SIMULATIONS OF CARBON DYNAMICS AND GREENHOUSE GAS EMISSIONS IN BIOENERGY SORGHUM PRODUCTION SYSTEMS IN TEXAS

A Dissertation

by

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ABSTRACT

Bioenergy sorghum [*Sorghum bicolor* (L.) Moench.] is a promising biofuel crop to mitigate greenhouse gas (GHG) emissions. However, optimum field management practices for its production in different regions and the effects of its long-term production on overall soil-plant-atmosphere carbon (C) dynamics are unknown. Our objectives were to evaluate the long-term regional effects of its production on C dynamics and GHG emissions in Texas, and find the best field management practices for its production in order to maximize yield, sustain soil fertility, and minimize GHG emissions by using the process-based biogeochemical model, DAYCENT.

The model was parameterized by using field measurements of soil temperature, soil water, aboveground biomass C, soil organic C (SOC), and GHG emissions including carbon dioxide (CO_2) and nitrous oxide (N_2O) from a 8-year field trial with treatments of residue return, nitrogen (N) fertilization, and tillage (6 combinations). The results showed an overall satisfactory fit when comparing simulated outputs to measured data, with an r^2 range of 0.49-0.90. DAYCENT was able to simulate the pattern and magnitude of measurement variation caused by treatment and seasonal change.

Life cycle analysis (LCA) of net GHG emissions in different treatments mentioned above (8 combinations) at our field trial site was conducted and accounted for main C sources and sinks. Of all C sinks, displaced fossil fuel during bioethanol conversion was the largest one, followed by SOC sequestration and methane (CH_4) oxidation. Of all C sources, N_2O emissions was the largest one, followed by energy

requirements for fertilizer N manufacture and field machinery operations. Most management combinations were able to sequester atmospheric CO_2 except treatments with high N fertilization and residue return, mainly due to high N_2O emissions and low displaced fossil fuel C emissions.

County-level net GHG emissions using different irrigation availabilities and the management treatments mentioned above (135 combinations) were evaluated by integrating representative weather and soil conditions, field management schedules, and verified bioenergy sorghum growth parameters. As a result, 0% residue return, no-till, and 150 kg ha^{-1} of N fertilization under limited irrigation was the best consideration for optimum management of bioenergy sorghum production in most cases.

DEDICATION

To my family.

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This work was supervised by a dissertation committee consisting of Dr. Frank M. Hons [advisor] and Dr. Fugen Dou [co-advisor] of the Department of Soil and Crop Sciences, Dr. X. Ben Wu of the Department of Ecosystem Science and Management, and Dr. Huiyan Sang of the Department of Statistics.

Dr. Frank M. Hons, Dr. Fugen Dou, and Yong Wang designed this work. Drs. Jason P. Wight, Joseph O. Storlien, and Hamid Shahandeh, conducted the field/lab work and data analysis, Yong Wang conducted the model simulation and data interpretation, and wrote this dissertation with advice from Dr. Frank M. Hons, Dr. Fugen Dou, Dr. X. Ben Wu, and Dr. Huiyan Sang.

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CHAPTER I

INTRODUCTION

The U.S. Energy Independence and Security Act (EISA) of 2007 mandated annual production of 36 billion liters of biofuels by the year 2022, approximately 20%-25% of the U.S. transportation fuel requirement, with 16 billion liters from cellulosic ethanol, 15 billion liters from grain ethanol, and 5 billion liters from other advanced fuels. One important issue with large-scale biofuel production is whether high biomass yields can be achieved at limited cost to soil and environmental quality. Optimal balance between high biomass yields and agricultural and environmental sustainability must be attained for successful deployment of biofuel production. Biofuels represent a potential opportunity to provide renewable energy with relatively low greenhouse gas (GHG) emissions. However, land conversion to bioenergy crops may deplete soil fertility and increase soil GHG emissions, thereby offsetting the potential global warming benefits associated with biofuel production. The 2007 EISA enhanced research efforts related to cellulosic biofuel production, including various potential feedstocks.

1.1 Literature Review

Bioenergy sorghum [*Sorghum bicolor* (L.) Moench.] is different from grain, forage, and sweet sorghums, and along with switchgrass (*Panicum virgatum* L.), miscanthus (*Miscanthus*×*giganteus*), and sugarcane (*Saccharum* spp.), has been identified by the U.S. Department of Energy (DOE) as a promising bioenergy crop. This ranking is based on its high biomass yield potential, energy productivity, nitrogen (N) and water use efficiency, genetic tractability, and production adjustability. Dry biomass yields of bioenergy sorghum ranging from 8.0-60.0 Mg ha^{-1} have been reported. Compared with grain sorghum, forage sorghum, and corn (*Zea mays* L.), higher biomass yields were observed in both bioenergy sorghum and sweet sorghum systems, which also performed better than switchgrass and miscanthus during first two years of production (Gill, et al., 2014, Propheter, et al., 2010, Rocateli, et al., 2012). The current genetic composition of bioenergy sorghum and associated agricultural production practices may only achieve 25% of its yield potential (Mullet, et al., 2014). A study of six ligno-cellulosic crops [cardoon(*Cynara cardunculus* L.), giant reed (*Arundo donax* L.), switchgrass, miscanthus, bioenergy sorghum, and poplar (*Populus* spp. L.)] for biofuel production purposes showed that bioenergy sorghum, next to giant reed, ranked second for net energy yield (319 GJ ha^{-1}) and following giant reed and miscanthus, ranked third for energy efficiency (16.4 GJ GJ^{-1}) (Fazio and Barbanti, 2014). Bioenergy sorghum for cellulosic ethanol production was able to offset 63%-78% of GHG emissions (Olson, et al., 2012). Compared with the other sorghum types and corn, bioenergy sorghum had higher N use efficiency, averaging 111-370 g DM g^{-1} N, comparable with sugarcane and miscanthus, mainly due to its long growth duration, high stem to leaf biomass ratio, and efficient N remobilization (Olson, et al., 2013). The epicuticular wax structure, osmotic adjustment, antioxidant capacity, and C4 photosynthetic pathway help bioenergy sorghum become adapted to hot dry environments (Sanchez, et al., 2002). Unlike other C4 crops, however, bioenergy sorghum has smaller genomes, which is conducive for genetic tracking and development, making it a genetic model for designing C4 grass bioenergy crops (Mullet, et al., 2014). Bioenergy sorghum production can also be adjusted annually, reducing the risks associated with perennial crops that require longer-term allocation of land to a crop that may take several years to reach optimal yield (Mullet, et al., 2014, Rocateli, et al., 2012).

Different from traditional crops where only grain is removed, most aboveground biomass is harvested with biofuel crops. Little information is available as to whether all bioenergy sorghum biomass can be harvested for biofuel production without detrimental impacts on crop production, soil quality, and the environment. Crop residues serve as important sources of soil organic carbon (SOC) and various nutrients, protect topsoil from erosion, and modify soil water and temperature, thus offering potentially higher crop production (Wilhelm, et al., 1986). Research showed that excessive biomass removal in forage and grain sorghum production systems decreased subsequent biomass yield (Powell and Hons, 1992). However, excessive return of crop residue can also cause wetter and colder soils, poor seed placement, lowered plant populations, and N immobilization (Karlen, et al., 2014). Consequently, contradicting results have been observed on crop responses to residue return due to site-specific characteristics and differences in agricultural operations (Karlen, et al., 2014, Malhi and Lemke, 2007, Wilhelm, et al., 1986). Additionally, agricultural residues favor SOC through increased soil aggregation, which further improves soil structure, increases soil water holding capacity, and improves soil aeration as well (Wilhelm, et al., 2004). Higher total and active organic carbon (C) pools as well as improved soil aggregation were found at different residue return rates in various cropping systems (Malhi and Lemke, 2007, Osborne, et al., 2014, Saffigna, et al., 1989). In contrast, SOC and nutrients were significantly decreased with all stover removed in grain and forage sorghum production systems (Powell and Hons, 1991). However, residue return will lessen the amount of biomass available for possible biofuel production and may potentially increase soil microbial activity and GHG emissions, thereby offsetting the benefits associated with biofuel production (Saffigna, et al., 1989). Generally, GHG emissions of carbon dioxide (CO_2) and nitrous oxide (N_2O) have been increased with residue returned (Huang, et al., 2004, Jin, et al., 2014, Saffigna, et al., 1989), with the magnitudes modified by residue C:N ratios, N fertilization, and tillage (Baggs, et al., 2000, Baggs, et al., 2003, Huang, et al., 2004), while exceptions existed where parallel or lower N_2O emissions were observed with residue incorporated (Baker, et al., 2014, Hao, et al., 2001). Past studies were mainly focused on corn stover and cereal residues for biofuel production and their environmental impacts, and minimum return rates for corn stover were estimated to establish sustainable harvest criteria (Graham, et al., 2007, Johnson, et al., 2014). However, information is generally lacking on the impacts of bioenergy sorghum residue return on subsequent biomass yield, SOC, and GHG emissions. A sustainable harvest rate needs to be estimated for sustaining both soil and environmental quality and biofuel production.

Additionally, other field management practices may also influence the production of bioenergy sorghum in various aspects including yield, soil fertility, and environmental quality of the agro-ecosystem.

Nitrogen fertilization has a vital impact on C and nutrient cycling. As the main yield-determining macronutrient, N fertilization often improves the production of various crops (Malhi and Lemke, 2007, Nyakatawa and Reddy, 2000, Sainju, et al., 2006). Nitrogen fertilization also plays a significant role in soil organic matter (SOM) formation and stabilization due to higher biomass input. Nitrogen fertilization has also resulted in higher total and aggregate-associated SOC levels over time in different cropping systems (Dou and Hons, 2006, Malhi and Lemke, 2007). However, N fertilization is also typically one of the largest factors contributing to GHG emissions, especially N_2O. Agricultural activities account for 20%-70% of anthropogenic N_2O emissions (Mosier, et al., 1998), and fertilizer-induced N_2O emissions account for about 33% of the estimated total from cropland in North America (Snyder, et al., 2009). Nitrous oxide emissions from agriculture generally increase with increasing application of N fertilizers (Malhi and Lemke, 2007, Mosier, et al., 2006, Pelster, et al., 2011) and the positive role of N fertilization in facilitating production and sequestering C may be offset by N_2O emissions (Snyder, et al., 2009). It was estimated by Han, et al. (2011) that if the U.S. is to meet its goal of replacing 30% of petroleum consumption with biofuels by 2030, 58.2 Tg of N fertilizers would theoretically be required for overall bioenergy-focused agriculture. However, it’s unclear how SOC and GHG as well will react to the fertilization other than the yield response. Systematic research has to be conducted to analyze the effects of N fertilization on C cycling and GHG emissions in bioenergy cropping systems such as bioenergy sorghum. It is necessary to determine bioenergy sorghum’s optimum N requirement in order to improve biomass yield and SOC while minimizing N losses as GHGs.

Lower energy requirements and greater environmental benefits of reduced soil erosion and N leaching make conservation tillage more promising for optimizing crop productivity than tilled systems (Sainju, et al., 2006). However, the effect of tillage on crop yields is variable. Increased soil moisture content with no till (NT) practice has been reported to increase seed germination and root growth, thus improving crop production (Nyakatawa and Reddy, 2000, Plaza-Bonilla, et al., 2014, Triplett, et al., 1996). On the other hand, delayed emergence and maturity caused by decreased soil temperature, poor root penetration and difficulties in obtaining adequate stands and weed or pest control have also been observed in NT systems, thereby reducing crop yields (Stevens, et al., 1992, Triplett, et al., 1996, van Kessel, et al., 2013). Exposure of tilled soils to the air accelerates decomposition of previously sequestered organic C within the soil, releasing CO_2 via microbial activity. Numerous studies have shown that conservation tillage systems, especially NT, increased both total SOC and labile SOC as well as soil aggregation in comparison with conventional tillage (Dou and Hons, 2006, Dou, et al., 2008, Wright and Hons, 2005). Use of conservation tillage practices has been acclaimed as one of the most important approaches to reducing the rate of increase of the atmospheric CO_2 pool by decreasing disturbance and decomposition of organic C in the soil (Follett, 2001). However, it has been reported that the benefits obtained with the use of conservation tillage might be counterbalanced by an increase in N_2O emissions due to lower air diffusion caused by higher bulk density and greater amounts of water and soluble forms of C in the soil (Aulakh, et al., 1984, Ball, et al., 1999). Nevertheless, Six, et al. (2004) and Plaza-Bonilla, et al. (2014) suggested that the emissions of N_2O could be reduced when maintaining NT over time, possibly due to an improvement of soil structure under long-term NT. This indication was in agreement with the meta-analysis conducted by van Kessel, et al. (2013). In contrast, parallel or lower N_2O emissions were observed in short-term NT systems in some cases (Malhi and Lemke, 2007, Pelster, et al., 2011). Yet, information about how tillage affects C dynamics and GHG emissions in bioenergy sorghum cropping systems is still unavailable. Whether conservation tillage is needed in bioenergy sorghum production and to what extent it should be conducted to sustain production and SOC while minimizing GHG emissions needs to be determined.

A few field studies on the effects of management practices on bioenergy sorghum production have been conducted in several places in Texas and other southern states (Gill, et al., 2014, Hao, et al., 2014, Rocateli, et al., 2012). However, due to environmental factor differences such as climate and soil properties, as well as field management differences, results from these studies are varied and hard to compare. Additionally, most studies only lasted for 2-3 years and yield was measured in finite treatments (usually N fertilization) due to labor and funding limitations (Olson, et al., 2012, Propheter, et al., 2010), which were not enough to predict very long-term effects and generalize regional patterns. Alternatively, process-based biogeochemical models may be used to predict the overall performance of long-term bioenergy sorghum production in different regions and under more complex field management combinations, in order to provide regional estimations of planting feasibility and best soil and water management practices for bioenergy sorghum in different geographical areas.

DAYCENT is a process-based biogeochemical model used to simulate environmental factors such as soil temperature and water fluxes, plant and soil C and nutrient dynamics, and GHG fluxes (Del Grosso, et al., 2001, Parton, et al., 1998). It integrates weather, soil, and crop information along with field management practices such as planting, harvest, tillage, mineral and organic fertilization, irrigation, etc. (Campbell, et al., 2014, Chamberlain, et al., 2011, Chang, et al., 2013). This model has been tested in many ecosystems including cropland, grassland, and forest systems (Del Grosso, et al., 2006, Gathany and Burke, 2012, Parton, et al., 2001), and applied in varied spatial resolutions from site-related to national and even global scales (Chang, et al., 2013, Del Grosso, et al., 2005, Stehfest, et al., 2007). So far, DAYCENT has been widely employed and shown to be effective in many traditional agricultural systems (Cheng, et al., 2014, Del Grosso, et al., 2009, Hartman, et al., 2011). Few bioenergy crop production systems have been modeled to date. Grain yield, soil C, and N_2O emission data were collected from three states in the U.S. to test DAYCENT performance for modelling the impacts of corn stover removal for bioenergy production. Overall, DAYCENT performed well in simulating stover yields (r^2 = 0.53) and low N_2O emission rates, reasonably well when simulating average SOC change (r^2 = 0.54), and poorly when estimating high N_2O emissions (Campbell, et al., 2014). The model matched observed switchgrass yields within 25% of the mean across South Carolina and explained 66%-90% of the observed yield variation in California, making further predictions reasonable (Chamberlain, et al., 2011, Lee, et al., 2012). Growth dynamics of miscanthus, switchgrass, and corn from Europe and Illinois were successfully simulated (r^2 = 0.987) and biogeochemical cycling was evaluated (Davis, et al., 2010). Similar studies were implemented in Pennsylvania for corn, soybean (*Glycine max* (L.) Merr.), alfalfa (*Medicago sativa* L.), hybrid poplar (*Populus* spp.), reed canarygrass (*Phalaris arundinacea* L.), and switchgrass (Adler, et al., 2007). However, no evaluations of DAYCENT performance in simulating C dynamics and GHG emissions in bioenergy sorghum production have been conducted.

By verifying DAYCENT performance in bioenergy sorghum production systems, long-term regional effects of more complex field management practices can be projected using representative weather and soil conditions, field management operations, and bioenergy sorghum growth parameters. Best management practices can potentially be determined by evaluating the agricultural efficiency and environmental effects of long-term production of bioenergy sorghum in different areas through various modeled outputs, such as biomass yield, SOC, and GHG emissions. As indicated above, however, evaluating the production efficiency and environmental effects of field management practices through separate measurements alone, such as yield, SOC, or GHG emissions, sometimes results in conflicting conclusions. For example, as the main yield-determining macronutrient, N addition is able to increase crop yield and SOC (Dou and Hons, 2006, Franzluebbers, et al., 1995, Powell and Hons, 1992). However, N fertilization is also typically one of the largest factors contributing to GHG emissions, especially N_2O (Snyder, et al., 2009). Evaluating individual parameters may give ambiguous results when considering agricultural productivity and effects on the environment. Conservation tillage has also been championed as an important approach for reducing the rate of increase of atmospheric CO_2 by decreasing crop residue and

SOC decomposition (Follett, 2001). However, the benefits obtained with conservation tillage could potentially be counterbalanced by increased N_2O emissions due to lower air diffusion caused by higher bulk density, and greater water and soluble forms of C in these soils (Aulakh, et al., 1984, Ball, et al., 1999, Plaza-Bonilla, et al., 2014). Additionally, different from more traditional crops where only grain is removed, most aboveground biomass will be harvested with biofuel crops. Little information is available as to the amount of bioenergy sorghum yield that can be harvested for biofuel production without detrimental impacts on crop production, soil quality, and the environment (Wang, et al., 2017). Meanwhile, additional factors, such as energy to manufacture and operate farm machinery and produce inputs such as fertilizer and herbicide, also contribute to net GHG gain or loss during the process from sorghum production to bioethanol conversion.

To deal with this issue, life cycle analysis (LCA) of net GHG emissions may help. Life cycle analysis can serve a critical role in the development of advanced biofuels by determining the C intensity of new bioenergy crop systems and by linking particular environmental impacts to certain elements in the production cycle. Life cycle analysis also highlights areas of uncertainty within the production cycle and can inform design decisions (Murphy and Kendall, 2015). Life cycle analysis has been further used by many studies to quantify the GHG mitigation potential of bioenergy crop production systems using corn, soybean, sugarcane, alfalfa, hybrid poplar, swithgrass, and miscanthus (Adler, et al., 2007, Meyer, et al., 2016, Wang, et al., 2012). However, there is little reported research on LCA of net GHG emissions in bioenergy sorghum production systems. Most previous studies analyzed the overall GHG mitigation potential of one or more bioenergy crops on a site or regional scale compared with fossil fuel uses (Cooper, et al., 2011, Zhao, et al., 2016). Few, however, compared how differences in field operations impacted LCA, and no optimum set of field practices was suggested. Additionally, most studies applied empirical models to estimate C sequestration and GHG emissions, which overlooked the impacts of climate and soil properties (Daylan and Ciliz, 2016, Murphy and Kendall, 2015). Biogeochemical models, like DAYCENT, have been shown to be more accurate when analyzing C cycles and GHG fluxes because of their accounting for both temporal and spatial variations (Del Grosso, et al., 2005).

1.2 Objectives

Our overall objectives were to: 1. Determine the best field management practices (residue return, N fertilization, tillage) under different irrigation systems for bioenergy sorghum production in order to maximize yield, sustain soil fertility, and minimize GHG emissions; and 2. Evaluate the long-term effects of bioenergy sorghum production systems on C dynamics and GHG emissions in each county in Texas. These objectives were achieved by conducing LCA of net GHG emissions using the verified process-based biogeochemical model, DAYCENT.

First of all, simulations of the influences of bioenergy sorghum residue return and N fertilization on the soil environment including soil temperature and volumetric water content, and aboveground biomass C, SOC, and GHG emissions including CO_2 and N_2O were conducted using the DAYCENT model. The model test and mechanism for residue return and N fertilization were examined separately in Chapters 2 and 3, respectively. Due to a limited variety of field measurements (only aboveground biomass C and SOC) compared to residue return and N fertilization, no separate chapter was written for tillage practice. However, model performance for all three practices was tabulated and summarized in Chapter 4 via LCA. Model performance and parameterization were progressively increased through simulations of treatments, field measurements, and experimental span.

Secondly, LCA at our field trial scale was conducted using the optimized parameter values calibrated and validated in the first two chapters. Based upon the principle that above average yield and net SOC change above zero should be sustained and net GHG emissions minimized, optimum residue return rate, N fertilization rate, and tillage practice combinations at the experimental site were discussed in Chapter 4.

Finally, long-term, regional changes in biomass C and SOC dynamics and GHG emissions after conversion of conventional crops to bioenergy sorghum as influenced by climate, soil properties, water availability, and different management practices in Texas were predicted. Best management practice combinations that sustain SOC and biomass yield while minimizing GHG emissions for each county and the state in general were discussed in Chapter 5.

CHAPTER II

SIMULATING IMPACTS OF BIOENERGY SORGHUM RESIDUE RETURN ON SOIL ORGANIC CARBON AND GREENHOUSE GAS EMISSIONS USING THE DAYCENT MODEL*

2.1 Introduction

Bioenergy sorghum [*Sorghum bicolor* (L.) Moench.] has been promoted as a next-generation biofuel crop due to its characteristics of high biomass yield and nutrient and water use efficiency. Biomass yields of bioenergy sorghum have been reported to range from 8.0 to 60.0 Mg ha^{-1} depending on management practices and environmental conditions (Hao, et al., 2014, Olson, et al., 2012, Wight, et al., 2012). Compared with grain sorghum, forage sorghum, or corn (*Zea mays* L.), higher biomass yields have been observed in bioenergy sorghum systems, which also performed better than switchgrass (*Panicum virgatum* L.) and miscanthus (*Miscanthus* x giganteus) during their establishment years (Gill, et al., 2014, Propheter, et al., 2010, Rocateli, et al., 2012). Compared with other sorghum types and corn, bioenergy sorghum exhibited higher nitrogen (N) use efficiency, which was comparable to sugarcane (*Saccharum officinarum* L.) and miscanthus (Olson, et al., 2013). The C4 photosynthetic pathway increases bioenergy sorghum's adaption to hot dry environments, increasing its water use efficiency and drought tolerance.

Agricultural residues increase soil organic carbon (SOC) sequestration through

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enhanced aggregate formation. Higher SOC as well as improved soil aggregation have been reported at different residue return rates in various cropping systems (Malhi and Lemke, 2007, Osborne, et al., 2014, Saffigna, et al., 1989). Residue return, however, lowers the amount of available feedstock and may increase soil microbial activity and greenhouse gas (GHG) emissions, thereby offsetting benefits associated with biofuel production (Baker, et al., 2014, Jin, et al., 2014, Saffigna, et al., 1989). Previous studies have focused on corn stover and cereal residues for biofuel production and their environmental impacts, with minimum return rates being proposed for corn stover to establish sustainable harvest criteria (Johnson, et al., 2014, Karlen and Johnson, 2014). However, information is lacking on impacts of bioenergy sorghum residue return on the soil environment, SOC, and GHG emissions. Sustainable harvest rates need to be estimated in order to balance biofuel feedstock production, soil quality and environmental health.

