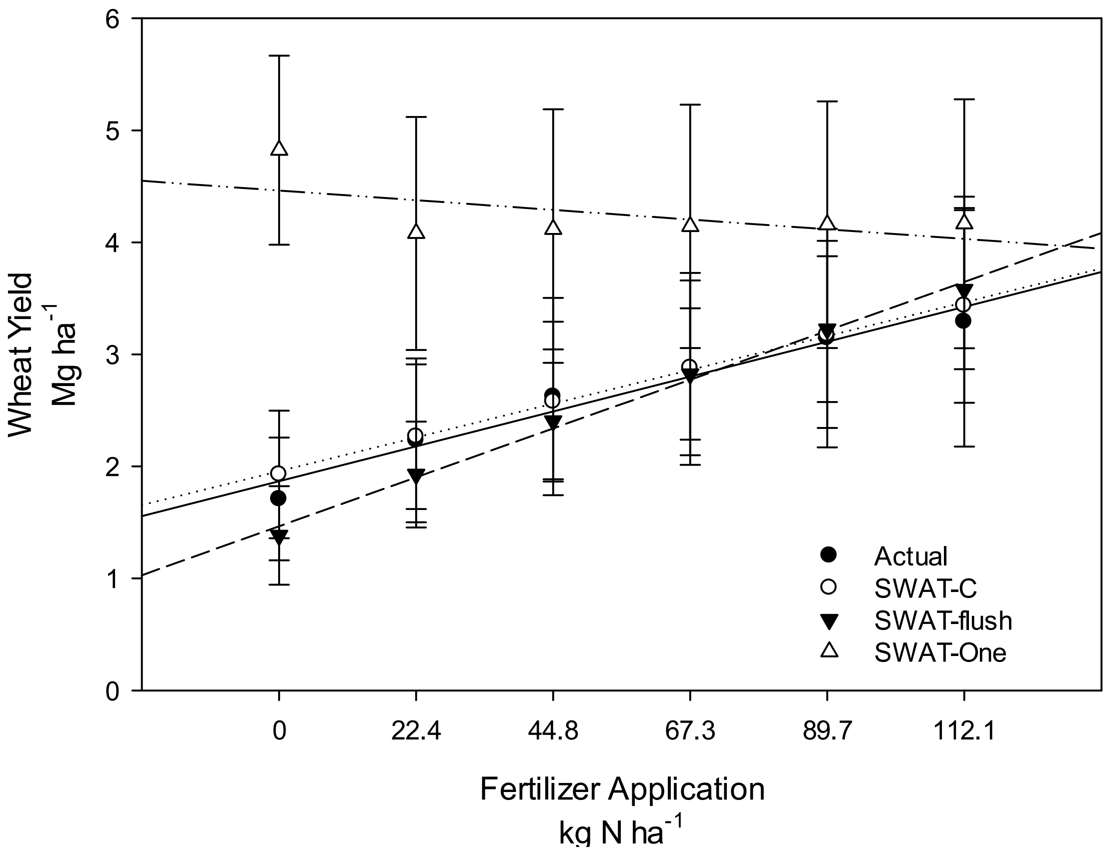

Figure 24. Relationship between N fertilizer additions and simulated and actual yield averaged over 28 years.

Table 4. Percent bias (PBIAS) Nash-Sutcliffe efficiency (NSE) and values of model simulated values at 0 kg N ha^{-1}, 112 kg N ha^{-1}, and the average of all fertilizer treatments.

	0 kg N ha^{-1}		**112 kg N ha^{-1}**		**Avg. All Fertilizer Treatments**	
	PBIAS	NSE	PBIAS	NSE	PBIAS	NSE
SWAT-flush	-19	-1.03	9	0.17	-3	-0.05
SWAT-One	182	-36.02	27	-0.97	61	-5.84
SWAT-C	13	-1.46	4	-0.06	2	-0.52