DAYCENT is a process-based biogeochemical model used to simulate soil environmental factors such as soil temperature and water fluxes, plant and soil carbon (C) and nutrient dynamics, and GHG fluxes (Parton, et al., 1998) and has been effective in simulating many traditional agricultural systems (Chang, et al., 2013, Del Grosso, et al., 2008). Few bioenergy crop production systems have been modeled to date. Corn, switchgrass, miscanthus, soybean [*Glycine max* (L.) Merr.], alfalfa (*Medicago sativa* L.), and hybrid poplar (*Populus* sp.) production systems have been simulated by DAYCENT, with observed crop yield, soil C, and nitrous oxide (N_2O) emission data compared with simulated results (Adler, et al., 2007, Chamberlain, et al., 2011, Davis, et al., 2010). The objective of this study was to parameterize and validate DAYCENT performance in simulating soil temperature and water content, SOC, and carbon dioxide (CO_2) and N_2O emissions in a bioenergy sorghum production system with variable biomass (residue) returns.

2.2 Materials and Methods

2.2.1 Site Description and Experimental Design

The field study associated with this research was established at the Texas A&M AgriLife Research Farm near College Station, Texas (30°32’15’’N, 96°25’37’’W) in 2008. This region has a mean annual temperature of 20°C and annual precipitation of 1017 mm. Soil at the site is classified as a Westwood silty clay loam (fine, mixed, thermic Udifluventic Ustochrept) consisting of 100, 560, and 340 g kg^{-1} of sand, silt and clay, respectively, in the top 15 cm, as well as a mean bulk density of 1.36 g cm^{-3} in the top 20 cm. The soil has a pH of 8.2 (1:2 soil/water) and initial SOC was 8.0 g kg^{-1} in the top 15 cm. The field was previously in a cotton (*Gossypium hirsutum* L.) and corn rotation.

The study used a randomized complete block design to study effects of bioenergy sorghum residue return: 0 or 50% of sorghum biomass yield return at harvest with each treatment replicated three times. Plots were 9.14 m long by 4.08 m wide, with four, 1.02-m rows. The bioenergy sorghum, “4-Ever Green”, a photoperiod-sensitive, one-cross hybrid with high biomass yield and low lodging potential (Walter Moss Seed Co, Waco, Texas, U.S.) was planted annually at a seeding rate of 160,000 seed ha^{-1}. A non-limiting N rate of 336 kg ha^{-1} as urea was side-dress applied 15 cm deep in 2008, with 280 kg ha^{-}

^{1} applied annually thereafter. Each year, conventional disk tillage to a depth of 15-20 cm was conducted after harvest and prior to planting. Furrow irrigation was applied only as needed to prevent severe water stress. Specific field operation dates and irrigation amounts can be found in Table 2.1. Since data for 2010 and 2011 were used in this simulation, related field activities and irrigation amounts for these two years are shown. Additional detailed field setup and operation information was reported by Wight, et al. (2012) and Storlien, et al. (2014).

2.2.2 Field Observations

Soil temperature was measured hourly by type T thermocouples at 10-cm depth near gas sampling collars within each plot (Storlien, et al., 2014). Soil volumetric water content was determined every 6 h by time domain reflectometry at 15-cm depth in the vicinity of the temperature sensors. Both temperature and moisture data were collected within the field with a CR1000 data logger (Campbell Scientific, Inc., Logan, UT), with hourly data for each sensor aggregated into daily values.

Composite soil samples from each experimental unit were collected from three, 4-cm i.d. soil cores in March each year at depth increments of 0-5, 5-15, 15-30, 30-60, and 60-90 cm, and oven dried at 105 °C for 7 d. However, only SOC data in the 0-20 cm depth were used to compare with DAYCENT output due to the model limitation. Soil organic C content for 0-20 cm was computed by accumulating SOC contents from 0-5, 5-15, 15-20 cm using SOC concentrations and bulk densities from 0-5, 5-15, 15-30 cm. Soil organic C were measured using an Elementar Americas Inc, VarioMAX CN analyzer (Mt. Laurel, NJ, U.S.).

Table 2.1 Field operation dates and irrigation amounts at College Station, Texas

Operation	2010	Amount	2011	Amount
Soil sampling	17th March		14th March	
Preplant cultivation	17th March		24th March	
Planting	13th April		25th March	
Fertilization	22nd May		5th May	
Inter-row cultivation	22nd May		5th May	
Irrigation	31st May	11 cm	12th April	11 cm
	-		9th May	9 cm
	-		14th July	11 cm
	-		4th August	11 cm
Harvest	7th October		1st September	
Bedding	12th October		5th September	

Soil GHG (CO_2, N_2O) fluxes were measured by integrating a Li-Cor 20-cm survey chamber (model 8100-103, Li-Cor Inc., Lincoln, NE) with an INNOVA 1412 photoacoustic gas analyzer (Innova AirTech Instruments A/S, Denmark) (Storlien, et al., 2014). Soil collars were installed near the middle of each plot to a depth of approximately 12 cm no less than 24 h before the initial gas sampling for each growing or fallow season and remained in place throughout the entire phase. Soil gas measurements were performed approximately weekly through the growing season and less intensively during the fallow period. More detailed observation and measurement information was included in previous publications (Storlien, et al., 2014, Wight, et al., 2012).

2.2.3 Model Description and Modification

The DAYCENT model runs on a daily time step and the key drivers include maximum and minimum daily air temperature, daily precipitation, soil properties, land management, and crop characteristics. The model simulation requires initializing the model based on the native ecosystem type at the site and using the best available information about land management during agricultural use.

Weather data from 1952 to 2012 at College Station Easterwood Field Climate Station used to drive model simulations for this study were obtained from the National Oceanic and Atmospheric Administration website (https://www.ncdc.noaa.gov/cdo-web/). Soil properties were described previously in Site Description and Experimental Design. Land management is given in Table 2.1, and other important site specific parameter modifications are presented in Table 2.2.

The model was started with a 5000-year equilibrium simulation to obtain the native vegetation SOC level, followed by a baseline simulation accompanied by agriculture initialization after the 1830's with increasing fertilization according to the land use change described by the Burleson county soil survey (https://www.nrcs.usda.gov/wps/portal/nrcs/surveylist/soils/survey). Given the planting history before our field experiment, cotton and corn were chosen to run the baseline simulations and default parameterizations. Soil organic C contents were adapted from Potter and Derner (2006) as well as field observations before the study was initiated.

Before biomass sorghum production simulation was initiated, cultivation and crop parameters were modified accordingly. Cropping and cultivation practices were parameterized based on the field management schedule (Table 2.1). Field cultivators and tandem disk, row cultivator, and field cultivators and tandem disk functions in DAYCENT were applied to represent preplanting cultivation, inter-row cultivation, and bedding, respectively, in the study.

Table 2.2 Site parameters for DAYCENT

Site parameter	Unit	Value
Field capacity	Volumetric	0.2907
Wilting point	Volumetric	0.0578
Damping factor for calculating soil temperature	-	0.005
N_2/N_2O ratio adjustment coefficient	-	1.0
Proportion of nitrified N that is lost as N_2O	-	0.9
Maximum daily nitrification amount	g N m^{-2}	0.7
Fraction of new net mineralization that goes to NO_3	-	0.8

Other than climate, site, and management parameterization, each crop to be simulated had a set of specific parameters representing its own characteristics. Carbon partitioning between shoots and roots, C:N ratio and lignin concentration in biomass of the crop compartments, and coefficients affecting plant growth and senescence were modified through other study results, our own measurements, and default values before simulation (Rocateli, et al., 2012, Rooney, et al., 2007). Key relevant parameters are included in Table 2.3. Lignin concentrations of shoots and roots were set to 8% and 6-10%, respectively. Ranges of C:N ratios for shoots and roots were set to 20-90 and 40-60, respectively. Data for soil temperature, soil water content, SOC, and daily CO_2 and N_2O fluxes in the control treatment (0% residue return) were used for model calibration, while data in the 50% residue return treatment were used for model validation.

2.2.4 Statistical Analyses

Statistical analyses were completed using the PROC GLIMMIX procedure of SAS 9.3 (SAS Institute Inc, 2013). The two-year combined data set was analyzed to test year and residue return effects for SOC and GHG annual emissions. Measurements with different residue return rates in the same year were compared first, followed by the

Table 2.3 Crop parameters for DAYCENT

Parameter	Definition	Value	Default
PRDX(1)	Coefficient for calculating potential production	0.625	0.5
PPDF(1)	Optimum temperature for production	35	30
PPDF(2)	Maximum temperature for production	50	45
FRTC(2)	Fraction of C allocated to roots in mature plants	0.3	0.1
CKMRSPMX(2)	Maximum fraction of juvenile live fine root C that goes to maintenance respiration for crops	1.0	0.5
CKMRSPMX(3)	Maximum fraction of mature live fine root C that goes to maintenance respiration for crops	1.0	0.5
CGRESP(2)	Maximum fraction of juvenile fine root live C that goes to growth respiration for crops	1.0	0.5
CGRESP(3)	Maximum fraction of mature fine root live C that goes to growth respiration for crops	1.0	0.5

measurement comparisons in different years with the same return rate. Return rate and year were taken as fixed factors, and block as a random factor. Means separation was at $P < 0.05$ level using Tukey's test. Linear regression analyses were used to compare measured vs. modeled soil temperature, soil water content, SOC, and annual GHG emissions, with coefficient of determinations (r^2) computed.

2.3 Results and Discussion

2.3.1 Soil Temperature and Soil Water Content

Crop residues have the capability of increasing soil water content and mitigating soil temperature fluctuations. The 50% residue return treatment increased soil water content by 23.13% during the 2011 growing season and decreased soil temperature by 0.73% across the 2010 and 2011 growing seasons (Figures 2.1 and 2.2).

Soil moisture dynamics and soil temperature profiles are major drivers of C flows and nutrient cycles in the DAYCENT model, thus potentially affecting plant

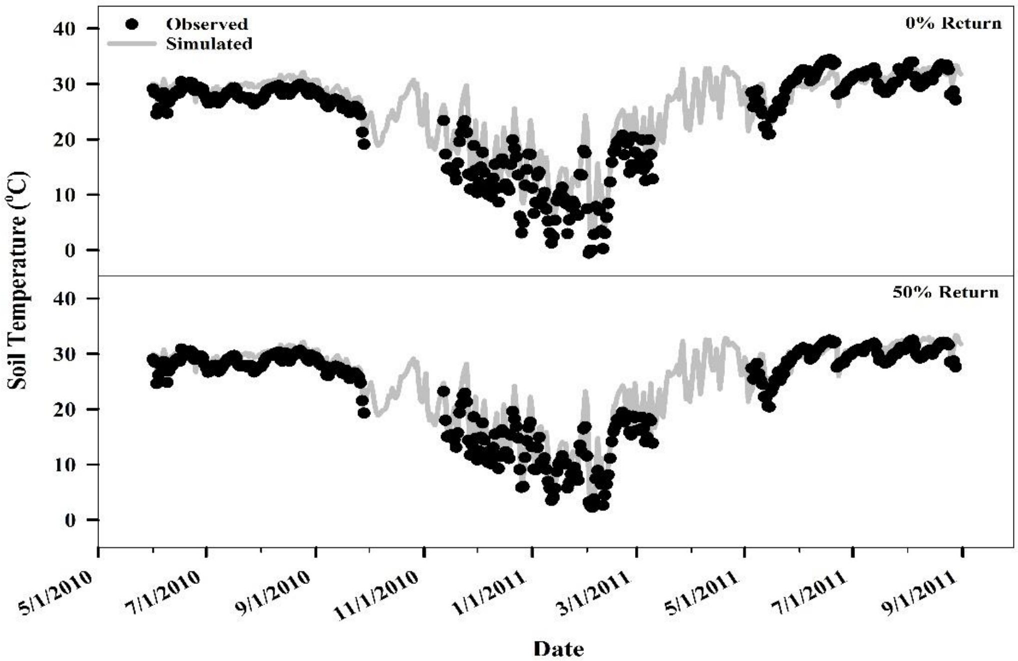

Figure 2.1 Observed and simulated soil temperature under 0% and 50% residue returns from the beginning of the 2010 growing season through the end of the 2011 growing season

growth and trace gas fluxes. Across the different return rates, r^2 values between observed and simulated soil temperature and soil water content were 0.94 and 0.81, respectively, indicating that the model adequately captured the patterns of soil temperature and water fluxes for the residue return treatments. However, the simulated control (0% residue return) and the simulated 50% residue return treatment showed little difference in soil water content and temperature if taken separately (Figures 2.1 and 2.2), implying that DAYCENT might underestimate the effects of residues in water holding capacity and temperature flux mitigation.

The reason little difference in soil water content between 0% and 50% residue

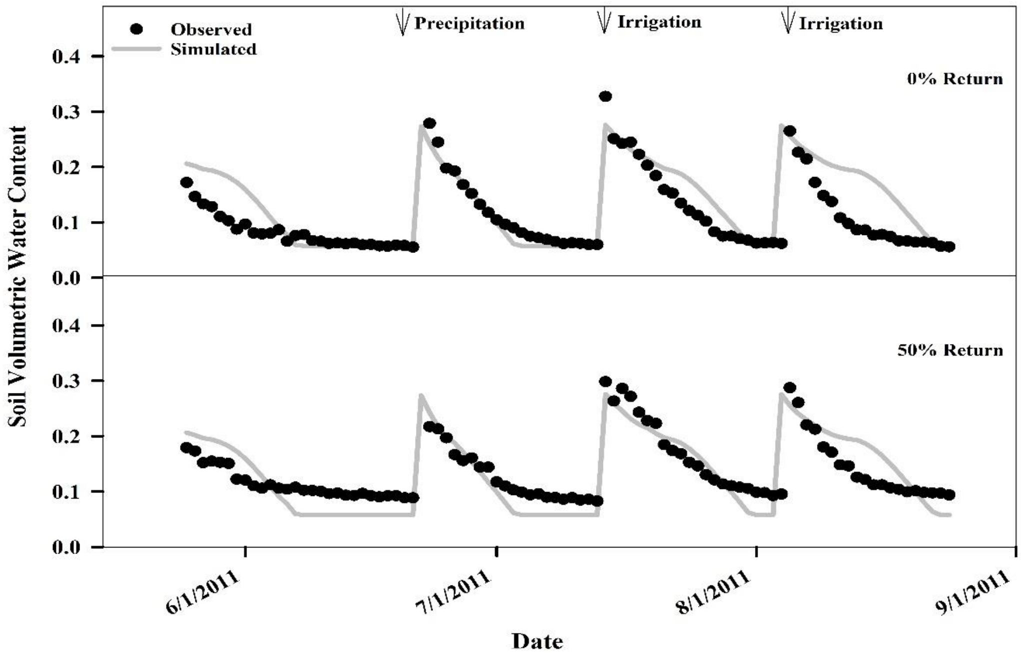

Figure 2.2 Observed and simulated soil water content under 0% and 50% residue returns during the 2011 growing season

returns was observed for the simulated output could possibly be associated with decreased bare soil evaporation in the 50% return treatment being offset by increased transpiration and intercepted water loss. Better model performance might be achieved by taking into account increased water holding capacity and reduced evaporation by litter, which was returned biomass in this study. The soil temperature submodel in DAYCENT is a function of air temperature and plant biomass (Parton, et al., 1998). Smaller live biomass difference between the two return rates from the simulated output than for field observations or a less sensitive temperature mitigation coefficient for litter effect in the submodel could be reasons for similar simulated soil temperatures between the two residue return rates.

2.3.2 Soil Organic Carbon (SOC)

Residue return increased SOC in both years (Figure 2.3). Soil organic C with 50% residue return was 7.77% greater than that under the control across both years. Similar results have been reported by other studies (Malhi and Lemke, 2007, Powell and Hons, 1991, Saffigna, et al., 1989). For example, Saffigna, et al. (1989) reported that SOC in the surface layer was 8% greater in the sorghum residue-retained than in the residue-removed treatment. Powell and Hons (1991) reported that removing all sorghum stover significantly decreased SOC.

Compared with 2010, SOC in 2011 was greater regardless of residue return, indicating that root biomass and root exudates may contribute to a significant increase in SOC. Our result was consistent with those reported by others (Johnson, et al., 2006, Menichetti, et al., 2015, Zhao, et al., 2014) who reported that belowground C inputs play a critical role in building and maintaining SOC.

Simulated SOC increased as bioenergy sorghum residue return increased in both years. Modeled SOC in 2011 was higher than that in 2010, regardless of the rate of residue return. Residue return and temporal effects on SOC were favorably modeled with an r^2 value of 0.75. The DAYCENT model has previously been shown by numerous studies to be effective at modelling SOC dynamics for conventional crops (Del Grosso, et al., 2002, Smith, et al., 2012). In this study, the results simulated by DAYCENT matched well with the observed changes in SOC for both different residue return rates and years. Campbell, et al. (2014) also reported similar effects of differential

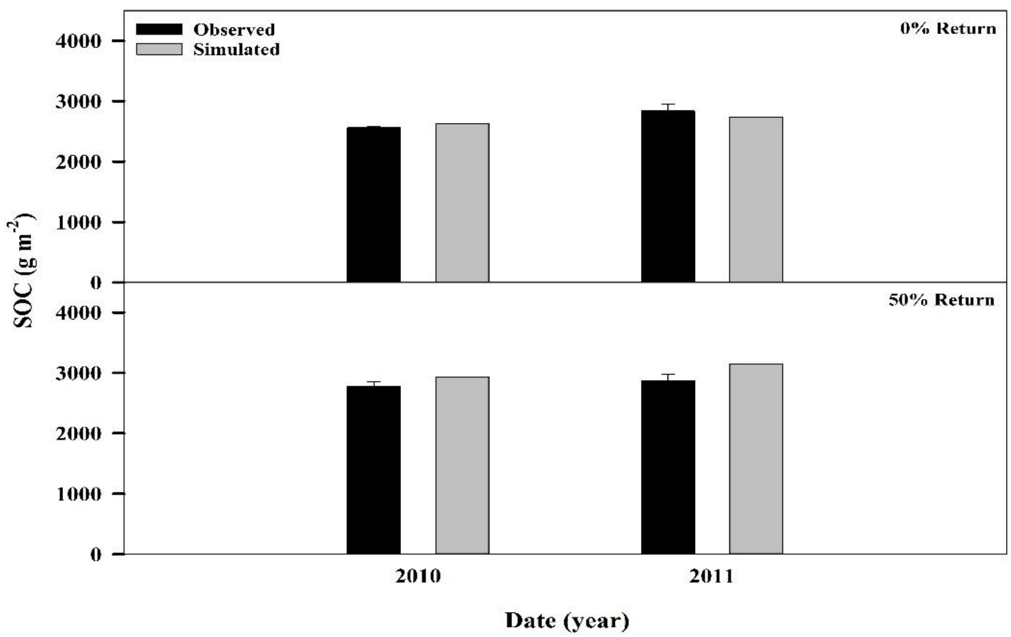

Figure 2.3 Observed and simulated SOC at 0-20 cm depth under 0% and 50% residue returns in 2010 and 2011

residue removal on SOC.

2.3.3 Carbon Dioxide (CO_2)

During most gas sampling events, higher daily CO_2 fluxes were observed for 50% compared with 0% residue return, though differences weren't always significant (Figure 2.4). Compared with the 2010 growing season, higher daily CO_2 fluxes occurred during the 2011 growing season for both return rates. Average measured soil temperatures for June, July and August 2011 vs. 2010 were +1.4, +1.2 and -0.4°C, respectively, for 2011. Daily peak fluxes were observed after irrigation, precipitation, and fertilization when soil moisture was relatively high (Figure 2.4).

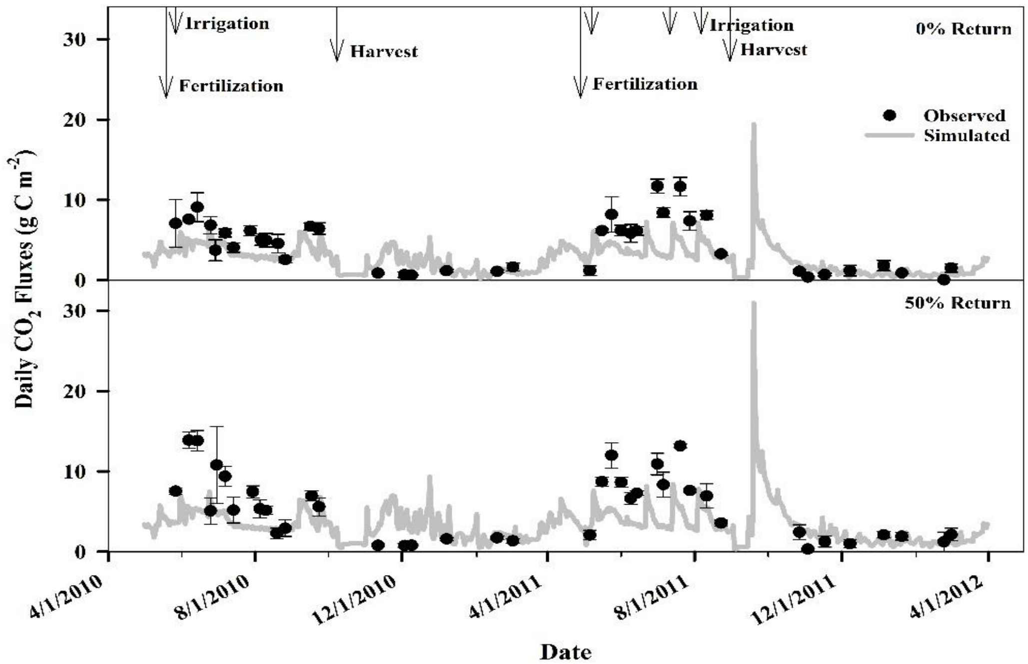

Figure 2.4 Observed and simulated CO_2-C fluxes under 0% and 50% residue returns during growing seasons and fallows in 2010 and 2011

Higher cumulative CO_2 emission for the 50% residue return treatment was found when combined across years, though results were not significantly different compared with 0% residue return in either year (data not shown). Compared with 2010, higher annual CO_2 losses were measured in 2011 for both return rates, indicating that conditions in 2011 were more favorable for decomposition. Jin, et al. (2014) summarized static chamber estimates of GHG emissions from nine corn production systems under various crop residue and tillage management practices across the U.S. Corn Belt and found that stove harvest generally reduced total soil CO_2 emissions by 4%. Baker, et al. (2014) summarized automated continuous chamber CO_2 data collected between spring 2010 and spring 2012 for three levels of stover harvest and found that CO_2 loss from plots with complete stover removal was lower than from plots with zero removal.

Similar daily flux patterns generally existed in the measured and simulated results (Figure 2.4), though annual cumulative CO_2 emissions were underestimated by the model. Like observed results, modeled outputs also indicated that 50% residue return increased CO_2 emissions in both years and showed higher CO_2 emissions in 2011 than in 2010 for both residue returns. DAYCENT performed very well in simulating annual cumulative CO_2 emissions with an r^2 value of 0.97.

2.3.4 Nitrous Oxide (N_2O)

Fluxes of N_2O were highly variable compared with CO_2, especially in 2011 when more irrigation was required because of the hot dry conditions (Storlien, et al., 2014) (Figure 2.5). During 2010, daily N_2O fluxes were mostly higher with the 50% residue return treatment, while in 2011, the situation was the opposite, with 0% residue return exhibiting more high daily N_2O fluxes, maybe due to more frequent water addition. Higher and more variable daily N_2O fluxes were observed for the 2011 compared to the 2010 growing season for both return rates. Peak daily N_2O fluxes were generally observed following fertilization and water addition from irrigation and precipitation (Figure 2.5).

Annual cumulative N_2O emissions showed the same pattern as daily N_2O fluxes, with 50% residue return having greater annual cumulative emission in 2010 and 0% residue return having higher annual cumulative emission in 2011, but no significant difference was found in either case (data not shown). When averaged over the 2 years,

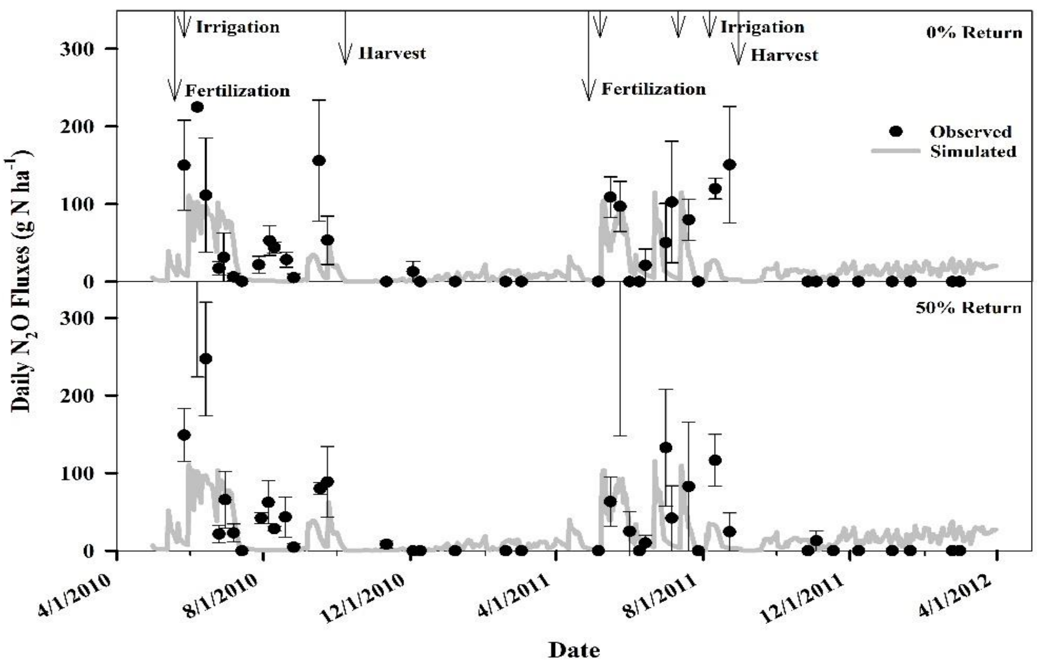

Figure 2.5 Observed and simulated N_2O-N fluxes under 0% and 50% residue returns during growing seasons and fallows in 2010 and 2011

higher N_2O loss was measured with 50% compared with 0% residue return, though the difference was not significant. This effect might be associated with enhanced microbial activity and C and N cycling due to the additional organic matter added. Annual cumulative N_2O emission was higher in 2011 than in 2010 for the control treatment (0% residue return), but the reverse pattern was found for the 50% residue return treatment.

Similar to the simulated annual cumulative CO_2 emissions, lower annual cumulative N_2O losses than measured were produced by the model. Simulated daily N_2O fluxes underestimated the observed results during the growing seasons, while overestimating fluxes during the fallow periods. Simulated results also showed higher

N_2O emissions with the return of 50% of the aboveground biomass after harvest. DAYCENT, however, did not accurately simulate annual N_2O losses (r^2=0.0057).

Due to both the transience and the magnitude of N_2O flux changes across growing and fallow seasons, continuously measured N_2O data would be of great value for comparison against DAYCENT model results, especially after rainfall or irrigation and N fertilization. Continuous monitoring would provide better information for simulating the magnitude and timing of peak flux events as well as more accurately estimating annual emissions. When using DAYCENT to evaluate N_2O emissions from different production practices, care should be taken not to underestimate emissions in systems of potentially high flux (Campbell, et al., 2014). Trace gas fluxes can also only be modeled well on the premise of accurate simulation of nutrient uptake and mineralization and soil water and temperature dynamics (Parton, et al., 1998).

2.4 Conclusions

The DAYCENT model simulated soil temperature, soil water content, SOC, and CO_2 very well, with corresponding r^2 values of 0.94, 0.81, 0.75 and 0.97, but was much less accurate in estimating N_2O emissions (r^2=0.0057). For both greenhouse gases, DAYCENT produced lower annual cumulative emissions than measured, especially for N_2O. These biases should be considered when DAYCENT is used as a decision support tool for recommending sustainable sorghum stover removal practices for bioenergy production.

CHAPTER III

DAYCENT SIMULATIONS OF THE IMPACTS OF NITROGEN FERTILIZATION IN BIOENERGY SORGHUM PRODUCTION

3.1 Introduction

Bioenergy sorghum [*Sorghum bicolor* (L.) Moench.] is a promising bioenergy crop due to its high biomass yield potential, drought tolerance, and genetic tractability (Mullet, et al., 2014, Rooney, et al., 2007, Wight, et al., 2012). Nutrient management is important to improve biomass yield and nitrogen (N) use efficiency for this emerging sorghum type. As a main yield-determining macronutrient, N application can increase bioenergy sorghum yields (Hao, et al., 2014, Olson, et al., 2013), and also plays a significant role in soil organic matter (SOM) stabilization due to greater input of plant residue and root exudates (Wilhelm, et al., 2004). Nitrogen fertilization has resulted in higher soil organic carbon (SOC) levels over time (Dou and Hons, 2006), but typically is also one of the largest factors causing greenhouse (GHG) emissions, especially nitrous oxide (N_2O) (Snyder, et al., 2009). Nitrous oxide emissions from agriculture generally increase with greater N fertilization (Johnson, et al., 2005, Mosier, et al., 2006, Pelster, et al., 2011) and its emission from bioenergy cropping systems has the potential to undermine the strategy of producing biofuels to reduce net GHG emission. However, little research has been done to establish the effects of N fertilization on both carbon (C) cycling and GHG emissions in bioenergy sorghum production. Determination of an optimal N application rate is necessary for increasing biomass yield and SOC, while minimizing GHG losses.

Field experiments generally reveal short-term results with limited factor levels due to labor and time constraints. Process-based models, however, are able to predict longer-term effects by integrating weather, soil, and crop information along with additional management practices. DAYCENT is a process-based biogeochemical model used to simulate environmental factors such as soil temperature and water fluxes, plant and soil C and nutrient dynamics, and GHG emissions (Del Grosso, et al., 2001, Parton, et al., 1998). This model has been widely verified and applied to many traditional agricultural systems (Cheng, et al., 2014, Del Grosso, et al., 2006, Stehfest, et al., 2007) and some bioenergy cropping systems (Campbell, et al., 2014, Chamberlain, et al., 2011, Lee, et al., 2012). However, evaluations of DAYCENT performance in simulating C dynamics and GHG emissions in bioenergy sorghum production are limited. Model fit using a site experiment can help determine proper N fertilization rates for maintaining yield and soil productivity, while mitigating GHG emissions. Based on the calibrated and validated model, additional regional predictions may also be realized by incorporating climate, soil parameters, and field management practices at the appropriate resolution needed for the intended generality. The objective of this study was to determine DAYCENT model performance in simulating the effects of N fertilization on soil N_2O fluxes and biogeochemical C cycling in soil and biomass under bioenergy sorghum production.

3.2 Materials and Methods

3.2.1 Site Description and Experimental Design

The field study associated with this research was established at the Texas A&M

AgriLife Research Farm near College Station, Texas (30°32’15’’N, 96°25’37’’W) in 2008. The region has a mean annual temperature of 20°C and annual precipitation of 1017 mm. Soil at the site is classified as Weswood silty clay loam consisting of 100, 560, and 340 g kg^{-1} of sand, silt and clay, respectively, in the top 15 cm, as well as a mean bulk density of 1.36 g cm^{-3} in the top 20 cm. The soil has a pH of 8.2 (1:2 soil/water) and initial SOC concentration was 8.0 g kg^{-1} in the top 15 cm. Before the start of the bioenergy sorghum study in 2008, the field was in cotton (*Gossypium hirsutum* L.) in 2007, and rotated annually with corn (*Zea mays* L.) under conventional disk tillage for the previous 10 yr. Soil nutrient properties at the initiation of the study were reported by Wight, et al. (2012).

Data for modelling were taken from the randomized complete block field experiment with three replications of all combinations of N rates of 0 and 280 kg N ha^{-1}, sorghum biomass removal rates of 100, 75, and 50%, and either continuous sorghum or a biannual rotation of corn and sorghum that was conducted in 2008-2015. For the purpose of this study, the two N rates in continuous sorghum with 100% biomass removal were used. Biomass yield was estimated for each plot in 2008-2014. Samples for SOC at 0-90 cm depth were collected in late February-early April in 2008-2015. Soil temperature, moisture, and GHG emissions were measured during the 2010 and 2011 growing seasons and in following fallow periods which spanned from May to the next March. All plots were 9.14 m long by 4.08 m wide, with four, 1.02-m rows. The bioenergy sorghum variety, “4Ever Green”, used within the study was a photoperiod-sensitive, one-cross hybrid with high biomass and low lodging potential (Walter Moss Seed Co, Waco, Texas, U.S.). Plots were disked to a depth of 15-20 cm and bedded into rows after harvest and prior to planting, with additional inter-row cultivation in the spring. Nitrogen was applied in a subsurface band at about 15-cm depth as urea and approximately 15 cm from plant rows at the 4-leaf stage for sorghum. Limited furrow irrigation was performed as needed to prevent severe water stress. After biomass yield weights were collected, remaining biomass was removed from plots. Additional detailed field setup and operation information were included in Wight, et al. (2012) and Storlien, et al. (2014).

3.2.2 Field Observations

Biomass yield was estimated from the entire length of the middle two rows of each plot using a mechanical harvester with a load cell. Weights of biomass subsamples from plots were determined before and following oven-drying at 60°C for 7 d to determine moisture content. Oven-dried plant tissue samples were ground in a ring and puck mill for elemental C determination via combustion analysis with an Elementar Americas Inc., VarioMAX CN analyzer (Mt. Laurel, NJ). Aboveground biomass C was calculated by multiplying biomass dry weight by elemental C concentration.

Results of SOC at the 0-20 cm depth were used to calibrate and validate the performance of DAYCENT. Three composited 4-cm diameter soil cores were collected annually from each plot, oven-dried (105°C) for 7 d and weighed to determine bulk density. A subsample of each composite sample was finely ground and analyzed for organic C via combustion analysis with the same equipment used to measure C concentration in plant tissue. Differential heating was used to separate inorganic and organic C. For organic C, the primary furnace was set at 650 ^{0}C and a 2 L min^{-1} O_2 flow rate. Total C was analyzed with the same instrument at 900 ^{0}C. Soil organic C content (g C m^{-2}) for 0-20 cm was calculated using the determined SOC concentrations (g C kg^{-1} soil) and corresponding bulk densities (g cm^{-3}) from 0-5, 5-15, and 15-30 cm.

Soil GHG emissions including carbon dioxide (CO_2) and N_2O were directly measured by integrating a Li-Cor 20-cm survey chamber (model 8100-103, Li-Cor Inc., Lincoln, NE) with an INNOVA 1412 Photoacoustic gas analyzer (Innova AirTech Instruments A/S, Denmark). Polyvinyl chloride soil collars with 20-cm diameter were installed near the middle of each plot to a depth of approximately 12 cm no less than 24 h before the initial gas sampling for each growing or fallow season and remained in place throughout the entire season. Soil gas flux measurements were performed approximately weekly through the growing season and less intensively during the fallow period. Measurements for year 1 (2010) occurred from May 27, 2010 through March 3, 2011 and for year 2 (2011) from May 6, 2011 to March 1, 2012.

Soil temperature was measured hourly by type T thermocouples at 10-cm depth near gas sampling collars within each plot. Soil volumetric water content was determined every 6 h by time domain reflectometry (TDR) (model TDR100, Campbell Scientific, Inc., Logan, UT) at 15-cm depth in the vicinity of the temperature sensors. Both temperature and moisture data were collected within the field with a CR1000 data logger (Campbell Scientific, Inc., Logan, UT), with hourly data for each sensor aggregated into daily values. More detailed observation and measurement information was reported in previous publications (Storlien, et al., 2014, Wight, et al., 2012).

3.2.3 Model Description and Parameterization

DAYCENT is the daily time step version of the CENTURY biogeochemical model (Parton, et al., 1987, Parton, et al., 1988). Key submodels include plant production, organic matter decomposition, soil water and temperature flows, and trace gas fluxes. Major model inputs are daily weather data, soil properties, best available information about native vegetation and historical agricultural use, as well as current land management and crop characteristics.

Weather data including daily maximum and minimum air temperature and precipitation during 1952-2015 were downloaded from College Station's Easterwood Field Climate Station (https://www.ncdc.noaa.gov/cdo-web/). Soil properties were described previously.

Modelling was initiated with a 5000-year equilibrium simulation to obtain the native SOC level, followed by a baseline simulation accompanied by agricultural initialization after the 1830's with increasing fertilization and residue return, and less intensive cultivation according to the land use change described by the Burleson county soil survey (https://www.nrcs.usda.gov/wps/portal/nrcs/surveylist/soils/survey). Given the planting history before our field experiment, cotton and corn with a two-year rotation cycle were chosen to run the baseline simulations, and default parameterizations for these two crops were adopted. Soil organic C contents were adapted from Potter and Derner (2006), as well as our field observations.

Current land management information including field operation dates and irrigation amounts is given in Table 3.1, and other important site specific parameters are

Table 3.1 Information for main field operation practices in bioenergy sorghum production during 2008 to 2015

Operation	2008	2009	2010	2011
Soil sampling	24th March	6th April	5th April	14th March
Preplant cultivation	25th March	6th April	17th March	24th March
Planting	26th March	7th April	13th April	25th March
Inter-row cultivation	24th April	5th May	22nd May	5th May
Fertilization	1st May	20th May	22nd May	5th May
Irrigation	10th June (9 cm)	16th July (6 cm)	31st May (11 cm)	12th April (11 cm)
	10th July (9 cm)	24th August (6 cm)	-	9th May (9 cm)
	-	-	-	14th July (11 cm)
	-	-	-	4th August (11 cm)
Harvest	14th October	5th November	7th October	1st September
Bedding	15th October	6th November	12th October	5th September

	2012	2013	2014	2015
Soil sampling	7th March	27th March	28th February	11th March
Preplant cultivation	8th March	27th March	23rd March	
Planting	19th March	28th March	30th March	
Inter-row cultivation	19th May	21st May	11th May	
Fertilization	26th April	21st May	11th May	
Irrigation	-	13th June (9 cm)	10th July (11 cm)	
	-	26th June (11 cm)	-	
	-	10th July (9 cm)	-	
	-	31st July (11 cm)	-	
Harvest	13th August	3rd September	23rd September	
Bedding	20th August	5th September	26th September	

presented in Table 3.2. Carbon partitioning between shoots and roots, C:N ratio and lignin concentration in biomass of the crop compartments, and coefficients affecting plant growth and senescence were modified against other published results (Olson, et al., 2012, Rocateli, et al., 2012, Rooney, et al., 2007), our own measurements, and default values. Key relevant crop parameters and defaults used are included in Table 3.3. Lignin concentrations of shoots and roots were set to 7.6% and 6-10%, respectively. Ranges of C:N ratios for shoots and roots were set to 20-100 and 30-70, respectively, according to our field measurements.

3.2.4 Model Calibration and Validation

For the soil environmental factors and GHG emissions, soil temperature at 10-cm depth, soil volumetric water content at 15-cm depth, and daily GHG emissions in 2010 were used for DAYCENT model calibration. The same measurements in 2011 were then used for model validation. For aboveground biomass C and SOC, data from 2008-2011 (half of the project period) were selected for model calibration, while data from the remaining years were used for validation.

3.2.5 Model Projection

Based on model performance, projection was conducted with N rates ranging from 0 to 350 kg ha^{-1} in increments of 70 kg ha^{-1}. Model projection to the middle of this century (2008-2050) was implemented to determine the long-term effects of different N rates on C dynamics and GHG emissions in bioenergy sorghum production. In the model projection, sorghum growth parameter values calibrated and validated in our field trials were adopted. Field operation dates in the projection process were set from the average

Table 3.2 Selected site parameters for DAYCENT simulation

Site parameter	Unit	Value
Field capacity	Volumetric	0.2869
Wilting point	Volumetric	0.0426
Damping factor for calculating soil temperature	-	0.005
Minimum water/temperature limitation coefficient for nitrify	-	0
Proportion of nitrified N that is lost as N_2O	-	1
Maximum daily nitrification amount	g N m^{-2}	1
Fraction of new net N mineralization nitrified to NO_3	-	1
Adjustment on inflection point for water filled pore space effect on denitrification	-	0.8
N_2/N_2O ratio adjustment coefficient	-	1

Table 3.3 Selected crop parameters for DAYCENT simulation

Parameter	Definition	Value	Default
PRDX(1)	Coefficient for calculating potential production	0.8	0.5
PPDF(1)	Optimum temperature for production	35	30
PPDF(2)	Maximum temperature for production	50	45
FRTC(2)	Fraction of C allocated to roots in mature plants	0.35	0.1
CKMRSPMX(2)	Maximum fraction of juvenile live fine root C that goes to maintenance respiration for crops	1.0	0.5
CKMRSPMX(3)	Maximum fraction of mature live fine root C that goes to maintenance respiration for crops	1.0	0.5
CGRESP(2)	Maximum fraction of juvenile fine root live C that goes to growth respiration for crops	1.0	0.5
CGRESP(3)	Maximum fraction of mature fine root live C that goes to growth respiration for crops	1.0	0.5

dates in the 2008-2015 period including soil sampling, preplant cultivation, planting, inter-row cultivation, fertilization at each supposed rate, harvest, and post-harvest cultivation. We assumed that averages from 8 years of field trials were adequate to represent the custom field operation dates for bioenergy sorghum production. Historical weather data from 1981-2015 were used to represent future weather data in 2016-2050. No irrigation was scheduled in projected simulations. After projection, annual aboveground biomass C, SOC change, N_2O emission, and methane (CH_4) uptake in 2008-2050 were calculated to determine N fertilization effects. Annual net GHG emission was then determined by combing annual SOC change, N_2O emission, and CH_4 uptake (Sainju, 2016). Results were presented as CO_2-C equivalents by assuming 296 and 23 times the global warming potential (GWP) for N_2O and CH_4 compared to CO_2, respectively.

3.2.6 Statistical Analysis

Statistical analyses were completed using the PROC GLIMMIX procedure of SAS 9.3 (SAS Institute Inc, 2013). The data set was analyzed to test N effects and yearly variation on aboveground sorghum biomass C, SOC, and annual GHG emissions. Nitrogen fertilization rate and year were taken as fixed factors, and block as a random factor. When factors were significant at $P < 0.05$, mean separation was conducted at $P < 0.05$ using Tukey's test.

Linear regression analyses were used to compare observed vs. modeled soil temperature, soil water content, aboveground biomass C, SOC, daily GHG fluxes, and annual GHG emissions, with coefficient of determinations (r^2), slope, intercept, and root mean square error (RMSE) computed in calibration and validation processes, and over all study years (Table 3.4).

Table 3.4 Statistical tests between simulated and observed values of aboveground biomass C, SOC, daily CO_2-C fluxes, daily N_2O-N fluxes, annual CO_2-C emissions, and annual N_2O-N emissions

Measurement	r^2	Slope	Intercept	RMSE*
		Calibration		
Soil temperature	0.87	0.72	8.31	3.14
Soil moisture	0.91	1.13	-0.03	0.03
Aboveground biomass C	0.62	0.69	112.34	152.71
SOC	0.68	0.72	723.50	100.80
Daily CO_2	0.64	0.70	0.44	1.50
Daily N_2O	0.61	0.60	0.47	32.94
		Validation		
Soil temperature	0.91	0.77	6.75	3.68
Soil moisture	0.77	0.86	0.04	0.04
Aboveground biomass C	0.75	1.42	-210.62	113.42
SOC	0.36	0.58	1136.20	201.88
Daily CO_2	0.57	0.39	0.85	2.94
Daily N_2O	0.10	0.14	11.91	49.21
		Overall		
Soil temperature	0.90	0.77	7.24	3.43
Soil moisture	0.78	0.96	0.01	0.03
Aboveground biomass C	0.57	0.78	80.25	137.26
SOC	0.47	0.64	952.94	159.56
Daily CO_2	0.55	0.48	0.89	2.32
Daily N_2O	0.34	0.36	6.86	41.98
Annual CO_2	0.49	1.14	-354.73	254.37
Annual N_2O	0.97	1.11	-2888.60	2200.78

* RMSE indicates root mean square error

3.3 Results and Discussion

3.3.1 Soil Temperature and Moisture

For both observed and simulated data, higher average soil temperature was observed in the 0 N control treatment compared with the fertilized treatment during the whole study period (Figure 3.1). This difference might be attributed to greater shading due to the increased biomass and plant canopy in the fertilized treatment. Soil without N application and less sorghum growth likely received more solar radiation due to a sparser canopy (Nyakatawa and Reddy, 2000).

The model was capable of simulating the observed soil moisture peaks caused by precipitation and irrigation events (Figure 3.2). Compared with the 0 N treatment, slightly higher soil water content was observed in the N fertilized treatment. The difference might be attributed to higher belowground litter associated with greater biomass from N application. However, this difference was not reproduced by the model. A similar scenario for observed soil water content differences caused by residue return effects in bioenergy sorghum production was also not captured by the model in the study of Wang, et al. (2017).

Across the different N fertilization rates, r^2 values between observed and simulated soil temperature and soil water content were 0.90 and 0.78 (Table 3.4), respectively, indicating that the model could adequately capture the observed patterns of soil temperature and water fluxes.

3.3.2 Aboveground Biomass Carbon (C)

The observed aboveground biomass C provided with N fertilization was higher

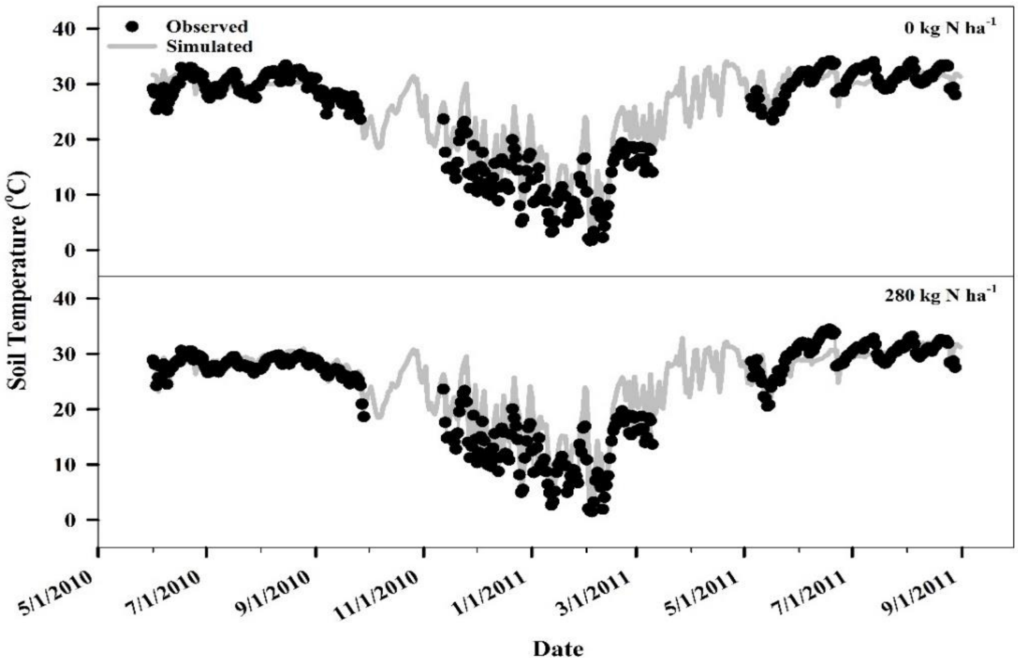

Figure 3.1 Observed (point) and simulated (line) soil temperature under 0 kg N ha^{-1} (upper panel) and 280 kg N ha^{-1} (lower panel) fertilization rates during 2010 and 2011

than that for the control in all study years (Figure 3.3). Annual variation of aboveground biomass C for the two N fertilization rates both demonstrated a pattern of higher yields the first two study years, lower yields during the middle years, and slightly increased yields toward the end of the study. A portion of the yield decline with time might be attributed to continuous sorghum production plus drought experienced in 2010-2012, which reduced the water input and growing season durations in those years. The growing days, average daily temperature and total water input (precipitation and irrigation) in the 2008-2014 growing seasons were 288, 309, 280, 244, 226, 246, 266 days, 26.24, 26.46, 27.71, 28.43, 26.65, 26.39, 25.95 ^{0}C, and 65, 78, 63, 59, 36, 70, 76 cm, respectively.