Yield under- or over-estimates result in erroneous estimates of percent NUE. NUE ranges from 23 - 50% in winter wheat cropping systems (Raun et al., 1998, Thomason et al., 2000). Oklahoma State University reports that NUE for Experiment 502 averages 32% (Raun et al., 1998), although we calculated the average actual NUE values at less than 25%, decreasing with increasing fertilizer applications to 14% at 112.1 kg N ha^{-1} treatment. Simulated NUE values for the submodels also decreased with increasing amounts of N fertilizer (25 to 20% for SWAT-flush, 15% to 14% for SWAT C, and all negative NUE values for SWAT One). The percent of N removed in grain relative to N uptake was 66% for SWAT-C and 70% and SWAT-flush. This value was 37% for SWAT-One, partially explaining the negative NUE values for SWAT-One. SWAT-flush most accurately represented field NUE values. Nitrogen use efficiency can be an important indicator of N dynamics in the soil and is reflective of nitrification, management, weather and plant growth (Thomason et al., 2000). Factors affecting low NUE in the field include losses of N from volatilization, which can be as great as 50% when urea or urea-containing products are applied (Macnack et al. 2013). In addition, N runoff losses range between 1% and 13% (Raun and Johnson, 1999). Certainly, biomass growth, pest, weed, temperature, and moisture stress also affects NUE in the field.

Deviations between simulated and actual yields and NUE values can be partly explained by variations in the way each model handled specific nitrogen pools and transformations (Figure 25). Volatilization varied among the sub-models. On average 81% of fertilizer applied was lost to volatilization with SWAT-One versus a 37% loss with SWAT-flush and SWAT-C. All sub-routines utilize the same volatilization and nitrification subroutines; however, SWAT-One may have simulated higher volatilization compared to SWAT-flush because all N mineralized is added to the NH_4^+ pool, instead of the NO_3^- pool. SWAT-flush does not simulate volatilization unless an NH_4^+ based fertilizer is used. We expected SWAT-C to have greater volatilization, but the average values were similar to those from SWAT-flush.

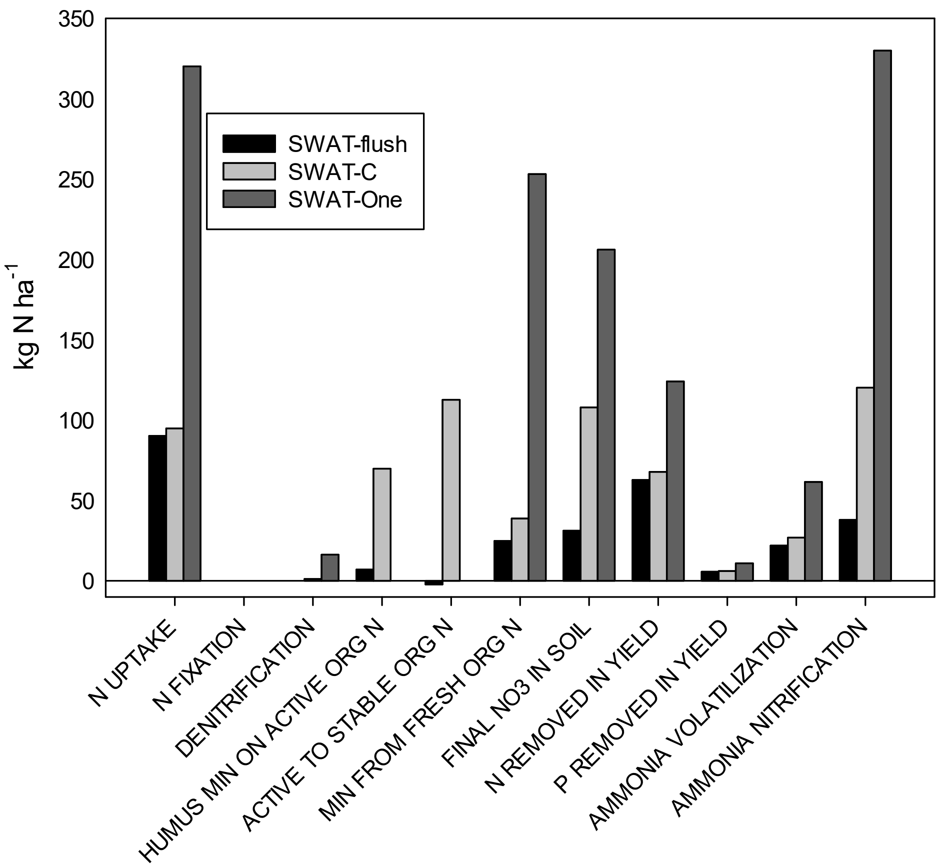

Figure 25. Simulated N cycling values for each of the three N-cycling subroutines. Mineralization values were not available for the SWAT-One model.