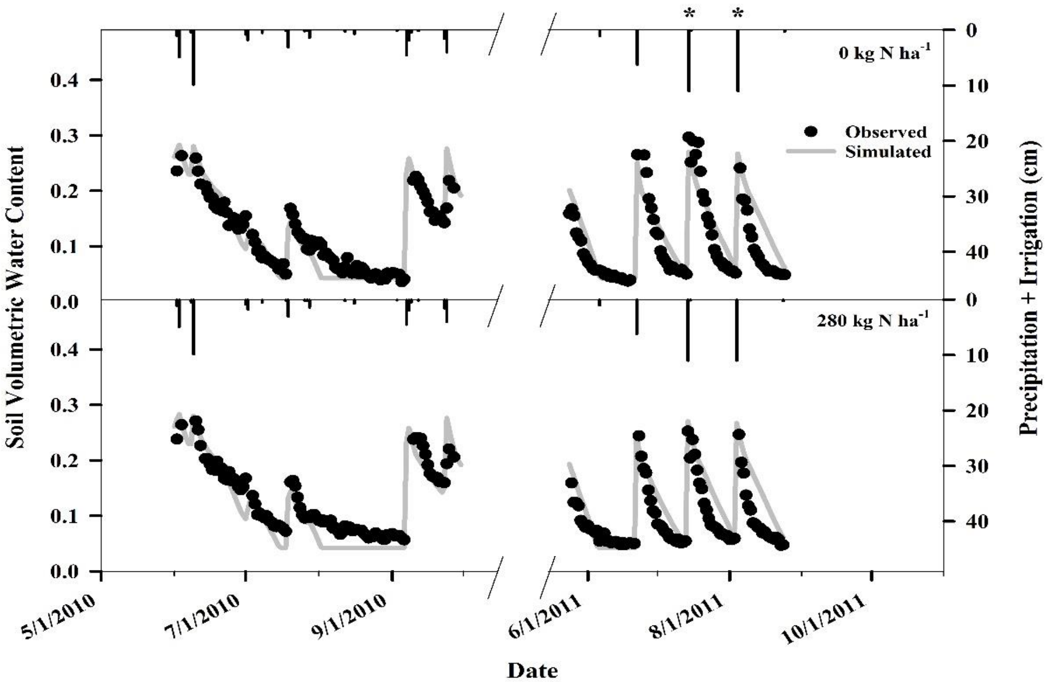

Figure 3.2 Observed (point) and simulated (line) soil volumetric water content under 0 kg N ha^{-1} (upper panel) and 280 kg N ha^{-1} (lower panel) fertilization rates during 2010 and 2011. * signs indicate irrigation operations. Lines on the top horizontal lines of the graph represent precipitation and irrigations amounts

Simulated aboveground biomass C was increased by applied N in all years (Figure 3.3), with results showing the same patterns as field observations. Within the same N treatment, simulated aboveground biomass C was higher at the beginning and end of the modelling period and lower in the middle, and were consistent with field observations.

To test the model's performance stability, the observed aboveground biomass C yields for 2008-2011 were selected to calibrate the model, while data from 2012-2014 were used for validation. As a result, the validation process presented parallel

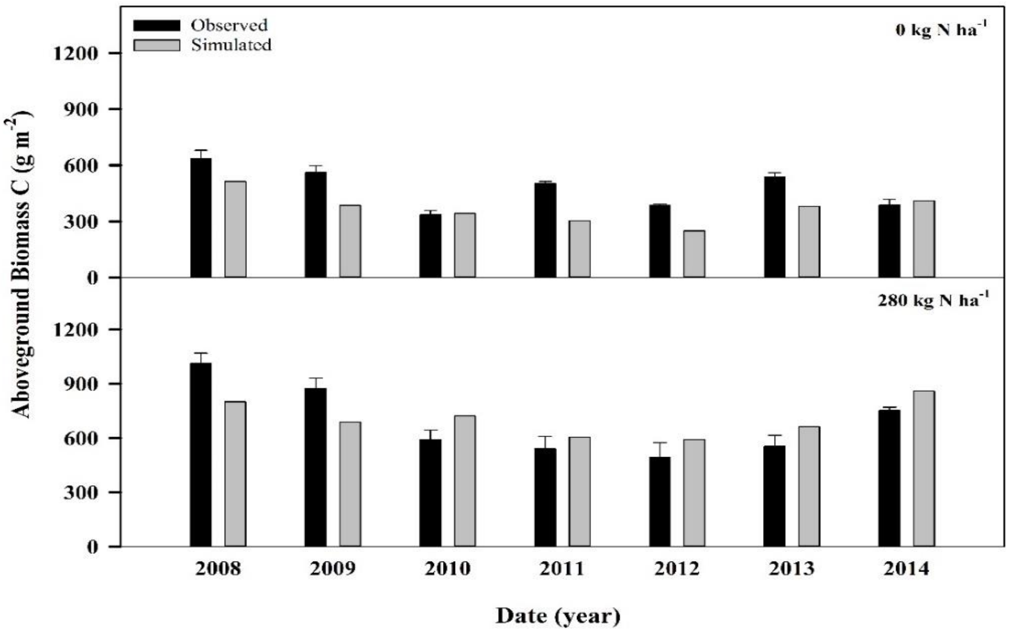

Figure 3.3 Observed (black bar) and simulated (gray bar) aboveground biomass C under 0 kg N ha^{-1} (upper panel) and 280 kg N ha^{-1} (lower panel) fertilization rates in 2008-2014

performance (r^2 = 0.75, slope = 1.42, intercept = -210.62, RMSE = 113.42) compared with the calibration process (r^2 = 0.62, slope = 0.69, intercept = 112.34, RMSE = 152.71) (Table 3.4). Overall, the model was able to simulate aboveground biomass C reasonably well (r^2 = 0.57, slope = 0.78, intercept = 80.25, RMSE = 137.26).

Sorghum yields in this study (7.0-27.0 Mg ha^{-1}) were within the range reported by several studies utilizing bioenergy sorghum (2.8-41.1 Mg ha^{-1}) (Gill, et al., 2014, Hao, et al., 2014, Propheter, et al., 2010). Lower yields in 2010-2012 might have been due to increased water stress and shorter growing seasons. Lower bioenergy sorghum water use efficiency was also observed in the Texas High Plains in 2010 and 2011, with lower yields compared with 2009 (Hao, et al., 2014). Nitrogen fertilization increased biomass yield compared to the treatment without N. Many other studies have demonstrated that N fertilization positively influenced soil N availability and thus sorghum yields (Hao, et al., 2014, Powell and Hons, 1992, Sainju, et al., 2006).

In the DAYCENT model, net primary productivity (NPP) is a function of nutrient availability, soil water and temperature, shading, vegetation type, and plant phenology. As anticipated, N fertilization increased biomass C assimilation over the unfertilized treatment in all study years, illustrating the need for N fertilization to sustain high yields across years. Our results were consistent with those of Meki, et al. (2013) who did long-term modelling of bioenergy sorghum production in the U.S. and also showed that N addition was required to sustain high yield over time. Input data on a daily basis, including weather and field operations, helps the model successfully reproduce observed annual variation (Kelly, et al., 2000). However, larger yield differences due to N fertilization were indicated by our model results compared with the actual measured data. One reason may be that simulated mineralized N was limited to only the 0-20 cm depth, likely underestimating the total N supply for plant growth from the deeper soil profile. In our study, only 30.80% of SOC content to a 90-cm depth was stored at 0-20 cm. Mineralized N from deeper soil profile could potentially supply bioenergy sorghum growth needs, even though the mineralization rate of deeper SOM may be lower. The DAYCENT model also underestimated soil mineral N concentration from five different short grass steppe sites in northeastern Colorado, except for a silty loam soil with N fertilization (Parton, et al., 2001). In our study, total simulated soil

NO_3^--N content in the 0 N control treatment at soil sampling dates was 13.11% lower compared to that from measured data at a 90-cm depth and it was the dominant available N form in the soil.

3.3.3 Soil Organic Carbon (SOC)

Soil organic C in the treatment receiving N fertilization was higher than that in the 0 N control in all study years (Figure 3.4). On average, SOC with N fertilization was 5.93% greater than that of the control when considered across all study years. Soil organic C with both N fertilization rates increased from the initial year until 2012, then dropped in 2013 and 2014, followed by an increase in the last study year.

Simulated SOC increased with applied N in all the years when compared to the simulated 0 N control. Modeled SOC also captured the annual variation as observed in the field (Figure 3.4). However, the variation of modeled results was conservative compared with actual observations, especially for decreases after year 2012.

Model performance in the calibration process was satisfactory (r^2 = 0.68, slope = 0.72, intercept = 723.50, RMSE = 100.80) (Table 3.4). During validation, however, the model was not able to adequately represent the SOC decline observed in 2013 and 2014. As a result, the model didn’t perform adequately in the validation process (r^2 = 0.36, slope = 0.58, intercept = 1136.20, RMSE = 201.88). Over the course of the entire study, field observations and modeled results showed similar patterns for SOC for the different N rates and years, with both showing higher SOC content in the added N treatment compared with the control and the variation caused by seasonal change (r^2 = 0.47, slope = 0.64, intercept = 952.94, RMSE = 159.56).

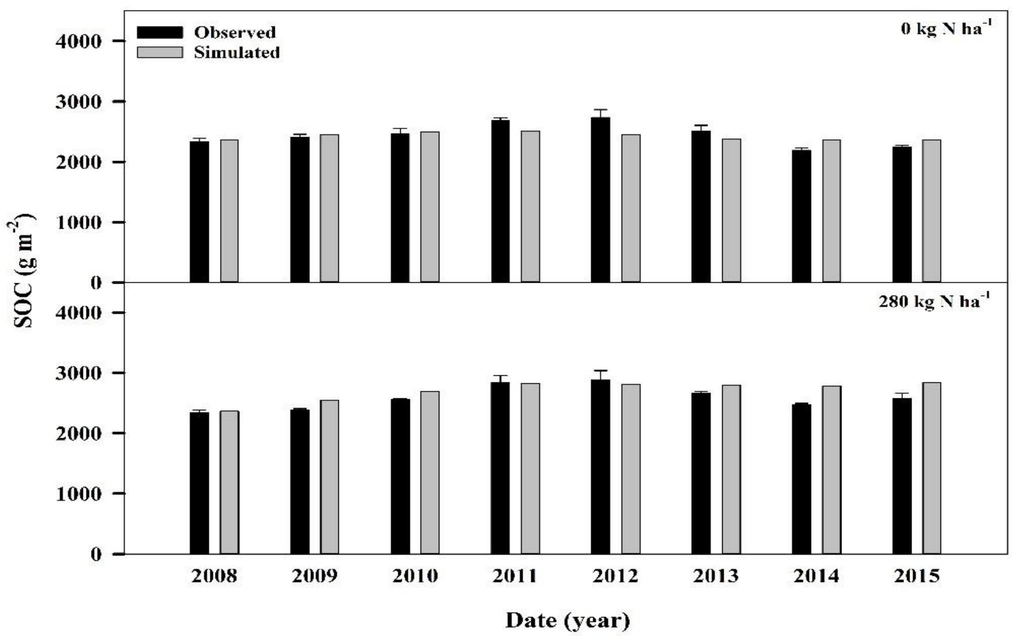

Figure 3.4 Observed (black bar) and simulated (gray bar) SOC at 0-20 cm depth under 0 kg N ha^{-1} (upper panel) and 280 kg N ha^{-1} (lower panel) fertilization rates in 2008-2015

Nitrogen fertilization increased SOC, which may result mainly from increased NPP. Both field trials and model simulation showed greater aboveground biomass with N application. Nitrogen fertilization increased biomass C assimilation, which often translates to more crop residues returned to the soil, including both aboveground dead material and root systems left after harvest (Wilhelm, et al., 2004).

Nitrogen fertilization may have stimulated greater root activity compared with the control. The greater mass of root-C or greater density of roots may have directly contributed to increased SOC. The bioenergy sorghum crop likely had an extensive root system that was distributed deep within the soil profile (Ferchaud, et al., 2015, Monti and Zatta, 2009). A crop with high aboveground biomass also usually produces comparably high belowground biomass. The DAYCENT model outputs the total biomass (above plus belowground) first, and then allocates the root/shoot ratio. The development of aboveground and belowground biomass are correlated and ratios can be modified with time, water, nutrient availability, and additional factors (Del Grosso, et al., 2001). Unfortunately, few studies are available that use sorghum root-to-shoot ratios to estimate the potential mass of belowground C based upon known aboveground C quantities. Preliminary data on shoot to root biomass ratios of bioenergy sorghum TX08001 obtained in 2011 showed the root biomass was 20% of the total biomass accumulated (Olson, et al., 2012). Samples collected from the fertilized treatment in our field study in 2013 indicated root biomass to be as high as 30% of the total biomass (data not shown).

Additionally, dead plant material falling from aboveground biomass during the growing season might be another contributor to SOC. Bioenergy sorghum is a photo-period sensitive C4 plant with high aboveground productivity, large leaves and a tall, dense canopy (Mullet, et al., 2014, Rooney, et al., 2007). Throughout the growing season, as the crop develops, older leaves periodically senesce from the plant and fall onto the soil, of which the cumulative mass across the entire growing season may have been substantial enough to increase SOC near the surface of the soil, particularly considering the relatively high C:N of sorghum plant tissue. In DAYCENT, the death rate of plant compartments is controlled by soil water, temperature, season, and plant-specific senescence parameters. Due to the severe drought and high biomass parameterization, dead biomass during the growing season could also be a significant contributor to SOC, especially for those plots with N fertilization.

Another possible reason for greater SOC with N fertilization was that bioenergy sorghum can provide a large shaded canopy over the soil surface throughout much of the middle and later portions of the growing season. With less probable shading from the crop canopy in 0 N control plots, the soil surface may have received greater solar radiation and became warmer than that under the shaded canopy. Both higher observed and simulated soil temperatures in the 0 N control treatment in our study may have enhanced the heterotrophic decomposition of organic C and soil respiration (Kirschbaum, 1995, Pietikainen, et al., 2005).

Temporal changes in SOC observed in the field were overall captured by the model, except that simulated results were too conservative compared to observations, especially for the observed declines in 2013 and 2014. The declines might be attributed to relatively early harvests followed by high intensity precipitation which provided favorable conditions for soil microorganisms to decompose unstable stored SOC from previous years. The weather record showed average air temperature in August, September, and October during 1952-2015 to be 29.27, 26.34, and 21.13 ^{0}C, respectively. According to the temperature effect on decomposition rate, the later harvest is conducted, the lower risk that SOC will be decomposed, especially for fresh residue and unstable SOC, because of lower temperatures. Biomass was harvested prior to October in 2011, 2012, and 2013 (Table 3.1). In these years, post-harvest precipitation before the end of October was 8.14, 17.3, 36.31 cm, respectively, indicating potentially greater decomposition, especially in 2012 and 2013. The reason DAYCENT didn't capture the SOC reductions well might be due to poorer model sensitivity for the effect of soil moisture on SOC decomposition rate (Campbell, et al., 2014, Paustian, et al., 1992).

3.3.4 Carbon Dioxide (CO_2)

During most gas sampling events, higher daily CO_2 fluxes were observed from plots receiving N fertilization compared with the control (Figure 3.5). Higher daily CO_2 fluxes generally occurred during the 2011 compared with the 2010 growing season regardless of N application, possibly because of higher daily temperatures and more frequent irrigations in 2011.

Greater annual CO_2 emission was observed with N fertilization compared with 0 N control in both years (Figure 3.6). Additionally, higher annual CO_2 loss was observed in 2011 compared with 2010 for both fertilization rates.

DAYCENT performed favorably in simulating both daily and annual CO_2 emissions, and demonstrated similar model fit for daily fluxes (r^2 = 0.55, slope = 0.48, intercept = 0.89, RMSE = 2.32) and annual emissions (r^2 = 0.49, slope = 1.14, intercept = -354.73, RMSE = 254.37) (Table 3.4). Similar daily flux patterns generally occurred for both observed and simulated results (Figure 3.5), though annual CO_2 emissions were underestimated by the model (Figure 3.6). Like observed results, modeled outputs also indicated that N fertilization increased CO_2 emission in both years and showed higher CO_2 emissions in 2011 than in 2010 for both N fertilization rates.

The treatment receiving N fertilization produced greater biomass, and likely both

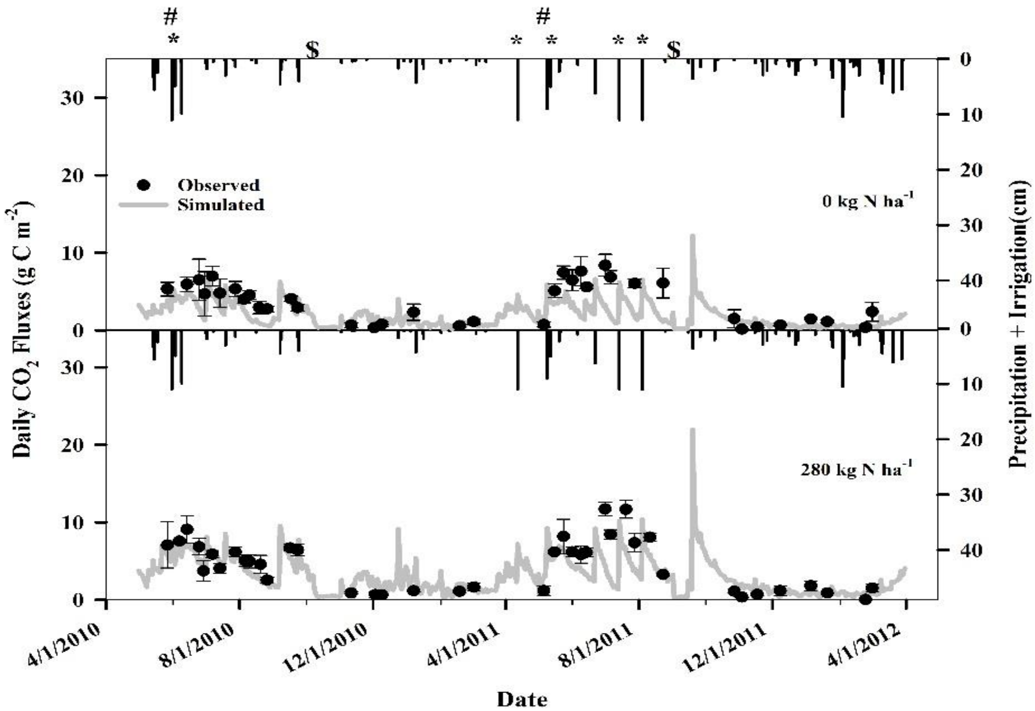

Figure 3.5 Observed (point) and simulated (line) daily CO_2-C fluxes under 0 kg N ha^{-1} (upper panel) and 280 kg N ha^{-1} (lower panel) fertilization rates during growing and fallow seasons in 2010 and 2011. # represents fertilization, * represents irrigation, and $ represents harvest. Lines on the top horizontal lines of the graph represent precipitation and irrigations amounts

autotrophic and heterotrophic respiration. Enhanced SOM mineralization (heterotrophic respiration) due to N fertilization has been reported for other cropping systems (Follett, 2001, Mosier, et al., 2006).

In the DAYCENT model, the potential decomposition rate is influenced by multiplicative functions of soil moisture and soil temperature. Microbial activity increases with increasing temperature which directly influences soil respiration (Franzluebbers, et al., 2001, Kirschbaum, 1995, Pietikainen, et al., 2005). Carbon dioxide emissions in 2011 were larger than those from 2010. Higher temperatures

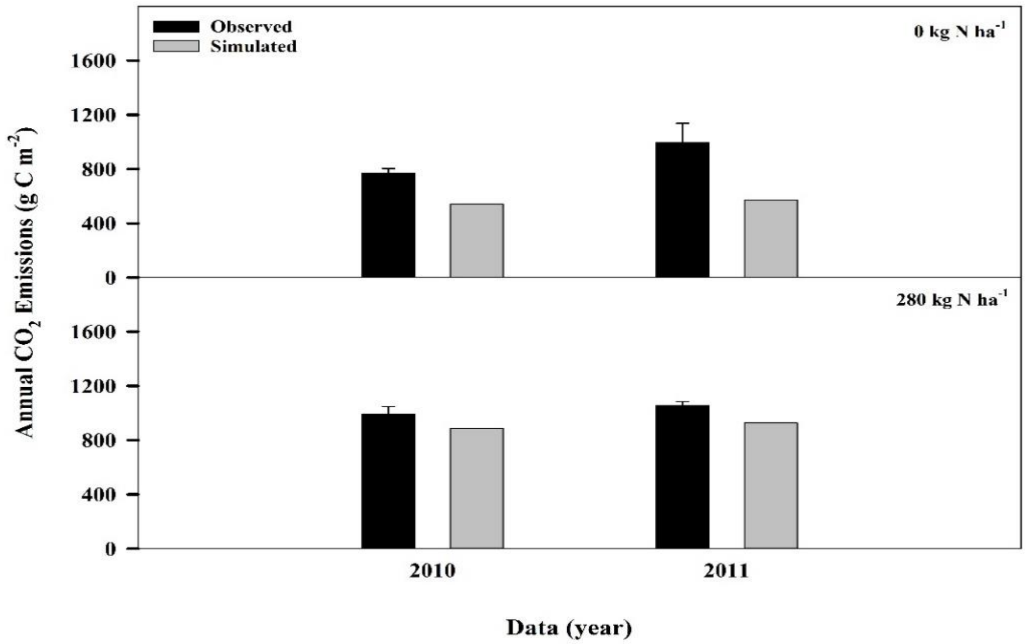

Figure 3.6 Observed (black bar) and simulated (gray bar) annual CO_2-C emissions under 0 kg N ha^{-1} (upper panel) and 280 kg N ha^{-1} (lower panel) fertilization rates in 2010 and 2011

throughout 2011 may partially explain this difference. Mean growing season and annual temperatures in 2010 and 2011 were 27.71 ^{0}C vs. 28.43 ^{0}C and 20.72 ^{0}C vs. 22.07 ^{0}C, respectively. In addition, more frequent irrigation events in the severe drought year of 2011 might also have contributed to higher CO_2 fluxes. Even though total water input (precipitation plus irrigation) in the growing season was slightly lower in 2011 compared to that in 2010 (58.71 cm vs. 63.18 cm), single water input events greater than 5 cm were 6 in 2011 compared to 2 in 2010, and annual water input amounts were 92.61 cm in 2011 compared to 88.87 cm in 2010. A long-term study on the effects of irrigation on CO_2 emissions in soybean [*Glycine max* (L.) Merr.] production systems showed higher growing season CO_2 emissions under irrigated than under dryland management, especially during dry growing seasons (Smith and Brye, 2014).

Based on favorable simulations of soil environmental factors and sorghum biomass yield, DAYCENT successfully reflected the daily CO_2 fluxes and annual emissions in the different N fertilization treatments and growing seasons observed in our field trial. The highest CO_2 fluxes were generally observed during the growing season, particularly after tillage, N fertilization, and precipitation/irrigation events. However, the model missed some high fluxes during growing seasons, in particular those after higher water input either by precipitation or irrigation. The model underestimation of those high fluxes and annual emissions might be the combined effect of not accounting for SOC decomposition at deeper depths and inadequate sensitivity for the effect of soil moisture on SOC decomposition rate.

3.3.5 Nitrous Oxide (N_2O)

In both 2010 and 2011, daily N_2O fluxes were mostly higher from the added N fertilizer treatment (Figure 3.7). Compared with the 2010 growing season, higher daily N_2O fluxes occurred during the 2011 growing season regardless of N application treatment.

Annual N_2O emissions showed the same pattern as daily N_2O fluxes, with N application exhibiting greater annual emissions in both years (Figure 3.8). This effect might be associated with enhanced microbial activity, nitrification, and C and N cycling due to the additional mineral N added. Annual N_2O emissions were also higher in 2011 than in 2010 for both fertilization rates.

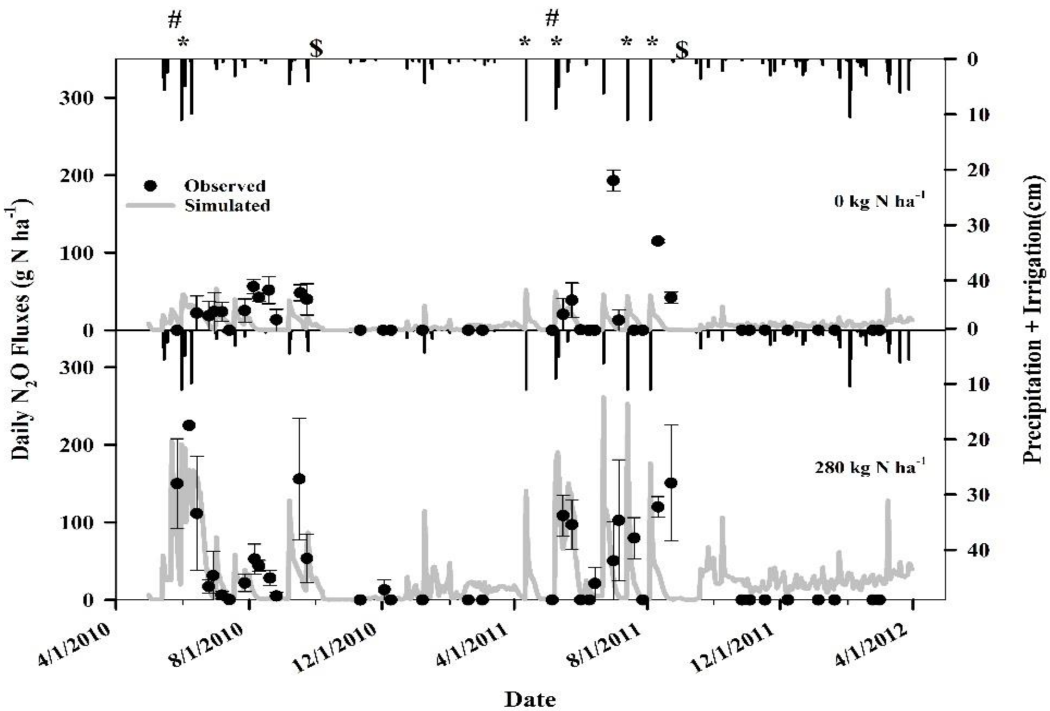

Figure 3.7 Observed (point) and simulated (line) daily N_2O-N fluxes under 0 kg N ha^{-1} (upper panel) and 280 kg N ha^{-1} (lower panel) fertilization rates during growing and fallow seasons in 2010 and 2011. # represents fertilization, * represents irrigation, and $ represents harvest. Lines on the top horizontal lines of the graph represent precipitation and irrigations amounts

Similar to the actual observations, lower daily fluxes and annual N_2O emissions were produced by the model in the control as opposed to the fertilizer added treatment in both years (Figures 3.7, 3.8). Additionally, simulated results also showed higher N_2O emission in 2011 with both N fertilization rates, which matched the observed tendency very well. Though model performance in simulating daily N_2O fluxes was not as satisfactory as it was for daily CO_2 fluxes due to several zero N_2O flux values (r^2 = 0.34, slope = 0.36, intercept = 6.86, RMSE = 41.98), DAYCENT accurately simulated annual N_2O losses under different N application rates (r^2 = 0.97, slope = 1.11, intercept = -

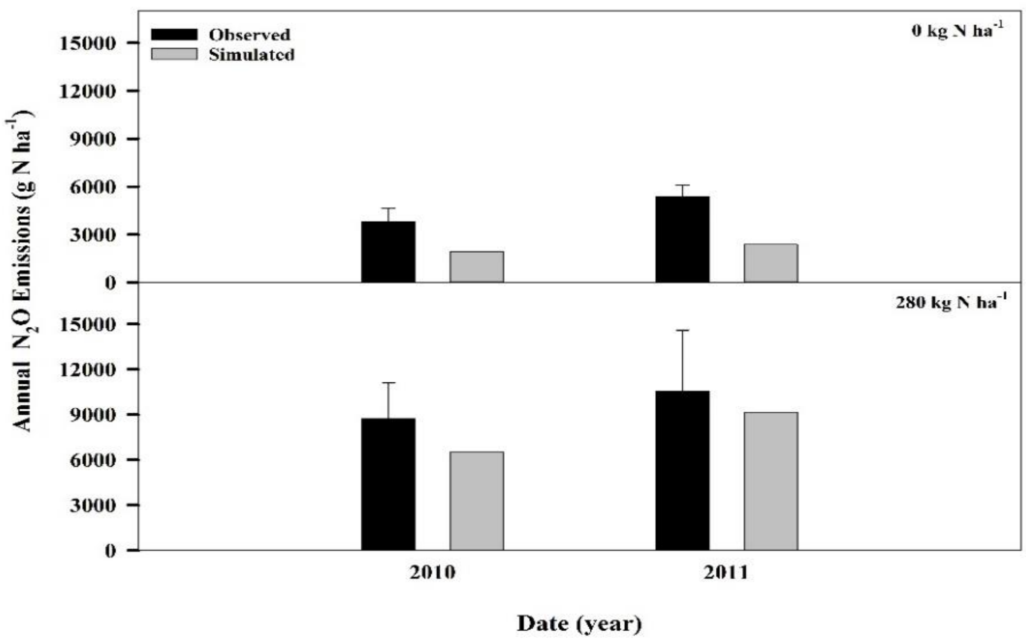

Figure 3.8 Observed (black bar) and simulated (gray bar) annual N_2O-N emissions under 0 kg N ha^{-1} (upper panel) and 280 kg N ha^{-1} (lower panel) fertilization rates in 2010 and 2011

2888.60, RMSE = 2200.78) (Table 3.4).

Increased N availability from fertilization often increases N_2O emissions and has been widely observed (Pelster, et al., 2011, Plaza-Bonilla, et al., 2014, Snyder, et al., 2009). Higher observed and simulated N_2O daily fluxes and annual emissions with added N might be associated with greater SOC and heterotrophic activity. Since urea was the fertilizer source, the added urea N was first hydrolyzed to NH_4^+ and then nitrified to NO_3^-, with N_2O being a potential byproduct of this conversion. Same as CO_2, increased SOC decomposition facilitated by favorable temperature and moisture conditions in 2011 resulted in more mineralized N for higher N_2O emissions compared to 2010.

Similar to CO_2 simulations, the model was able to capture N_2O emission pattern in different N fertilization treatments and its inter-annual variation, as well as flux patterns caused by field operations including tillage, N fertilization, and irrigation events, and intra-annual differences between growing seasons and fallows. Additionally, the model might underestimate high N_2O fluxes and annual emissions due to insufficiently reflecting N mineralization from SOC decomposition deeper in the soil profile and under higher water input conditions.

Generally, greater variation was observed in N_2O flux measurements. Growing season fluxes were particularly variable, ranging from no detectable flux to a maximum of approximately 225 g N_2O-N ha^{-1} day^{-1}, while the maximum flux during fallow seasons only reached 13 g N_2O-N ha^{-1} day^{-1} (Figure 3.7). This range might be attributed to the rather complex mechanisms of N_2O production from soil. Emissions of N_2O from soils are most often a byproduct of nitrification or denitrification (Del Grosso, et al., 2000, Parton, et al., 2001, Parton, et al., 1996). In DAYCENT, N gas flux from nitrification is assumed to be a function of soil NH_4^+ concentration, soil water content, temperature, and pH. Denitrification is a function of soil NO_3^- (e^- acceptor) concentration, labile C (e^- donor) availability, water-filled pore space (WFPS), and soil physical properties related to texture that influence gas diffusivity. Denitrification prevails under anaerobic conditions, commonly associated with excessively wet soils, although very high CO_2 concentrations in microsites within the soil may be conducive to denitrification on a small scale. When WFPS in soil reaches more than 80%, denitrification is anticipated to be the dominant N_2O-producing process, while lower soil moisture levels would be more conducive to nitrification (Del Grosso, et al., 2011). Since the WFPS in our study only peaked near a maximum of 56% in 2010 and 62% in 2011, we believe soil conditions were generally more conducive to nitrification being the dominant source of N_2O. This conclusion also aligns with our observation of higher fluxes shortly following fertilizer N application and with a number of studies which reported nitrification as the dominant mechanism producing N_2O, due to relatively low WFPS (Pelster, et al., 2011, Snyder, et al., 2009). The model also had a higher N_2O portion from nitrification (81%) compared with that from denitrification, which also has been reported in other studies (Parton, et al., 2001).

3.3.6 Model Projection

After model verification, projections (2008-2050) with N rates ranging from 0 to 350 kg ha^{-1} in 70 kg ha^{-1} increments were conducted. The results indicated that increasing N fertilization would increase aboveground biomass C, with projected aboveground biomass C yields being 307, 531, 646, 671, 678, and 682 g C m^{-2} for 0, 70, 140, 210, 280, and 350 kg N ha^{-1}, respectively. However, as expected, the N fertilizer productivity (biomass C divided by corresponding N fertilization rate) declined as N rate increased. All N fertilized treatments increased SOC, even though fluctuations existed over the course of the projection due to yearly weather variation (Figure 3.9). However, SOC content was potentially reduced when no N fertilizer was applied. When all GHG emissions (SOC change representing CO_2 emission, N_2O emission, and CH_4 uptake) were combined to quantify the net GHG emission for each N treatment, net GHG

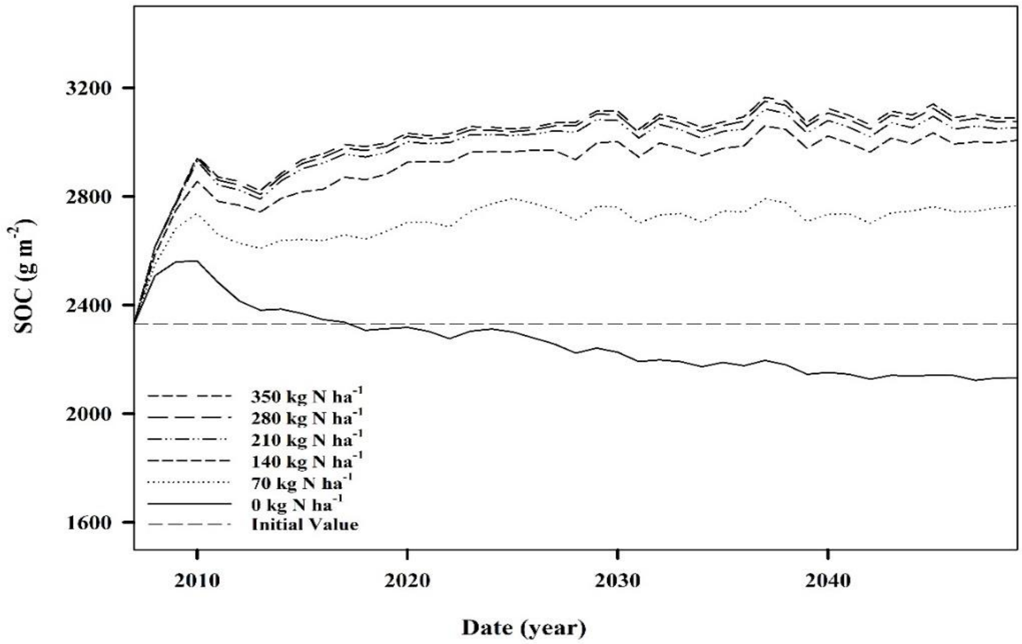

Figure 3.9 Projected SOC change under different N fertilization rates during 2008-2050

emissions increased as N fertilization rate increased, mainly due to greater N_2O emissions which exceeded the corresponding gain in SOC sequestration and soil CH_4 uptake (Table 3.5).

The projection results indicated that increasing N fertilization would increase aboveground biomass C. Average aboveground biomass C yields were 307, 531, 646, 671, 678, and 682 g m^{-2} when N rates increased from 0 to 350 kg N ha^{-1} in increments of 70 kg ha^{-1}. If the average C concentration in bioenergy sorghum (0.45 g C g^{-1} biomass) were used, then actual bioenergy sorghum dry matter yields ranged from 6.82 to 15.16 Mg ha^{-1} over the N fertilization range. The projected results agreed with several previous field trial results. Hao, et al. (2014) reported photoperiod-sensitive sorghum yields

Table 3.5 Projected GHG emissions (2008-2050) at different N fertilization rates

N rate (kg N ha^{-1})	SOC change	N_2O emission	CH_4 uptake	Net GHG emission
	Unit (g C m^{-2})			
0	4.90	29.61	-1.50	33.00
70	-9.59	67.87	-1.49	56.79
140	-15.89	110.02	-1.48	92.65
210	-17.04	140.17	-1.48	121.65
280	-17.55	163.14	-1.48	144.11
350	-17.81	184.40	-1.48	165.11

Positive values mean C source, negative values represent C sink

ranging from 12 to 18 Mg ha^{-1} planted near Amarillo, Texas with N rates of 0 to 344 kg ha^{-1}. The higher yields were attributed to full irrigation in both years. When the study was conducted by the same group in 2009-2011 with an N rate of 252 kg ha^{-1}, yields from 8 to 13 Mg ha^{-1} under dryland conditions were observed. Gill, et al. (2014) reported a broader range of biomass sorghum yield without irrigation in Texas, ranging from 4.3 to 20.9 Mg ha^{-1} in 2009-2012. Nitrogen fertilizer productivity (biomass C divided by corresponding N fertilization rate) in our study declined as N rates increased, which was caused by non-proportional increases in yield as N fertilization rate increased. Field trials of N use efficiency conducted by Hao, et al. (2014) also found a similar pattern, with greater yield increase with lower N rates and stabilizing at higher rates. All added N treatments were projected to raise the SOC level, even though yearly fluctuations were observed. However, long-term SOC content was potentially depleted when no N fertilization was applied (Figure 3.9). In this portion of our study, all aboveground biomass except plant crowns was removed at harvest, which resulted in roots likely being the major C input into the production system. Root biomass input without N fertilization apparently would not be sufficient to offset microbial decomposition according to the projected results. Chamberlain, et al. (2011) also found decreasing SOC stock without N fertilization and increasing SOC stocks at increasing N fertilization rates for a 30-year projection following the conversion of cotton or grass systems to switchgrass production. When all GHG emissions (SOC change representing CO_2 emission, N_2O emission, and CH_4 uptake) were combined to determine net GHG emissions, for all the N fertilized treatments, increasing net GHG emissions were observed as N fertilization rate increased, mainly attributed to higher N_2O emissions which offset the C sequestered by SOM and soil CH_4 uptake (Table 3.5). Similar results were observed in Colorado when conventional-till continuous corn was planted in 2002-2004 with N fertilizer rates ranging from 0 to 224 kg N ha^{-1} (Mosier, et al., 2006). Nitrous oxide fluxes increased linearly with increasing N fertilizer rate each year and offset the SOC sequestration and CH_4 uptake, thereby resulting in positive net GHG emissions and increased GWP. However, a corn–soybean field trial studying the interaction of N fertilization and tillage and a global scale DAYCENT model analysis of GHG emissions and mitigation strategies for corn, wheat (*Triticum aestivum* L.), and soybean systems demonstrated possible increased SOC storage and N_2O reduction by combining no tillage with a nitrification inhibitor or lower N rate (Del Grosso, et al., 2009, Pelster, et al., 2011). According to our model projections and other field trials or model projections, N fertilization between 140 and 210 kg N ha^{-1} may be optimal to maximize N use efficiency, sustain SOC content, and minimize net GHG emissions (Hao, et al., 2014, Pelster, et al., 2011).

3.4 Conclusions

Compared with the 0 N control, N fertilization in both field trial and model simulations resulted in greater aboveground sorghum biomass C, SOC, and annual CO_2 and N_2O emissions across the eight study years. Though the performance of the model in simulating aboveground biomass C was reasonably accurate, DAYCENT tended to underestimate crop yield when no N fertilization was applied. The model estimations of SOC were acceptable. However, simulated SOC variation caused by seasonal changes was smaller compared to field observations. DAYCENT also successfully reflected the daily GHG flux variation affected by fertilization treatments, other field operations, and seasonal changes. Although annual emissions were underestimated by the model, treatment effects and yearly variations were simulated fairly well for both CO_2 and N_2O emissions. The highest fluxes of CO_2 and N_2O were observed during the growing season and frequently followed tillage, N fertilization and/or precipitation or irrigation events. Addition of N fertilizer consistently increased GHG emissions each year of the study. Nitrogen fertilization was necessary for sustaining high yield and maintaining SOC, which will be vital to the feasibility and sustainability of the studied bioenergy cropping system. However, N fertilizer productivity decreased as N application rate increased, and potentially increased net GHG emissions also need attention. Our model projection results indicated that N fertilization between 140 and 210 kg N ha^{-1} may be optimal for maximizing N use efficiency and sustaining SOC content, while minimizing net GHG emissions.

CHAPTER IV

LIFE CYCLE ANALYSIS OF NET GREENHOUSE GAS EMISSIONS FOR DIFFERENT BIOENERGY SORGHUM MANAGEMENT PRACTICES

4.1 Introduction

Bioenergy sorghum [*Sorghum bicolor* (L.) Moench.] is a second-generation bioenergy crop with high biomass yield potential and nitrogen (N) and water use efficiency (Hao, et al., 2014, Olson, et al., 2013, Rocateli, et al., 2012). Bioenergy sorghum will potentially offset greenhouse gas (GHG) emissions by converting atmospheric carbon dioxide (CO_2) to crop biomass that may be used for bioethanol production to substitute for traditional fossil fuels. However, as an emerging hybrid crop to be used as a biofuel feedstock, bioenergy sorghum has received only limited research (Mullet, et al., 2014, Rooney, et al., 2007). Bioenergy sorghum yield is greatly affected by field management practices such as residue management, N fertilization, and cultivation intensity, and its production efficiency and environmental effects are largely unknown.

Evaluating the production efficiency and environmental effects of field management practices through separate measurements, such as yield, soil organic carbon (SOC), or GHG emissions, sometimes results in conflicting conclusions. For example, as the main yield-determining macronutrient, N addition is able to increase crop yield and SOC (Dou and Hons, 2006, Franzluebbers, et al., 1995, Powell and Hons, 1992). However, N fertilization is also typically one of the largest factors contributing to GHG emissions, especially nitrous oxide (N_2O) (Snyder, et al., 2009). Evaluating individual parameters may give ambiguous results when considering agricultural productivity and effects on the environment. Conservation tillage has also been championed as an important approach for reducing the rate of increase of atmospheric CO_2 by decreasing crop residue and SOC decomposition (Follett, 2001). However, the benefits obtained with conservation tillage could potentially be counterbalanced by increased N_2O emissions due to lower soil air diffusion caused by higher bulk density, and greater water soluble forms of carbon (C) in these soils (Aulakh, et al., 1984, Ball, et al., 1999, Plaza-Bonilla, et al., 2014). Additionally, different from more traditional crops where only grain is removed, most aboveground biomass will be harvested with biofuel crops. Little information is available as to the amount of bioenergy sorghum yield that can be harvested for biofuel production without detrimental impacts on crop production, soil quality, and the environment (Wang, et al., 2017). Meanwhile, additional factors, such as energy to manufacture and operate farm machinery and produce inputs such as fertilizer and herbicide, also contribute to net GHG gain or loss during the process from sorghum production to bioethanol conversion.

The objective of this study was to determine the effect of bioenergy sorghum production under different management practices on various C sinks and sources and net GHG emissions. The biogeochemical model DAYCENT was used to assess soil GHG fluxes, SOC change, and biomass yields for bioenergy sorghum. DAYCENT results were combined with estimates of fossil fuels used to provide farm inputs and operate agricultural machinery in order to calculate net GHG fluxes for the different practices considered. Net GHG fluxes represented by CO_2 equivalent C (CO_2e-C) were calculated by life cycle analysis (LCA), a technique to assess environmental impacts associated with all the stages of a product's life from raw material extraction through processing to disposal or recycling.

Life cycle analysis can serve a critical role in the development of advanced biofuels by determining the C intensity of a new bioenergy crop system and by linking particular environmental impacts to certain elements in the production cycle. Life cycle analysis also highlights areas of uncertainty within the production cycle steps and can inform design decisions (Murphy and Kendall, 2015). Life cycle analysis has been used by many studies to quantify the GHG mitigation potential of bioenergy crop production systems using corn (*Zea mays* L.), soybean [*Glycine max* (L.) Merr.], sugarcane (*Saccharum officinarum* L.), alfalfa (*Medicago sativa* L.), hybrid poplar (*Populus* sp.), swithgrass (*Panicum virgatum* L.), and miscanthus (*Miscanthus giganteus*) (Adler, et al., 2007, Meyer, et al., 2016, Wang, et al., 2012). However, there is little reported research on LCA of net GHG emissions in bioenergy sorghum production systems. Most previous studies analyzed the overall GHG mitigation potential of one or more bioenergy crops on a site or regional scale compared with fossil fuel uses (Cooper, et al., 2011, Zhao, et al., 2016). Few, however, compared how differences in field operations impacted LCA, and no optimum field management practice was suggested. Additionally, most studies applied empirical models to estimate C sequestration and GHG emissions, which often overlooked the impacts of climate and soil properties (Daylan and Ciliz, 2016, Murphy and Kendall, 2015). Biogeochemical models, like DAYCENT, have been shown to be more accurate when characterizing C cycles and GHG fluxes because of their accounting for temporal and spatial variations (Del Grosso, et al., 2005). In our study, a LCA including DAYCENT was used to evaluate the GHG mitigation potential of various bioenergy sorghum production systems and determine optimum field management practices.