Simulated nitrification also varied among the N sub-routines. SWAT-One simulated the greatest amount of nitrification, followed by SWAT-C and SWAT-flush. The fact that SWAT does not account for pH of the soil (average pH 5.7) in any N subroutine complicates replication of the N cycle and plant growth operations, which could influence yield prediction capabilities. Nitrification at pH 5.7 should be low as rates fall distinctly below pH 6 and nitrification should be almost non-existent below pH 5.0 (Coyne, 1960). SWAT-flush nitrification values were equal to that of the NH_4^+ fertilizer added minus the NH_4^+ volatilized. SWAT-one and SWAT-C will continually have significantly higher volatilization and nitrification values than SWAT-flush because they simulate the transformation of organic N to NH_4^+. It may be beneficial to add a pH control to these processes because the volatilization and nitrification values were unrealistically high given the actual pH of the soil simulated. Furthermore, SWAT-flush may benefit from converting mineralized N into NH_4^+ versus NO_3^- to more realistically simulate field N transformations.

Denitrification did not occur in any of the simulations, and therefore did not contribute to simulated yield estimates. Denitrification occurs in the absence of O_2, and varies depending upon soil moisture, temperature, organic matter content, C and NO_3^- concentration (Coyne, 1999). SWAT usually only simulates denitrification under flooded conditions, although it is well documented that this process occurs in small pockets of the soil profile where anaerobic conditions can take place, regardless of the level of the soil water table or complete saturation of the soil.

Simulation of NH_4-N or NO_3-N pools is also critical to accurate yield estimates. N fertilizer applied in excess of plant uptake should increase soil N pools (Raun et al., 1998). During simulations, total soil N (organic N + NO_3^--N) was only increased when yield was simulated using SWAT-One. SWAT-One simulated a marked increase in organic N and NO_3^--N in the soil. SWAT-C simulated an overall decrease in organic N. NO_3^--N values decreased when using SWAT-flush, but increased when using SWAT-One, and SWAT-C. Because this is a conventional till, wheat-fallow cropping system, we would expect that organic N values would decrease over time because of long-term losses in SOC (Doran et al., 1997). Because of the soil texture, we would expect NO_3^- values in the soil to decrease on average. Surprisingly, excess N was not lost to leaching using any of the sub-models even though the soil is a silt-loam and should drain well. Based on these data, it appears that none of the N subroutines are adequately simulating N cycling processes in the soil.

There was a significant correlation between SWAT-flush ($r^2 = 0.34$, $p < 0.001$) and SWAT-C ($r^2 = 0.20$, $p < 0.001$) predicted and actual annual yields (Figure 26). Although the trend is significant, the variability around the regression line indicates that neither model is precise in its predication of annual wheat yield. SWAT-One annual predicted yields were not correlated with actual annual yield. These data suggest that the N-cycling models may be ineffective at simulating mineralization, decomposition or the conversion of urea.

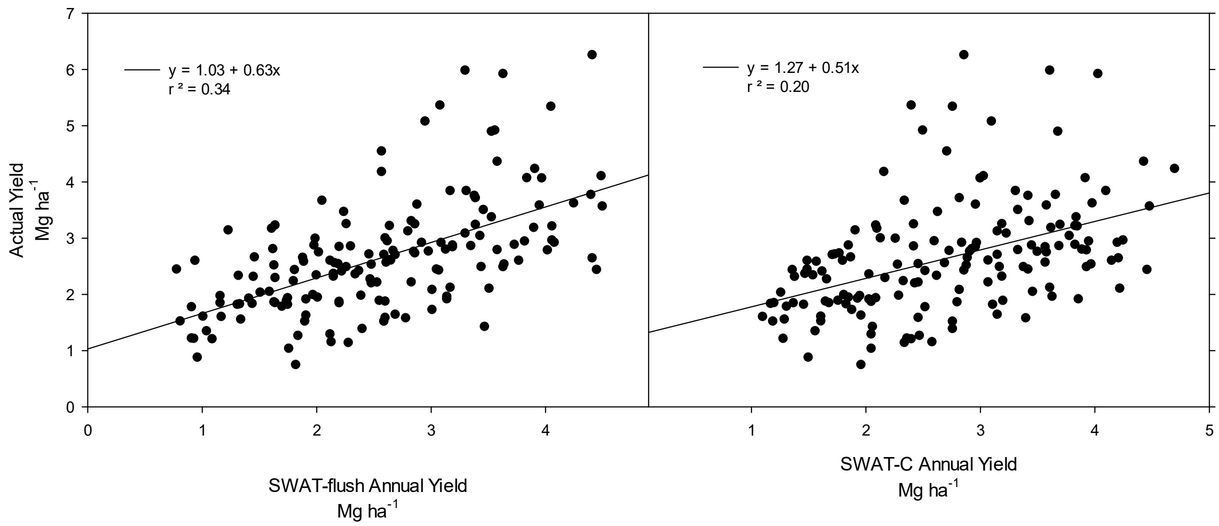

Figure 26. Regression between yearly SWAT-flush and SWAT-C predicted and actual yield for all fertilizer treatments.