4.2 Materials and Methods

4.2.1 Site Description

Field studies associated with this research were established at the Texas A&M AgriLife Research Farm near College Station, Texas (30°32’15’’N, 96°25’37’’W) in 2008 and 2009. The region has a mean annual temperature of 20°C and annual precipitation of 1017 mm. Soil at the site is classified as a Weswood silty clay loam (fine, mixed, thermic Udifluventic Ustochrept) consisting of 100, 560, and 340 g kg^{-1} of sand, silt and clay, respectively, in the top 15 cm, as well as a mean bulk density of 1.36 Mg m^{-3} in the top 20 cm. The soil has a pH of 8.2 (1:2 soil/water) in the top 15 cm, and the field was in a cotton [*Gossypium hirsutum* (L.)] and corn rotation prior to this study.

4.2.2 Experimental Design

Modelling data were taken from two experiments: one study used a randomized complete block design (RCBD) with four replications to compare effects of N fertilization (0 vs. 280 kg N ha^{-1}) and residue return (0% vs. 50% aboveground biomass return) under conventional tillage, and a second study utilized a completely randomized design (CRD) with five replications to compare the effects of tillage (conventional vs. reduced tillage) receiving 280 kg N ha^{-1} without residue return. The first study was conducted from 2008-2015 and the second was conducted from 2009-2015 adjacent to the first experiment. Initial SOC samples were collected in 2008 and 2009 before the field trials were started and thereafter samples were taken each spring before sorghum was planted. The final soil samples were gathered in 2015 and no sorghum was planted in this year. All plots were 9.14 m long by 4.08 m wide, with four 1.02-m rows. The bioenergy sorghum variety, "4Ever Green", used within the study was a photoperiod-sensitive, one-cross hybrid with high biomass and low lodging potential (Walter Moss Seed Co, Waco, Texas, U.S.). Annual planting at a seeding rate of 160,000 seed ha^{-1} was scheduled to occur after March 15th each year with harvest occurring between August and November. Conventionally tilled plots were disked to a depth of 15-20 cm and bedded into rows after harvest and prior to planting, with additional inter-row cultivation in the spring. Plots under reduced tillage received only spring inter-row cultivation to maintain rows. Nitrogen as urea was applied in fertilized treatments in a subsurface band about 7.5 cm deep and approximately 15 cm from plant rows at the 4-leaf stage for bioenergy sorghum. Limited furrow irrigation was performed as needed to prevent severe water stress. Weeds were controlled by minimal application of herbicides. Biomass was harvested from the entire length of the middle two rows of each plot. After biomass yield weights were collected, all the aboveground biomass was removed from plots having the 0% residue return treatment. To physically simulate harvest that would return 50% of the sorghum crop residue, biomass harvested from the middle two rows was collected and evenly distributed across the area of the entire plot following removal of biomass from the two outside rows. Field operations, dates and irrigation amounts are included in Table 4.1.

Table 4.1 Field operation dates in bioenergy sorghum production in College Station, Texas

Operation	2008	2009	2010	2011
Soil sampling	24th March	6th April	5th April	14th March
Preplant cultivation	25th March	6th April	17th March	24th March
Planting	26th March	7th April	13th April	25th March
Inter-row cultivation	24th April	5th May	22nd May	5th May
Fertilization	1st May	20th May	22nd May	5th May
Irrigation	10th June (9 cm)	16th July (6 cm)	31st May (11 cm)	12th April (11 cm)
	10th July (9 cm)	24th August (6 cm)	-	9th May (9 cm)
	-	-	-	14th July (11 cm)
	-	-	-	4th August (11 cm)
Harvest	14th October	5th November	7th October	1st September
Bedding	15th October	6th November	12th October	5th September

	2012	2013	2014	2015
Soil sampling	7th March	27th March	28th February	11th March
Preplant cultivation	8th March	27th March	23rd March	
Planting	19th March	28th March	30th March	
Inter-row cultivation	19th May	21st May	11th May	
Fertilization	26th April	21st May	11th May	
Irrigation	-	13th June (9 cm)	10th July (11 cm)	
	-	26th June (11 cm)	-	
	-	10th July (9 cm)	-	
	-	31st July (11 cm)	-	
Harvest	13th August	3rd September	23rd September	
Bedding	20th August	5th September	26th September	

4.2.3 Field Observations

For both field experiments, biomass yield, biomass C concentrations and SOC were measured for all replications during all study years. Soil temperature, soil volumetric water content, and GHG emissions were measured in three replications of the first experiment in 2010 and 2011 (Storlien, et al., 2014).

Total aboveground biomass yield was determined at harvest using a tractor-mounted mechanical harvester equipped with a catch compartment and load cell. Moisture content of aboveground biomass was determined from an approximately 600-g subsample taken from 5 randomly sampled plants within each plot which were mulched with a commercial chipper/shredder into approximately 0.04-m by 0.04-m pieces. Weights of subsamples were determined before and following oven-drying at 60°C for 7 d to determine moisture content. Oven-dried plant tissue samples were coarse ground in a large Wiley mill to pass a 1-mm sieve, then fine ground to pass a 0.5-mm sieve using a puck-and-ring mill in preparation for elemental C determination via combustion analysis with an Elementar Americas Inc., VarioMAX CN analyzer (Mt. Laurel, NJ). Aboveground biomass C was estimated by multiplying biomass dry weight by elemental C concentration.

Composite soil samples from each experimental unit were formed from three, 4-cm i.d. soil cores taken annually at depth increments of 0-5, 5-15, 15-30, 30-60, and 60-90 cm. However, only SOC data at 0-20 cm depth were used to compare with DAYCENT output due to model constraints. Samples were oven-dried (105°C) for 7 d, weighed to determine bulk density, coarse ground with a flail grinder, and sieved to pass

1.75 mm. A subsample of each composite sample was finely ground with a puck-and-ring mill and analyzed for organic C via combustion analysis as described previously. Soil organic C content for 0-20 cm was computed by accumulating SOC contents from 0-5, 5-15, 15-20 cm using SOC concentrations and bulk densities from 0-5, 5-15, 15-30 cm.

Soil GHG (CO_2, N_2O) emissions were directly measured in the first experiment by integrating a Li-Cor 20-cm survey chamber (model 8100-103, Li-Cor Inc., Lincoln, NE) with an INNOVA 1412 Photoacoustic gas analyzer (Innova AirTech Instruments A/S, Denmark) (Storlien, et al., 2014). A PVC flux chamber soil collar (20-cm diameter) was installed near the middle of each plot to a depth of approximately 12 cm no less than 24 h before the initial gas sampling for each growing or fallow season and remained in place throughout the entire phase. Soil gas flux measurements were performed approximately weekly through the growing season and less intensively during the fallow period. Measurements for year 1 (2010) occurred from May 26, 2010 through March 4, 2011 and for year 2 (2011) from May 5, 2011 to March 1, 2012.

Soil temperature and moisture data were collected during GHG sampling years (Storlien, et al., 2014). Soil temperature was measured hourly by type T thermocouples at 10-cm depth near gas sampling collars within each plot. Soil volumetric water content was determined every 6 hours by time domain reflectometry (TDR) at 15-cm depth in the vicinity of the temperature sensors. Both temperature and moisture data were collected within the field with a CR1000 data logger (Campbell Scientific, Inc., Logan, UT), with hourly data for each sensor aggregated into daily values. More detailed observation and measurement information was included in previous publications (Storlien, et al., 2014, Wight, et al., 2012).

4.2.4 Model Calibration, Validation, and Projection

The DAYCENT model runs on a daily time step and model inputs can be divided into four categories: weather data, soil properties, crop characteristics, and land management. The model simulation requires initializing the model based on the native ecosystem type at the site and using the best available information about land management during agricultural use.

Weather data, including daily maximum and minimum temperatures and daily precipitation from 1952 to 2015 used to drive site-scaled model simulations, was derived from the National Oceanic and Atmospheric Administration website (https://www.ncdc.noaa.gov/cdo-web/). Other weather statistics required were created by the file100 utility from the model.

Properties including latitude and longitude of the site, soil sand, silt, and clay contents, bulk density, pH, and other important site specific parameters were obtained either from preliminary field measurements or created by the file100 utility from the model.

Other than climate and soil data, the crop to be simulated (i.e. bioenergy sorghum) had a set of specific parameters representing its own characteristics. Carbon partitioning between shoots and roots, C:N ratio and lignin concentration in biomass of the crop compartments, and coefficients affecting plant germination, growth, senescence, and death were modified through our own measurements, published results, or default values before simulation (Olson, et al., 2012, Rocateli, et al., 2012, Rooney, et al., 2007). Important modified weather, soil, and crop parameters are included in Table 4.2.

Before a simulation was initiated, historic and current field management information was collected and edited, including grazing and fire in native vegetation, planting, harvesting, tillage, N fertilization and irrigation of past and current cropping systems.

The model started with a 5000-year equilibrium simulation to obtain the native vegetation SOC level, followed by a baseline simulation accompanied by agricultural initialization after the 1830's with increasing fertilization and residue and less intensity tillage according to the land use change described by the Burleson county soil survey (https://www.nrcs.usda.gov/wps/portal/nrcs/surveylist/soils/survey). Given the planting history before our field experiment, a two-year cotton and corn rotation system was chosen to run the baseline simulation and default parameterizations for these two crops were adopted. Soil organic C contents under native vegetation and initial status before the study began were from published data and field observations (Potter and Derner, 2006). Half the experimental data in chronological sequence for the measured bioenergy sorghum aboveground biomass C, SOC, GHG emissions, soil temperature and moisture were used for model calibration and corresponding data in the remaining half were used for validation.

Statistical analyses were completed using the PROC GLIMMIX procedure of SAS 9.3 (SAS Institute Inc, 2013). The data set was analyzed to test residue return, N fertilization, and tillage effects on aboveground biomass C yields, SOC, and annual

Table 4.2 Key parameters modified in DAYCENT model for bioenergy sorghum study

Parameter	Definition	Value	Default
DMPST	Damping factor for calculating soil temperature by layer	0.005	0.003
PMXTMP	Effect of biomass on maximum surface temperature	-0.0048	-0.0032
PRDX(1)	Coefficient for calculating potential production	0.8	0.5
PPDF(1)	Optimum temperature for production (℃)	35	30
PPDF(2)	Maximum temperature for production (℃)	50	45
FRTC(2)	Fraction of C allocated to roots in mature plants	0.3	0.1
CKMRSPMX(2)	Maximum fraction of juvenile live fine root C that goes to maintenance respiration for crops	1.0	0.5
CKMRSPMX(3)	Maximum fraction of mature live fine root C that goes to maintenance respiration for crops	1.0	0.5
CGRESP(2)	Maximum fraction of juvenile fine root live C that goes to growth respiration for crops	1.0	0.5
CGRESP(3)	Maximum fraction of mature fine root live C that goes to growth respiration for crops	1.0	0.5

GHG emissions. During analyses, residue return, N fertilization, and tillage were taken as fixed factors, and block and year as random factors. Mean separation was at $P < 0.05$ level using Tukey's test.

Linear regression analyses were used to compare observed vs. modeled soil temperature, soil water content, aboveground biomass C, SOC, daily GHG fluxes, and annual GHG emissions, with coefficient of determinations (r^2), slope, intercept, and root mean square error (RMSE) computed in calibration and validation processes, and over the whole duration (Table 4.3). At the same time, magnitude comparison of annual average values of observations and simulations was included in Table 4.4.

After model calibration and validation, projection from 2008 to the end of this century (2099) was conducted using updated parameters assuming there was a tillage x fertilization x residue return experiment initiated in 2008 on typical farming land [all the combinations of N fertilization, residue return, and tillage with levels of 0 vs. 280 kg N ha^{-1} (N0 vs. N280), 0% vs. 50% aboveground biomass return (R0 vs. R50), and conventional till vs. reduced till (CT vs. RT), respectively]. Weather data used for projection from 2016 was a circulation of historical data from 1952-2015. Field management dates for projection from 2015 was an average of corresponding dates from 2008-2015. According to SOC change characteristics, with most treatments showing relatively small SOC change after 30 years of simulation, all model outputs needed for LCA were calculated on an annual basis for three periods, 2008-2038, 2039-2099, and 2008-2099, in order to assess short-term, long-term, and average impacts.

Table 4.3 Statistical tests between simulated and measured values of aboveground biomass C, SOC, daily CO_2-C fluxes and N_2O-N fluxes, and annual CO_2-C and N_2O-N emissions

Measurements	r^2	Slope	Intercept	RMSE*
		Calibration		
Soil temperature	0.88	0.72	8.34	3.12
Soil moisture	0.87	1.12	-0.01	0.03
Aboveground biomass C	0.58	0.80	27.94	165.63
SOC	0.67	0.75	639.95	130.46
Daily CO_2	0.53	0.43	1.08	2.63
Daily N_2O	0.73	0.55	-0.23	38.70
Annual CO_2	0.28	0.72	-22.36	347.81
Annual N_2O	0.93	0.80	-1529.00	3145.58
		Validation		
Soil temperature	0.91	0.78	6.61	3.64
Soil moisture	0.73	0.88	0.02	0.04
Aboveground biomass C	0.72	1.11	-36.66	118.92
SOC	0.43	0.76	601.79	242.11
Daily CO_2	0.57	0.34	0.95	3.16
Daily N_2O	0.36	0.19	10.42	61.60
Annual CO_2	0.76	1.51	-822.88	312.93
Annual N_2O	0.92	1.35	-4084.60	1984.52
		Overall		
Soil temperature	0.90	0.76	7.17	3.40
Soil moisture	0.80	1.01	0.01	0.03
Aboveground biomass C	0.56	0.81	60.26	147.44
SOC	0.51	0.75	639.20	145.64
Daily CO_2	0.53	0.38	1.03	2.91
Daily N_2O	0.51	0.35	6.48	51.51
Annual CO_2	0.49	1.08	-371.47	330.83
Annual N_2O	0.81	1.04	-2508.90	2629.92

* RMSE indicates root mean square error

4.2.5 Life Cycle Analysis (LCA)

The protocol used by Adler, et al. (2007) for LCA of net GHG emissions in different bioenergy cropping treatments was followed in this study. Net GHG emissions were calculated as the total of C sinks (negative) and C sources (positive), where the

Table 4.4 Comparison of observed (Obs) and simulated (Sim) annual soil temperature, soil volumetric water content, aboveground biomass C, SOC, CO_2-C, and N_2O-N emissions among treatments from CRBD and RCD field trials

Field data source	Treatment	Soil temperature (°C) Obs	Sim	Soil moisture - Obs	Sim	Aboveground biomass C ($g\ m^{-2}$) Obs	Sim
RCBD	CT-N0-R0	24.17	25.74	0.1122	0.1303	487	347
	CT-N0-R50	24.34	25.70	0.1226	0.1304	489	376
	CT-N250-R0	23.44	24.95	0.1135	0.1273	654	726
	CT-N250-R50	23.34	24.95	0.1256	0.1271	747	728
CRD	CT-N250-R0	-	-	-	-	582	684
	RT-N250-R0	-	-	-	-	589	682

Field data source	Treatment	SOC ($g\ m^{-2}$) Obs	Sim	CO_2 ($g\ C\ m^{-2}$) Obs	Sim	N_2O ($g\ N\ ha^{-1}$) Obs	Sim
RCBD	CT-N0-R0	2433	2289	884	486	4597	2107
	CT-N0-R50	2511	2477	1027	596	5249	2510
	CT-N250-R0	2555	2555	1023	835	9636	7702
	CT-N250-R50	2742	2889	1187	1030	10878	9177
CRD	CT-N250-R0	2233	2288	-	-	-	-
	RT-N250-R0	2377	2315	-	-	-	-

CT, RT, N0, N280, R0 and R50 represent conventional and reduced tillage, 0 and 280 kg N ha^{-1}, and no or 50% biomass return, respectively

sinks were (a) the amount of C released from fossil fuel combustion replaced by bioethanol, (b) the change in SOC and belowground biomass C (this can be negative or positive depending on specific field management practices), (c) the amount of C emitted from fossil fuels used in feedstock transport to biorefinery, conversion to bioethanol, and subsequent distribution (this can also be negative or positive depending on the size of the electricity credit from combustion of the coproduct lignin at the biorefinery during production of ethanol from biomass), and (d) C from CH_4 uptake by the soil; sources were (e) C from direct N_2O emissions including nitrification and denitrification, (f) C from indirect N_2O emissions including offsite denitrification of leached NO_3 and volatilized N (NO_X + NH_3), (g) C emitted from manufacture of chemical inputs, and (h) C emission from fuel used by agricultural machinery for tillage, planting, fertilizer application, and harvesting. The ethanol yield for cellulosic biomass crops was determined by multiplying the harvested aboveground biomass by 90% of the theoretical ethanol yield from U.S. Department of Energy theoretical ethanol yield calculator and biomass feedstock composition and property database (https://www.afdc.energy.gov/fuels/ethanol_feedstocks.html), with ethanol yield being 381 L Mg^{-1} dry matter as corn stover. The quantity of fossil fuel displaced by bioethanol was calculated from the product of bioethanol yield and the fuel economy ratio of fossil fuel to biofuel, which was 6.75 km L^{-1} ethanol divided by 10.3 km L^{-1} gasoline (Sheehan, et al., 2004). The quantity of GHGs from the life cycle of fossil fuel displaced by bioethanol was calculated from the product of the quantity of fossil fuel displaced by bioethanol (aforementioned) and the total C emission during the fossil fuel life cycle. Based on Sheehan, et al. (2004), approximately 671.3 g CO_2e-C will be emitted per liter of gasoline consumed. Due to the simulated output unit being g C m^{-2}, a coefficient 0.45 was used to convert from biomass C to biomass yield, assuming 1 g C per 2.2 g dry matter (Hartman, et al., 2011). So sink (a) was calculated as harvested biomass C/0.45/1,000,000*90%*381*6.75/10.3*671.3, where 1,000,000 was yield unit conversion from g to Mg. Soil organic C change, sink (b), was collected from

DAYCENT output. The conversion factor was calculated to be -135.2 g CO_2e-C L^{-1} ethanol produced from corn stover at the biorefinery, because various coproducts are also generated during the production of ethanol from biomass (Sheehan, et al., 2004). Coproducts such as lignin from biomass converted to ethanol were factored into the conversion factor for biomass and was the reason it was negative. The negative value results from an electricity credit at the conversion facility from combustion of the lignin fraction of biomass (Sheehan, et al., 2004). The lignin fraction of biomass was not converted to ethanol, but to electricity when combusted. Thus, sink (c) was calculated as harvested biomass C/0.45/1,000,000*90%*381*135.2. Methane uptake, sink (d), was determined from DAYCENT simulation, and converted to CO_2e-C by assuming its global warming potential (GWP) is 23 times that of CO_2 on a mass basis (IPCC 2001). Two ways in which N fertilizer contributes to GHG emissions, sources (e) and (f), were modeled by DAYCENT: direct N_2O emissions from the soil (e) and indirect N_2O emissions from offsite denitrification of NO_3 and volatilized N that is deposited offsite and converted to N_2O (f). The direct N_2O emissions were from DAYCENT output. To calculate indirect N_2O, DAYCENT output and IPCC methodology (IPCC, 2000) were combined. IPCC assumes that 2.5% of NO_3 leached is eventually denitrified to N_2O in water ways and that 1% of volatilized N (NO_X + NH_3) is deposited on soil and converted to N_2O. Nitrous oxide emissions were converted to CO_2e-C by assuming its GWP is 296 times that of CO_2 on a mass basis (IPCC, 2001). The CO_2 emissions associated with the manufacture of chemical farm inputs (fertilizers, herbicides, insecticides), source (g), were from West and Marland (2002). Fuel usage by agricultural machinery, source (h), was organized by Adler, et al. (2007) using agricultural machinery management data documented in the American Society of Agricultural Engineers (ASAE) machinery management standards (Table 4.5).

4.3 Results and Discussion

4.3.1 Model Performance

Soil temperature and moisture data are major drivers of ecosystem processes in the DAYCENT model. Plant productivity, decomposition of dead plant material and SOC, nutrient uptake and leaching, and trace gas fluxes can only be modeled well on the premise of accurate simulation of soil water and temperature dynamics (Del Grosso, et al., 2001, Parton, et al., 1998). In the model output, sorghum biomass, SOC change, and CH_4 uptake were used for C sinks in LCA, and direct and indirect N_2O emissions were used for C sources in LCA. Thus, the modelling performance of all these measurements was based on how well the model simulated soil water and temperature. The model simulated soil temperature satisfactorily well, reflecting the temperature difference caused by residue return and N fertilization, with both observed and simulated results showing higher average soil temperature in treatments with lower fertilization and residue return, and lower average soil temperature in treatments with higher fertilization and residue return (Table 4.4). The model simulated soil moisture peaks caused by precipitation and irrigation events quite well (Chapters 2 and 3). However, simulated soil water differences among treatments were minute. This might be the reason the model underestimated biomass differences caused by the residue return treatment (Table 4.4). DAYCENT does not reflect the improvement of water holding capacity by soil

Table 4.5 Fossil-fuel energy requirements and CO_2 emissions from agricultural machinery

Operation	Fuel usage (L ha^{-1})	Energy (GJ ha^{-1})	CO_2 emissions (kg C ha^{-1})
Tillage	5.12	0.20	4.34
Planting	4.64	0.18	3.94
Fertilization	1.58	0.06	1.34
Harvesting	8.80	0.34	7.47

incorporated litter, which could have been another reason why biomass produced in the 50% residue return treatment was higher than that with 0% residue return, besides the higher nutrient level in the 50% residue return treatment. DAYCENT performed fairly well in simulating aboveground biomass C when enough N fertilization was applied (Chapters 2 and 3). However, the model tended to underestimate yield when N fertilization was insufficient (Table 4.4). Both observed and simulated results indicated higher SOC with higher N fertilization and residue return and lower SOC with lower fertilization and residue return (Table 4.4). However, the model was not sensitive enough in simulating yearly SOC changes, especially when severe drought existed (Chapters 2 and 3). The model performance in simulating GHG fluxes demonstrated a similar pattern as with aboveground biomass C, with better performance when sufficient N was applied and a less accurate fit when more N was required in the system (Chapters 2 and 3). DAYCENT only simulates SOC at 0-20 cm depth, which neglects SOC mineralization and N availability in deeper soil layers and thus may underestimate crop yield and GHG fluxes when insufficient fertilizer N was applied. Overall, DAYCENT was able to simulate observations of soil temperature, soil water content, aboveground biomass C, SOC, daily GHG fluxes, and annual GHG emissions reasonably well and captured variations caused by field management and seasonal changes (Table 4.3). Thus, model outputs were reliable for LCA of net GHG emissions under different field management practices when considering all C inputs and outputs from bioenergy sorghum production to bioethanol combustion.

4.3.2 Greenhouse Gas (GHG) Sinks

4.3.2.1 Displaced Fossil Fuel by Biofuel

Bioenergy sorghum yield was mainly determined by N fertilization (Figure 4.1a). On average, aboveground biomass C produced was 740 g m^{-2} in treatments receiving 280 kg N ha^{-1} and only 227 g m^{-2} without N application as predicted by the model. Though the model tended to underestimate yield when mineral N was insufficient as also shown in other studies (Parton and Rasmussen, 1994, Paustian, et al., 1992), dry matter yields were still in the range reported for similar field management practices (coefficient 0.45 was used to represent the average C concentration in the sorghum biomass, resulting in 5.04-16.44 Mg ha^{-1} dry matter yield) (Gill, et al., 2014, Hao, et al., 2014). Under the same N fertilization rate, higher yields were indicated by the model with 50% residue return compared with 0% return, particularly where no N was applied. Similar results were also observed and modeled by Campbell, et al. (2014) who assessed the biomass production impact of corn stover management by assembling a series of data from published literature evaluating two sites in Rosemount and Morris, MN. Powell and Hons (1992) also found that sorghum stover removal adversely affected yields during a two-year study. Given the same N fertilization and residue return rates, reduced till

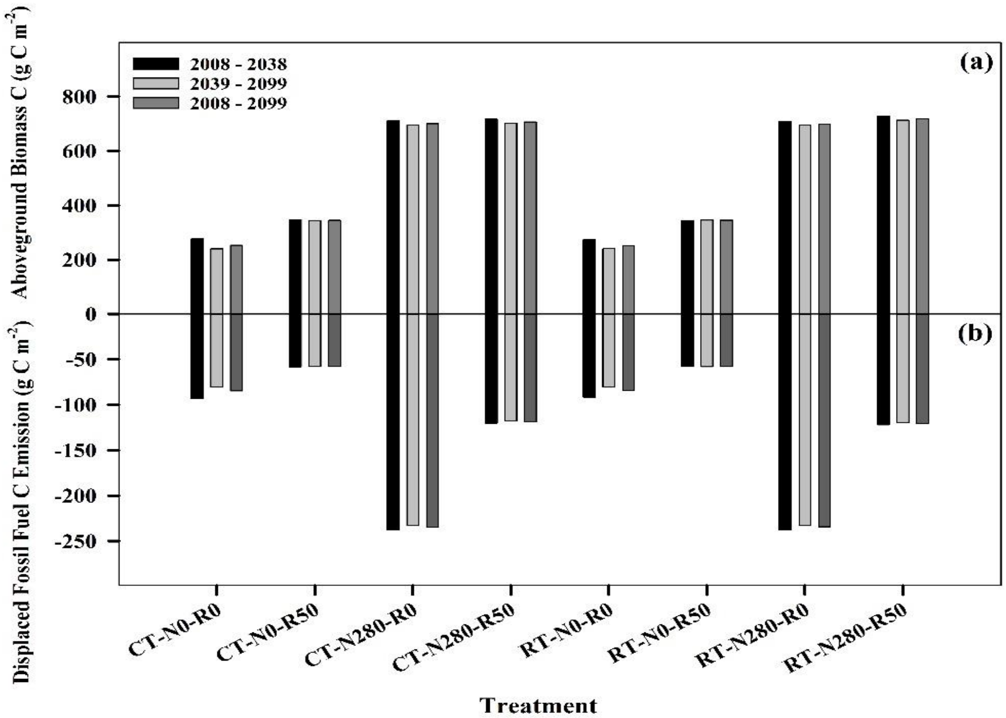

Figure 4.1 Annual aboveground biomass C (a) and displaced fossil fuel C (b) under different management practices during 2008-2038, 2039-2099, and 2008-2099. CT, RT, N0, N280, R0 and R50 represent conventional tillage, reduced tillage, no fertilizer N, 280 kg ha^{-1} fertilizer N, no residue return and 50% residue return, respectively

yielded slightly less biomass than conventional tillage (Fig. 4.1a), which might be caused by lower mineral N available for sorghum growth due to less intensive cultivation and slower mineralization in reduced tillage.

As mentioned in the LCA protocol, biofuel production was directly and linearly related to crop yield because the same C composition and conversion efficiency were used for sorghum in different treatments in this study. Thus, differences in displaced fossil fuel as affected by management practices can be explained by variation in biomass yield between different treatments, except those with 50% residue return which exhibited higher biomass yield yet had lower displaced fossil fuel since only 50% of the biomass was removed for conversion to bioethanol. As with biomass yield, displaced fossil fuel was impacted the most by N fertilization (Figure 4.1b). Treatments receiving 280 kg N ha^{-1} had the highest displaced fossil fuel, irrespective of residue return and tillage. Under the same N fertilization level, 0% residue return was able to displace more fossil fuel than 50% return since it used all aboveground biomass for bioethanol production. Reduced till had slightly lower displaced fossil fuel compared with conventional till under the circumstance of the same N fertilization and residue return levels.

For all C sinks, displaced fossil fuel was the largest GHG sink (Table 4.6). Since the composition between non-grain biomass sources is somewhat similar and ethanol yield differences per unit mass are generally small (Adler, et al., 2007, Rocateli, et al., 2012, Wang, et al., 2012), biomass yield is usually the most important factor determining biofuel production. As expected, the crop with the highest biomass yield is generally the one with the highest biofuel yield. Thus, bioenergy sorghum has an advantage in this respect. Compared with grain sorghum, forage sorghum, and corn, higher biomass yields have been observed with bioenergy sorghum, which also performed better than switchgrass and miscanthus during the first two years of production (Gill, et al., 2014, Propheter, et al., 2010, Rocateli, et al., 2012). Based on the current genetic composition of bioenergy sorghum and associated agricultural production practices, only 25% of its yield potential is being achieved (Mullet, et al., 2014). Thus, bioenergy sorghum is a promising crop for biofuel production in the future.

Table 4.6 Carbon sinks under different management practices during 2008-2038, 2039-2099, and 2008-2099. CT, RT, N0, N280, R0 and R50 represent conventional tillage, reduced tillage, no fertilizer N, 280 kg ha^{-1} fertilizer N, no residue return and 50% residue return, respectively

Treatment	Duration	C sinks (g CO_{2e}-C m^{-2} $year^{-1}$)			
		Displaced fossil fuel	Feedstock conversion	SOC change	CH_4 uptake
CT-N0-R0	2008-2038	-92.64	-28.47	13.27	-1.48
	2039-2099	-80.59	-24.77	5.31	-1.47
	2008-2099	-84.65	-26.02	7.95	-1.47
CT-N0-R50	2008-2038	-58.21	-17.89	-5.22	-1.47
	2039-2099	-57.59	-17.70	3.64	-1.46
	2008-2099	-57.80	-17.76	0.33	-1.46
CT-N280-R0	2008-2038	-238.01	-73.15	-16.22	-1.45
	2039-2099	-232.97	-71.60	1.49	-1.44
	2008-2099	-234.67	-72.12	-4.65	-1.44
CT-N280-R50	2008-2038	-120.14	-36.92	-43.78	-1.45
	2039-2099	-117.55	-36.13	-0.86	-1.44
	2008-2099	-118.42	-36.39	-15.75	-1.44
RT-N0-R0	2008-2038	-91.57	-28.14	10.35	-1.49
	2039-2099	-80.67	-24.79	4.62	-1.48
	2008-2099	-84.34	-25.92	6.47	-1.48
RT-N0-R50	2008-2038	-57.71	-17.74	-8.39	-1.47
	2039-2099	-57.95	-17.81	3.17	-1.46
	2008-2099	-57.87	-17.79	-1.21	-1.46
RT-N280-R0	2008-2038	-237.78	-73.07	-21.72	-1.46
	2039-2099	-232.67	-71.50	0.78	-1.44
	2008-2099	-234.39	-72.03	-7.01	-1.45
RT-N280-R50	2008-2038	-121.99	-37.49	-48.01	-1.41
	2039-2099	-119.56	-36.74	-0.63	-1.39
	2008-2099	-120.38	-36.99	-16.94	-1.40

Nitrogen fertilization was a major contributor to high biomass production, as demonstrated by higher average aboveground biomass C in 280 kg N ha^{-1} treatments regardless of residue return rate and tillage practice (Figure 4.1a). Since only 50% of the aboveground biomass was used for bioethanol production in treatments with 50% residue return, higher fossil fuel replacement was observed with 0% residue return when N fertilization and tillage practices were fixed (Figure 4.1b). According to the displaced fossil fuel pattern affected by these management practices, high N fertilization and low residue return rate seemed to be most favorable for bioethanol production, while the effect of tillage appeared to be minimal.

4.3.2.2 Soil Organic Carbon (SOC) Sequestration

Changes in SOC were variable and dependent on treatment (Figure 4.2a). All treatments exhibited increased SOC for the first two years after the study initiation, but treatments without added N and no residue return declined with time after that. Treatments receiving no N, but 50% residue return had elevated SOC levels compared to no N and no residue return, but then also declined with time. Treatments with N but no residue return had much greater SOC than the similar treatment without N, but the concentration stabilized after approximately 30 years. Greatest SOC was observed with added N and 50% residue return, with values increasing very slightly with time, but again generally stabilizing after 25-30 years. This prediction was consistent with the inference drawn by Lal (2004) that soil sink capacity will be filled in 20 to 50 years if recommended best management practices are conducted. Reduced tillage typically resulted in greater SOC compared to conventional, especially where N was added. Soil

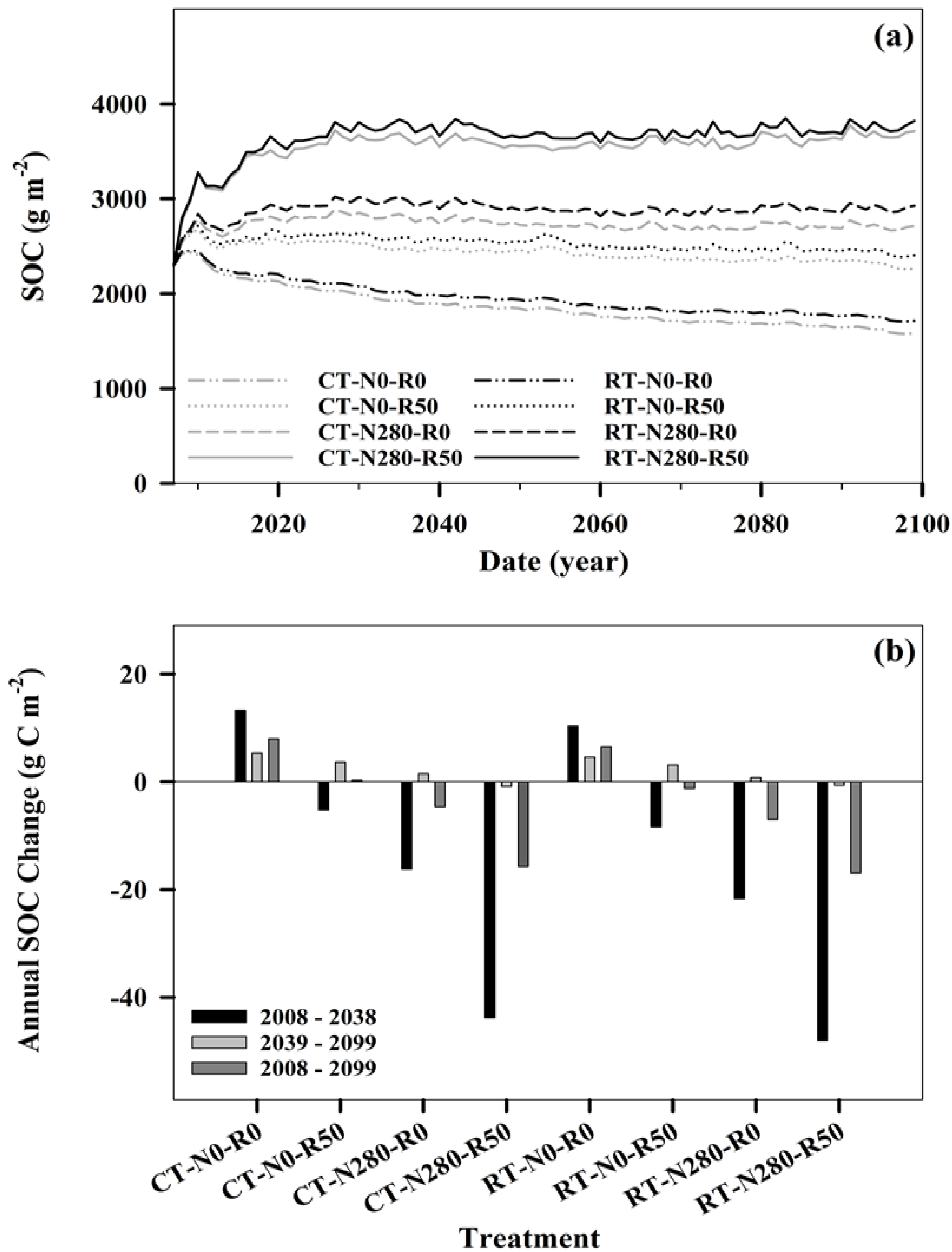

Figure 4.2 Projected SOC content at 0-20 cm under different management practices in 2008-2099 (a) and annual SOC change at 0-20 cm under different management practices during 2008-2038, 2009-2099, and 2008-2099 (b). As a sink, negative values in (b) indicate sequestration. CT, RT, N0, N280, R0 and R50 represent conventional tillage, reduced tillage, no fertilizer N, 280 kg ha^{-1} fertilizer N, no residue return and 50% residue return, respectively

organic C increase was mainly attributed to N fertilization, followed by residue return and reduced tillage, respectively. Nitrogen fertilization has been reported to result in higher total and aggregate-associated SOC levels over time in different cropping systems (Dou and Hons, 2006, Malhi and Lemke, 2007), mainly being attributed to higher yields in fertilized treatments. Higher total and active organic C pools as well as improved soil aggregation were also found with residue return in various cropping systems (Malhi and Lemke, 2007, Osborne, et al., 2014, Saffigna, et al., 1989). In contrast, SOC and available nutrients were significantly decreased when all stover was removed in both grain and forage sorghum production systems (Powell and Hons, 1991). Declines of SOC were also simulated when residues were removed from 14 residue removal experiments within temperate climatic areas of Canada and the Midwestern U.S. (Kim, et al., 2009). Numerous studies have shown that conservation tillage systems, especially no-tillage, increased both total SOC and labile SOC as well as soil aggregation in comparison with conventional tillage (Dou and Hons, 2006, Dou, et al., 2008, Wright and Hons, 2005). Reported model results also have shown that dryland soils that were depleted of C due to conventional till can store additional C upon conversion to no till (Del Grosso, et al., 2002).

Of all C sinks, SOC sequestration was the second largest sink. Treatments without N fertilization, however, were at most risk of losing SOC unless using residue return and reduced tillage practices to partially compensate for low C input and high tillage disturbance (Figure 4.2b). The change in SOC and belowground biomass C (root biomass) will approach zero with time as soil C levels reach equilibrium for a given quantity of C inputs and C losses from decomposition (Paustian, et al., 2000). However, even though changes in soil C will approach zero, some cropping systems will still have higher long-term SOC storage due to higher inputs and/or reduced decomposition. According to Figure 4.2, treatments with N fertilization appeared to better sustain SOC, even with 100% aboveground biomass removal and conventional tillage.

4.3.2.3 Methane (CH_4) Uptake

In DAYCENT, CH_4 oxidation is a function of soil water content, temperature, porosity, and field capacity. Soil water content and physical properties are the primary controls on CH_4 uptake, and the potential for soil temperature to affect CH_4 uptake rate increases as soils becomes less limited by gas diffusivity (Del Grosso, et al., 2000). In our study, soil water content differences among treatments were minimal, and higher soil temperatures were indicated in treatments with lower N fertilization and residue return rates, causing slightly higher CH_4 uptake in these treatments (Figure 4.3). Overall, however, annual CH_4 uptake was similar among different management practices, ranging from around 1.43 to 1.5 g C m^{-2}, with results being comparable with other studies for upland crops (Adler, et al., 2007, Del Grosso, et al., 2009).

4.3.3 Greenhouse Gas (GHG) Sources

4.3.3.1 Nitrous Oxide (N_2O) Emissions

As expected, both direct and indirect N_2O emissions were higher in treatments with 280 kg N ha^{-1} than those with none (Figure 4.4a, b), irrespective of residue return and tillage intensity. A similar pattern of total N_2O emissions influenced by field management practices can also be found in other field and modelling studies. Fertilizer-

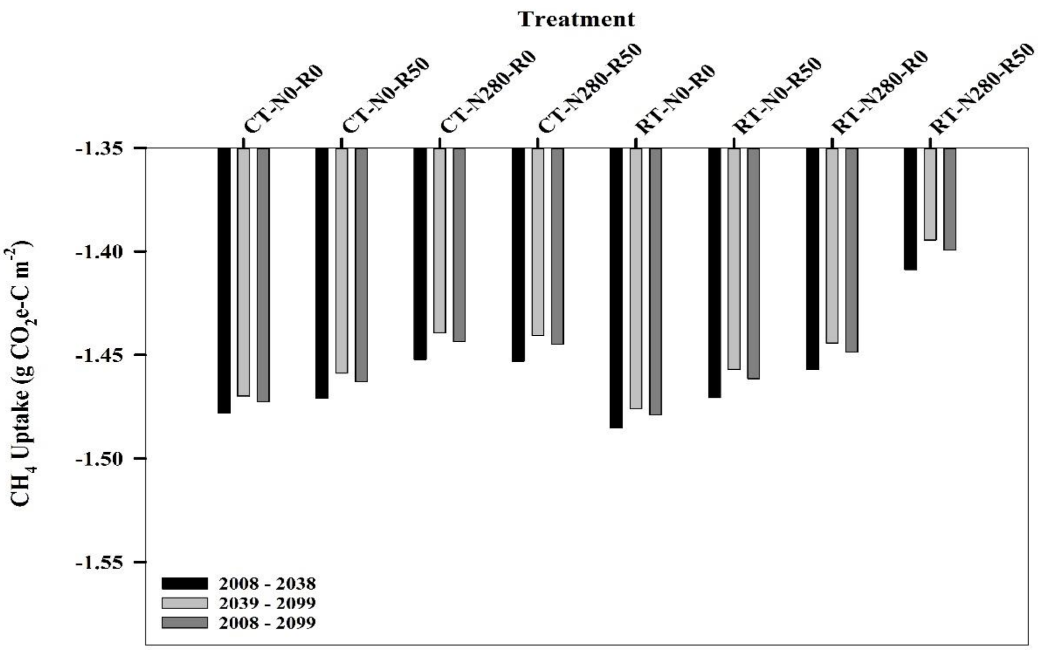

Figure 4.3 Annual soil CH_4 uptake under different management practices during 2008-2038, 2039-2099, and 2008-2099. CT, RT, N0, N280, R0 and R50 represent conventional tillage, reduced tillage, no fertilizer N, 280 kg ha^{-1} fertilizer N, no residue return and 50% residue return, respectively

induced N_2O emissions account for about 33% of the estimated total N_2O emitted from cropland in North America (Snyder, et al., 2009), and N_2O emissions from agriculture generally increase with increasing application of N fertilizer (Malhi and Lemke, 2007, Mosier, et al., 2006, Pelster, et al., 2011). Higher total N_2O emissions resulted from higher N fertilization rates in both conventional crop systems and bioenergy crop systems when DAYCENT was used for the simulations (Chamberlain, et al., 2011, Del Grosso, et al., 2009). In addition, higher total N_2O emissions were also indicated by the model in our treatments with 50% residue return (Figure 4.4a, b). Finally, higher total

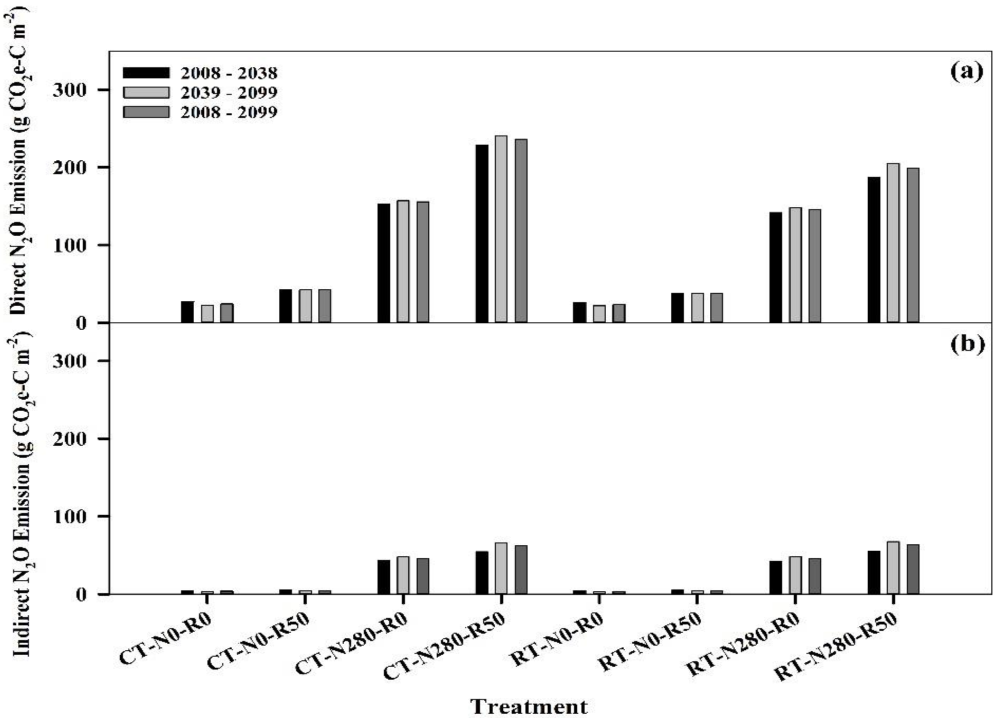

Figure 4.4 Annual direct (a) and indirect (b) soil N_2O emissions under different management practices during 2008-2038, 2039-2099, and 2008-2099. CT, RT, N0, N280, R0 and R50 represent conventional tillage, reduced tillage, no fertilizer N, 280 kg ha^{-1} fertilizer N, no residue return and 50% residue return, respectively

N_2O emissions were also observed for conventional compared with reduced till. It has often been observed that N_2O emissions increase with conversion of conventional tillage land to no-till. However, Six, et al. (2004) found that while N_2O emissions were higher the first 10 years after conversion to no-till from conventional tillage, after 20 years after no-till adoption, N_2O emissions were higher in conventional tillage systems as was observed in this study. Our simulations were for almost a century and estimating higher N_2O emissions with conventional tillage would be consistent with what has been observed in other studies (Six, et al., 2004). Less N_2O emissions were also indicated after converting to no till from conventional till in a 100-year simulation of corn production in the U.S. Corn Belt (Kim, et al., 2009).

Indirect N_2O emissions from NO_3 leaching and volatilization, like direct soil N_2O emissions, varied the same way across treatments as a function of N inputs from fertilizer and other sources (Figure 4.4b). This result was because other factors that influence N losses (soil texture, weather, etc.) were considered constant for this study.

As the biggest contributor of C sources, N_2O emissions offset quite a portion of the C which could have been sequestered by fossil fuel replacement, especially in the treatments with N fertilization and 50% residue return (Table 4.7). According to the N_2O emission patterns among different treatments, total emissions were most determined by N fertilization, followed by residue return, and tillage, respectively. Although treatments releasing as little gaseous N emissions as possible would be favorable, biomass yield and SOC should also be taken into account when selecting the best management practice combinations.

4.3.3.2 Nitrogen (N) Fertilization and Machinery

Only treatments receiving 280 kg N ha^{-1} had N fertilizer manufacture as a C source. The CO_2 emissions associated with the manufacture of chemical farm inputs (fertilizers, limestone, herbicides, insecticides) were taken from West and Marland (2002). The CO_2 emissions associated with the manufacture of chemical farm inputs were the same, with 24.01 g C m^{-2} for all fertilized treatments.