As it is in nature, plant growth is moderated in the SWAT model due to water, nutrient, and temperature stress. SWAT calculates the amount of stress for water, temperature, N and P stress daily and reduces plant growth as a percentage of optimal growth when the plant is not dormant. Potential biomass production for each day is calculated as the potential increase in total plant biomass on a given day multiplied by the plant growth factor (Neitsch, 2009):

$$\gamma_{reg} = 1 - \max(wstrs,\ \ tstrs,\ \ nstrs,\ \ pstrs)$$

where γ_{reg} is the plant growth factor (0.0-1.0), *wstrs* is the water stress for a given day, *tstrs* is the temperature stress for a given day expressed as a fraction of optimal plant growth, *nstrs* is the nitrogen stress for a given day, and *pstrs* is the phosphorus stress for a given day. Potential leaf area added on a given day is also adjusted daily for plant stress in the same manner.

All three N cycling options utilize the one maximum stressor for each day. For example, if temperature stress is at 30% and water stress is at 20% for the day, the 30% temperature stress is used to regulate plant growth on that day. Annually, the wheat plants in all simulations were under stress (below optimal conditions for plant growth) between 126 and 177 days per year (Table 5). Phosphorus stress (not shown) was negligible and therefore not reported. Overall, SWAT-One had the least amount of stress days (especially N), which corresponds to its consistent over-prediction of yield. SWAT-flush had the highest N stress days, most likely due to under-prediction of N mineralization at low N fertilization rates. Temperature stress was the same throughout the three N submodels. It appears that water stress was low for all N subroutines and was overshadowed by temperature or N stress on most days.

Table 5. Average annual water, temperature, N, and P stress days for each N cycling routine for the 28-year run.

	SWAT-flush	SWAT-One	SWAT-C
Water stress days	24	15	11
Temperature stress days	109	108	108
N stress days	44	3	35
Total stress days	177	126	154

These results indicate that, except under extreme wet or dry conditions, temperature and N have a stronger influence over simulated yield on a yearly basis than soil moisture. Simulated yields did not differ significantly regardless of yearly precipitation, which indicates that rainfall is not the significant controlling factor in predicted yield. In fact, this research has shown that annual precipitation, spring precipitation, and growing season precipitation were not directly correlated to predicted or actual crop behavior. Lobell et al. (2004) found that in the field soil variability is greater than variability in weather when water availability is not a limiting factor. Based on the results shown in Table 5, it appears that the SWAT model may be overly sensitive to temperature stress, thereby reducing the importance of both N and water stress.

Conclusions

I found that although multi-year average simulated crop yields were well correlated with actual average yields, SWAT-flush under-estimates yield at low N fertilizer levels then over-estimates at higher N fertilization. SWAT-flush most accurately represented field NUE values. On average, SWAT-One was unsuccessful at predicting yields. SWAT-C most closely estimates average yield according to calculated PBIAS values, while NSE calculations indicate that SWAT-flush is more capable of predicting average yield. The N removed in yield relative to N uptake and N volatilization were surprisingly similar between SWAT-C and SWAT-flush; however, nitrification, final NO_3^- in soil, and the amount of water and N stress varied between the two models. Annually, SWAT-flush and SWAT-C yields were correlated with actual yield, but showed a high degree of variability indicating that these submodels may not be reliable for predicting annual wheat yield at sites similar to the study area.

Overall, this research indicates that SWAT-C or SWAT-flush provide the most accurate prediction of average wheat yield and can be used for wheat cropland yield assessment. However; none of the N-cycling routines included in the SWAT model predict annual variations in wheat yield with great certainty. Further research is needed to determine the effectiveness of SWAT-C and SWAT-flush in determining average and annual yield in various farming regions and with numerous agronomic crops.

CHAPTER V

CONCLUSIONS

A N cycling routine simulating the flush of N after significant rainfall events using the measurement of microbial activity and water-extractable N and C was added to the SWAT model (SWAT-flush). SWAT-flush and SWAT predicted wheat yields were first compared to compared to field soil analyses and NDVI greenness in Texas. Yields predicted by SWAT were strongly correlated with fertilizer inputs and yields were insignificant at simulated low fertilization rates. SWAT predicted wheat yields in Texas were not sensitive to changes in the default soil properties associated with soil series descriptions or elevation changes. These results indicate that the SWAT N model is under-predicting N mineralization processes in the soil. In addition, because the N model in SWAT is based on the very large pools of soil organic C and N, which are 40 times larger than the active pool of N and C that the microbes utilize to cycle N, it is less sensitive to spatial variation of N mineralization.

The robust correlation between wheat yield, rainfall, N mineralization, and fertilizer when using the SWAT-flush shows improved simulation of field N mineralization processes. SWAT-flush yields were consistantly higher for each Texas field soil sample as would be expected with the additon of N mineralization resulting from microbial activity. Furthermore, annual yield values, inter-annual variability, and spatial variability were consistantly greater from the SWAT-flush than from the SWAT model. SWAT-flush naturally considers the spatial variability of soils over geographic areas when using field soil data because as the C:N ratio of a soil varies, the MAC_WEON calculation will vary accordingly. For example, spatial analyses of soil properties indicate that healthier soil is located at the north end of the field, which corresponds to lower elevations where the soil holds more moisture and microbial activity is increased. The SWAT model predicts that this area has the lowest yield, when historically it has the highest yield.

To better under-stand forcing factors controlling yields in the field, actual yields from the long-term experiment in OK were compared to precipitation, temperature, and varying fertilizer application rates. There was no significant difference between actual yields at higher fertilization rates (> 22.4 kg N ha^{-1}) or a significant correlation between yield and precipitation or temperature. While gains in actual yields on a yearly basis were correlated with increasing fertilizer applications in most years, the response to fertilizer was highly variable from year to year. The data indicate that fertilization rates exceeding 44.8 kg N ha^{-1} have no significant effect on wheat yield, signifying that, annually, there is no predictable yield or economic gain from fertilizing at high rates. Furthermore, NUE values were considerably low in the field which may be a contributing factor to N nonpoint pollution. These data are noteworthy as model assumptions, as well as agronomist expectations, are that N fertilization and weather greatly affect annual grain yield. The agricultural producers are not only losing money by applying fertilizer at rates that do not significantly affect yield, but also potentially threatening our environment.

Soil organic C values were used as a proxy for microbial activity and WEOC and WEON for the long-term wheat study in Lahoma, OK. SWAT, SWAT-flush, SWAT-One, and SWAT-C predicted yields were compared to actual yields. SWAT-One did not predict average annual or yearly yield effectively. Average annual actual from the long-term study in OK and computed yields from SWAT, SWAT-flush, and SWAT-C were strongly correlated. SWAT consistently under-predicted yield. SWAT-flush and SWAT-C yield estimations were improved over basic SWAT and were closer to the 1:1 relationship between average predicted and actual yield. SWAT-C most closely estimates average yield according to calculated PBIAS values, while NSE calculations indicate that SWAT-flush is more capable of predicting average yield. SWAT-flush tends to under-estimate yield at low N fertilizer levels and over-estimate yield at higher N fertilization. SWAT-flush most accurately represented field NUE values. The N removed in yield relative to N uptake and N volatilization were similar between SWAT-C and SWAT-flush; however, nitrification, final NO_3^- in soil, and the amount of water and N stress varied between the two models.

None of the N cycling models were precise in detecting inter-annual variability in actual yields. Annually, SWAT-flush and SWAT-C yields were correlated with actual yield, but showed a high degree of variability indicating that these submodels may not be reliable for predicting annual yield.

Overall, this research indicates that SWAT-C or SWAT-flush provide the most accurate prediction of average wheat yield and can be used for wheat cropland yield assessment. The equations used to model the complex biogeochemical N cycling relationships in SWAT-flush are elegant in their simplicity, yet capture the spatial complexity associated with their processes and improved yield prediction by SWAT significantly. SWAT-C is substantially more complex than SWAT and SWAT-flush and may be preferred if yield simulation and C cycling output is desired. However; none of the N-cycling routines included in the SWAT model predict annual variations in wheat yield with great certainty.

Future studies will need to include long-term yield data for varying soils, crops and management practices in varying climates. Research may also include variations in the approach to data attainment and management for larger projects at the watershed scale. While this study indicates that SWAT-C and SWAT-flush correctly predict average annual yield, inter-annual variability in yields may be better calculated by obtaining more detailed soils information. Data acquisition may be challenging for large scale projects as it will not be practical to soil test large areas. In addition to the impracticality of large-scale soil sampling, only a few laboratories throughout the United States offer the soil tests that the modified N model is based upon. Satellite imagery may play a critical role in further development for large-scale simulations.

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