Agricultural machinery used in our study included those used for tillage, planting, fertilization and herbicide application, and harvesting operations. Fuel used by

Table 4.7 Carbon sources under different management practices during 2008-2038, 2039-2099, and 2008-2099. CT, RT, N0, N280, R0 and R50 represent conventional tillage, reduced tillage, no fertilizer N, 280 kg ha^{-1} fertilizer N, no residue return and 50% residue return, respectively

Treatment	Duration	C sources (g CO_{2e}-C m^{-2} year^{-1})			
		Direct N_2O emission	Indirect N_2O emission	N Fertilizer manufacture	Field operations
CT-N0-R0	2008-2060	27.30	4.46	0.00	2.44
	2061-2099	22.69	3.39	0.00	2.44
	2008-2099	24.24	3.75	0.00	2.44
CT-N0-R50	2008-2060	42.79	4.99	0.00	2.44
	2061-2099	42.38	4.53	0.00	2.44
	2008-2099	42.52	4.69	0.00	2.44
CT-N280-R0	2008-2060	152.75	42.92	24.01	2.58
	2061-2099	157.03	47.60	24.01	2.58
	2008-2099	155.59	46.02	24.01	2.58
CT-N280-R50	2008-2060	228.40	54.49	24.01	2.58
	2061-2099	240.22	65.79	24.01	2.58
	2008-2099	236.23	61.98	24.01	2.58
RT-N0-R0	2008-2060	25.81	4.08	0.00	1.58
	2061-2099	21.99	3.19	0.00	1.58
	2008-2099	23.28	3.49	0.00	1.58
RT-N0-R50	2008-2060	37.38	4.88	0.00	1.58
	2061-2099	38.36	4.64	0.00	1.58
	2008-2099	38.03	4.72	0.00	1.58
RT-N280-R0	2008-2060	141.38	41.88	24.01	1.71
	2061-2099	148.16	47.74	24.01	1.71
	2008-2099	145.88	45.77	24.01	1.71
RT-N280-R50	2008-2060	187.47	55.53	24.01	1.71
	2061-2099	204.87	67.54	24.01	1.71
	2008-2099	199.01	63.49	24.01	1.71

agricultural machinery for these same operations were determined by using agricultural machinery management data documented in the ASAE machinery management standards and compiled by Adler, et al. (2007). The CO_2 emissions associated with each operation were 0.43, 0.39, 0.13, and 0.75 g C m^{-2}, respectively (Table 4.5). The machinery use difference was caused by differences in fertilization and tillage in various treatments, with two diskings before planting and after harvest, and one in-season cultivation for conventional tillage, while reduced tillage only received in-season cultivation. Treatments with both 280 kg N ha^{-1} and conventional tillage had the highest machinery emissions, and treatments with neither had the lowest emissions.

The C emissions from farm operations were similar to the compilation conducted by Lal (2004). The CO_2 costs of chemical inputs were mainly due to fertilizer production, followed by limestone, herbicides, and insecticides (West and Marland, 2002). Nitrogen fertilizer production was responsible for most of the CO_2 costs from fertilizer input for all studied cropping systems reported by Adler, et al. (2007), and it ranked in second place for GHG sources in our study. Kim, et al. (2009) also found the primary source of total fossil energy associated with crop biomass production was N fertilizer production and application. Thus, reducing synthetic N use is important for decreasing GHG emissions, especially N_2O, from cropping systems through use of more efficient N-use strategies (Del Grosso, et al., 2009).

4.3.4 Net Greenhouse gas (GHG) Emissions

The LCA integrated all GHG sinks and sources evaluated in this study, and considered how using biofuels would reduce net GHG emissions compared to continued fossil fuel use. Three sources of GHG emissions were quantified in this study, soil N_2O emissions, CO_2 emissions from manufacture of fertilizer, and CO_2 from fuel used by agricultural machinery for tillage, planting, fertilizer application, and harvesting. Three sinks for GHG emissions were also evaluated, the amount of C released from fossil fuel combustion replaced by ethanol production and conversion, the change in SOC and belowground biomass C, and C from CH_4 uptake by the soil. All sources and sinks were ordered in their contribution to C losses or gains.

Projections to the end of this century were conducted to undertake a LCA of net GHG emissions under eight management practices [all the combinations of N fertilization, residue return, and tillage with levels of 0 vs. 280 kg N ha^{-1} (N0 vs. N280), 0% vs. 50% aboveground biomass return (R0 vs. R50), and conventional vs. reduced till (CT vs. RT), respectively]. Since SOC reached equilibrium after approximately 30 years according to simulation, all model outputs needed for LCA were calculated on an annual basis for three periods, 2008-2038, 2039-2099, and 2008-2099, in order to assess short-term, long-term, and average impacts (Tables 4.6 and Table 4.7).

For both short-term and long-term scenarios, all treatments were promising for mitigating GHG emissions, except treatments with both 280 kg N ha^{-1} and 50% residue return, mainly due to higher N_2O emissions and lower displaced fossil fuel C emissions (Figure 4.5). Biofuels have been considered to have a near-zero net emission of GHGs since CO_2 released from bioethanol combustion will be reabsorbed through photosynthesis and fixed in the plant and soil again. Additionally, coproducts such as lignin and protein can also reduce net GHG emissions, making these system sinks

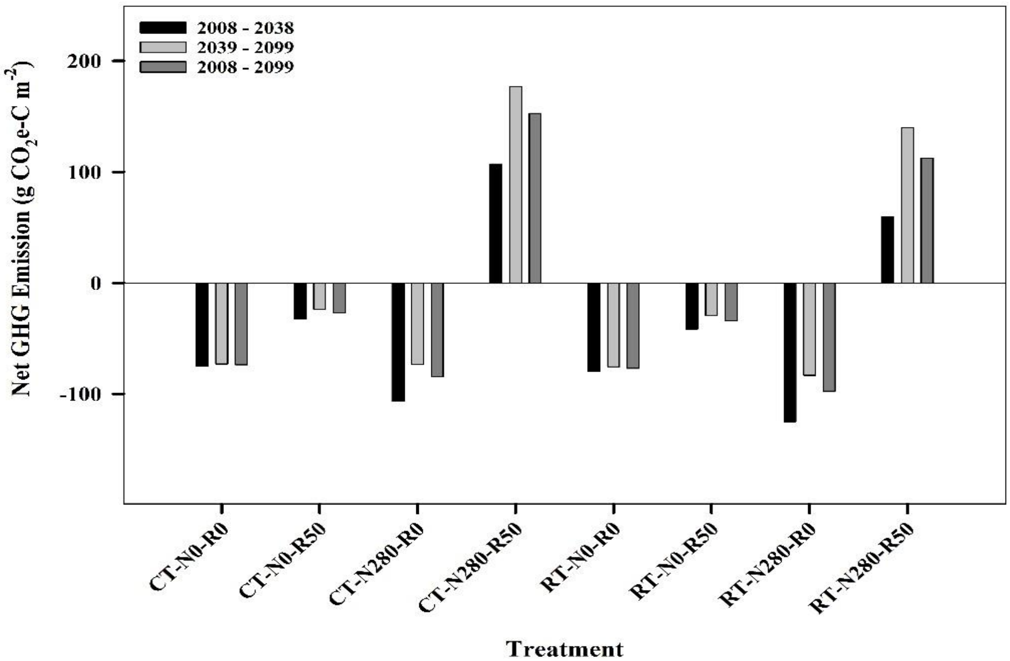

Figure 4.5 Annual net GHG emission under different management practices during 2008-2038, 2039-2099, and 2008-2099. CT, RT, N0, N280, R0 and R50 represent conventional tillage, reduced tillage, no fertilizer N, 280 kg ha^{-1} fertilizer N, no residue return and 50% residue return, respectively

(Adler, et al., 2007, Murphy and Kendall, 2015). When compared with the life-cycle GHG emissions of the displaced fossil fuel, our analysis also showed biofuels had net GHG benefits. Similar results were shown in other studies on LCA of net GHG for other bioenergy crops. Meyer, et al. (2016) did a LCA of GHG for seven biomass feedstocks [pine (*Pinus sp*.), tulip poplar (*Liriodendron tulipifera*), hybrid poplar, switchgrass, corn stover, and two blends consisting of either equal weights of pine, tulip poplar, and switchgrass, or two thirds of pine and one third of hybrid poplar] and found that the estimated GHG reduction compared to petroleum fuel was 60% or greater in all cases

(27.8-38.7 g CO_{2e} MJ^{-1} compared to 93.08 g CO_{2e} MJ^{-1} for fossil fuel). A study conducted by Murphy and Kendall (2015) for corn stover and switchgrass as feedstocks indicated that most of the conservative scenarios estimated GHG emissions of approximately 45-60 g CO_2 equivalent per MJ of delivered fuel without credit for coproducts, and 20-30 g CO_{2e} MJ^{-1} when coproducts were considered, reducing GHG emissions by 36%-79%. However, our study indicated a range of from 103% GHG reduction to 144% GHG addition compared to fossil fuel combustion depending on different field management practices, indicating the significance of selecting appropriate management practices for biofuel feedstock production. Adler, et al. (2007) used the same protocol to assess GHG fluxes for corn, soybean, alfalfa, hybrid poplar, reed canarygrass (*Phalaris arundinacea* L.), and switchgrass as bioenergy crops, and found that compared with the life cycle of fossil fuel, ethanol and biodiesel from corn reduced GHG emissions by ~40%, reed canarygrass by ~85%, and switchgrass and hybrid poplar by ~115%. The difference in Adler's and our study compared with the other two studies was that in our study DAYCENT was used to account for SOC sequestration and CH_4 uptake, both C sinks in the LCA, while the other two excluded these portions. The discrepancy between our study and Adler's was that Adler's work focused on LCAs for different bioenergy crops, while our work focused only on bioenergy sorghum but with different management scenarios in order to determine the optimum combination. It's also worth noting that Adler's study ran the model for only 30 years and the GHG reduction percentage aforementioned was based on a long-term estimation which assumed SOC was at equilibrium. The short term simulation actually indicated a ~155%

GHG reduction for switchgrass and hybrid poplar. Other factors such as differences in biomass yield and fertilization rate also contributed to differences in GHG reduction rate. The assumptive unlimited N fertilizer application in our study (28.3 g N m^{-2}) was much higher than the amount used in Adler's study, in which N fertilizer application rates were 12.7 g N m^{-2} for corn, 5.6 g N m^{-2} for switchgrass and 15.4 g N m^{-2} for reed canarygrass with half applied in the spring and the other after harvest. This might be the reason for much higher N_2O emissions in our study, which offset some benefit of C mitigation potential.

Overall, all our studied management combinations were able to sequester atmospheric C, except the treatment with 280 kg N ha^{-1} and 50% residue return under both conventional and reduced tillage. Taking into considerations all C sinks and sources, 280 kg N ha^{-1} with 0% residue return under reduced tillage produced the highest biomass yield for biofuel production, sustained adequate SOC, and sequestered the most atmospheric C among the eight management treatments, resulting in a net GHG emission reduction of approximately 150 g CO_2e-C m^{-2} yr^{-1} in the short term and 80 g CO_2e-C m^{-2} yr^{-1} in the long term. (Figure 4.5).

It has been demonstrated in previous studies that cellulosic crops had higher biofuel yield and lower GHG emissions per unit land area than grain crops (Adler, et al., 2007, Daylan and Ciliz, 2016, Murphy and Kendall, 2015). Cellulosic crops also had a greater reduction in GHG emissions per unit biofuel produced than grain crops, resulting in greater reductions in GHG emissions associated with energy use compared with fossil fuels. Currently, only a portion of total biomass C is convertible to ethanol due to technical obstacles. In an ethanol conversion facility for corn stover, for example, only about one third of the biomass C is converted to ethanol, with the remainder of biomass C being emitted as combustion exhaust and fermentation-generated CO_2 (Sheehan, et al., 2004). Capture of CO_2 from fuel production and energy generation using biomass would further increase the capacity of bioenergy crops for reducing net GHG emissions as refining techniques advance and optimum field management practices are adopted.

4.4 Conclusions

The DAYCENT model was able to simulate soil temperature, soil moisture, aboveground biomass C yield, SOC, and GHG emissions under different residue return rates, N fertilization rates, and tillage practices, enabling a reliable LCA of net GHG emissions under different field management practices in bioenergy sorghum production. Of all C sinks, displaced fossil fuel was the largest GHG sink, followed by SOC sequestration and CH_4 oxidation. For all C sources, N_2O emissions were the largest GHG source, followed by energy requirements for N fertilizer manufacture and field machinery operations. All management combinations were able to sequester atmospheric C, except the treatment receiving 280 kg N ha^{-1} fertilization and 50% residue return under both conventional and reduced tillage. Zero residue return with N fertilization under reduced tillage was able to yield highest biomass for biofuel production, sustain adequate SOC, and sequester the most atmospheric C among the eight management practice combinations studied.

CHAPTER V

BEST SOIL AND WATER MANAGEMENT PRACTICE FOR BIOENERGY SORGHUM PRODUCTION IN TEXAS

5.1 Introduction

Biofuel production must increase to 36 billion gallons by the year 2022 in order to meet U.S. government mandates, with the majority of this fuel to be produced from advanced or second-generation biofuel feedstocks after 2015 (U.S. Congress, 2007). Despite this mandate, the current production of biofuels from advanced feedstocks, including crop residue from annual crops such as sorghum [*Sorghum bicolor* (L.) Moench.] and corn (*Zea mays* L.), has been very low (Williams, et al., 2016). As 2022 draws closer, the urgency of establishing a lignocellulosic biofuel industry becomes more pressing. Many questions still remain as to the viability of the industry, including farm-level biomass production.

Bioenergy sorghum is a second generation biofuel crop with attributes of high biomass yield potential, drought tolerance and genetic tractability. As a C4 crop originally from Africa, it has potential to be successfully grown in the southern U.S. Texas is geographically located in the south central part of the U.S. and leads the nation in agricultural land and associated commodity production. Sorghum is well-adapted to Texas, and its ability to yield consistently in harsh environments makes it popular with growers. However, inappropriate crop management may occur due to the lack of information of the production efficiency and environmental effects, such as greenhouse gas (GHG) emissions, of this emerging crop, with merely 14 years since the development of hybrid sorghum for bioenergy at Texas A&M University in 2003 (Rooney, et al., 2007). Meanwhile, Texas has a wide diversity of climate and soils due to its large geographical area, second in size among the U.S. states. Thus, it is meaningful to explore suitable production areas and field management practices for bioenergy sorghum production in Texas, in order to maximize the crop productivity, effectively conserve and utilize soil and water resources, and mitigate GHG emissions.

A few field studies on the effects of management practices on bioenergy sorghum production have been conducted in several places in Texas and other southern states (Gill, et al., 2014, Hao, et al., 2014, Rocateli, et al., 2012). However, due to environmental factor differences such as climate and soil properties, as well as field management differences, results from these studies are varied and hard to compare. Additionally, most studies only lasted for 2-3 years and yield was measured in finite treatments due to labor and funding limitations (Olson, et al., 2012, Propheter, et al., 2010). One of the most systematic studies was conducted near College Station, Texas (Shahandeh, et al., 2016, Storlien, et al., 2014, Wight, et al., 2012). This study measured soil temperature, soil moisture, aboveground sorghum biomass and biomass carbon (C) and nutrient concentrations, soil organic carbon (SOC) and soil nutrient contents, and soil GHG fluxes including carbon dioxide (CO_2) and nitrogen oxide (N_2O) over 8 years. However, even 8 years of field data are still not enough to predict very long-term effects and generalize regional patterns. Process-based biogeochemical models can be used to predict the overall performance of long-term bioenergy sorghum production in different regions and under more complex field management combinations. These models potentially can provide regional estimations of planting feasibility and best soil and water management practices for bioenergy sorghum in different geographical areas.

DAYCENT, the daily time step version of the CENTURY biogeochemical model (Parton, et al., 1987, Parton, et al., 1988), simulates C and nitrogen (N) dynamics among atmosphere, vegetation, and soil (Del Grosso, et al., 2001, Parton, et al., 1998). Key submodels include plant production, organic matter decomposition, soil water and temperature flows, and trace gas fluxes. Plant production is a function of genetic potential, phenology, nutrient availability, water and temperature stress, and solar radiation. Decomposition of litter and SOC and nutrient mineralization are functions of substrate availability and quality, and water and temperature stress. Nitrogen gas fluxes from nitrification and denitrification are driven by soil ammonium (NH_4^+) and nitrate (NO_3^-) concentrations, water content, temperature, texture, and labile C availability. Major model inputs are daily weather data, soil properties, best available information about native vegetation and historical agricultural use, as well as current land management and crop characteristics. Major model outputs are soil water and temperature by soil layers, aboveground and belowground crop biomass, soil organic C and N to 20-cm depth, soil mineral N by soil layer, as well as soil CO_2 and N gas emissions. The DAYCENT model has been extensively tested at different resolutions and has been shown to be effective in simulating C and N dynamics in different ecosystems (Del Grosso, et al., 2009, Parton, et al., 2015, Zhang, et al., 2013).

The objective of this study was to conduct simulations of bioenergy sorghum production for each county in Texas under 45 residue return, N fertilization, and tillage management combinations under 3 different irrigation regimes. The process-based biogeochemical model DAYCENT integrated GIS-based county level representative weather, soil, and growing season information and predicted long-term sorghum biomass yield, SOC change, and soil N_2O emission potential in order to determine the suitability of each county for bioenergy sorghum production and to assess best management practices.

5.2 Materials and Methods

County level simulations were carried out for the state of Texas to predict C dynamics and GHG emissions following the conversion of conventional crops to bioenergy sorghum in the period of 2016-2050. The focus of simulations for all Texas counties during this period included: (1) annual aboveground biomass C of bioenergy sorghum under 45 management practices including all combinations of residue return (0%, 25%, and 50% of aboveground biomass return represented by RR0, RR25, and RR50, respectively), N fertilization (0 kg N ha^{-1}, 75 kg N ha^{-1}, 150 kg N ha^{-1}, 225 kg N ha^{-1}, and 300 kg N ha^{-1} represented by N0, N75, N150, N225, and N300, respectively), and tillage (conventional tillage, reduced tillage, and no till represented by CT, RT, and NT, respectively) under 3 different irrigation regimes (no irrigation, irrigation to field capacity when soil water content drops to wilting point, and irrigation to field capacity when soil water content drops to 50% available soil water content represented by non-irrigation, limited-irrigation, and full-irrigation, respectively); (2) annual SOC change in respective cropping treatments, and (3) annual net GHG budget for each cropping system, including crop/soil system CO_2 flux and direct N_2O emissions calculated both with and without GHG mitigation by harvested biomass conversion.

Simulations were divided into three major steps: 1) acquisition and formatting of model input data required to run DAYCENT, 2) modelling of native vegetation and conventional cropping systems to adjust SOC close to the initial value when projection was started, and 3) simulations of bioenergy sorghum cropping systems under different management practice and irrigation regime combinations.

5.2.1 Input data collection

Weather, soil properties, representative native vegetation and conventional crop data were collected in each county to initialize SOC to the closest to current value when each prediction was initiated. Plow-out time of native vegetation and progressive field management practices for conventional crop agricultural systems were estimated. Meteorological data required to drive DAYCENT were acquired from DAYMET (https://daymet.ornl.gov/), a dataset that provides gridded estimates of daily time step, 1-km^2 spatial resolution weather data. DAYMET daily weather data are available for the continental U.S. for 1980 through the latest calendar year. In this study DAYMET data in 1982-2016 were selected to represent future weather data in 2016-2050. Soil data were acquired from the web soil survey (https://websoilsurvey.sc.egov.usda.gov/App/HomePage.htm). Representative native vegetation was identified from Major Land Resource Areas Dataset maps from the Geospatial Data Gateway (https://gdg.sc.egov.usda.gov/) and described in Land Resource Regions and Major Land Resource Areas of the U.S., the Caribbean, and the Pacific Basin (USDA NRCS, 2006). Representative conventional crops were identified from Cropland Data Layer Dataset maps from the Geospatial Data Gateway (https://gdg.sc.egov.usda.gov/). The latitude and longitude of the center of the largest cluster of cropped land in each county were identified based on National Land Cover Dataset maps from the Geospatial Data Gateway (https://gdg.sc.egov.usda.gov/). For each county, soil data, climate data, the highest percentage of land use in major land resource areas, and crops planted in 2011-2015 of the area weighted geographic center of cropped land were used to drive DAYCENT. County-specific soil property data were acquired including percent sand, silt, and clay, bulk density, and pH. DAYMET climate data from the 1-km^2 cell that was closest to the geographic center were collected including daily maximum and minimum temperatures and precipitation. Approximate plow-out year of native vegetation and consequent management practices were derived from archived county soil surveys (http://www.nrcs.usda.gov/wps/portal/nrcs/soilsurvey/soils/survey/state/). Initial SOC data at the 0-20 cm depth when projections were started were obtained from Soil Survey Geographic Database (SSURGO) (https://gdg.sc.egov.usda.gov/).

5.2.2 Native vegetation and historical agriculture simulation

Two sets of simulations were performed for each county: one for native vegetation (year 1 to around 1850) and the other to represent conventional crop agricultural practices (around 1851 to 2015). Collected information and historical data including weather, soil, native vegetation, and conventional cropping systems were summarized into a set of 254 * 2 schedule files representing native vegetation and a full range of agricultural practices for conventional crops in each county. Simulation of about 1850 years of native vegetation was needed to ensure that SOM pools in the model were at steady state. Simulations of initial plow-out and conventional crop agricultural practices assumed conventional to less intensive tillage, gradual increases in synthetic fertilizer application and residue return, and progressively higher yielding crop cultivars, in order to approach as closes as possible to current SOC values before projections were started.

DAYCENT was calibrated by fitting final SOC values in conventional crop simulations to the SOC values collected from SSURGO, in order to develop initial soil fertility parameters for model projections. Discrepancies between modeled and observed SOC values at this stage provided more information about historical changes in crop varieties, fertilization and residue return levels, and tillage practices for each county, indicating how to adjust the model's parameters and inputs to improve the accuracy of schedule files at each point in time. For example, if actual SOC was greater than simulated SOC for a given county, more fertilizer (within historically realistic limits) could be applied, or a higher yielding variety could be chosen (Hartman, et al., 2011).

5.2.3 Projection of bioenergy sorghum production

The DAYCENT model was used to estimate bioenergy sorghum yields, SOC levels, and N_2O emissions for each county for 45 different management practice combinations under three irrigation regimes. Five N fertilization levels (N0, N75, N150, N225, and N300), three levels of residue return (RR0, RR25, and RR50), three tillage levels (CT, RT, and NT), as well as three irrigation regimes (non-irrigation, limited-irrigation, and full-irrigation) were assembled into 135 different scenarios (5*3*3*3) for analysis for bioenergy sorghum production in each one of 254 counties. The model was repeatedly run 34290 times (135*254) by programming using C language. Model parameters were adopted from the calibration and validation process by utilizing field aboveground biomass C, SOC, and GHG data under different N fertilization, residue return, and tillage practices for bioenergy sorghum production in 2008-2015 that were collected at the Texas A&M AgriLife Research Farm near College Station (Shahandeh, et al., 2016, Storlien, et al., 2014, Wight, et al., 2012). Key parameters are included in Table 5.1, and statistics about model performance in our verified simulations are included in Table 5.2.

According to our earlier work on life cycle analysis (LCA) of net GHG emissions in bioenergy sorghum production systems, major C sinks and sources were selected for county net GHG emission calculations. Net GHG budgets were calculated by accounting for crop/soil system CO_2 flux, direct N_2O emissions, and with or without C emissions replaced by harvested biomass conversion. It was assumed that net change in system C was due to the sequestration of CO_2 by plants and the release of CO_2 from heterotrophic respiration. Thus, crop/soil system CO_2 flux was calculated through system C change in the soil including SOC and residual C.

DAYCENT model outputs included system plant and soil C amounts in g C m^{-2} and N_2O flux in g N_2O-N m^{-2}. The units of these two variables were converted to CO_2-C equivalents so they could be added together to compute net GHG emissions. It was assumed that a kilogram of N_2O has 298 times the 100 year horizon global warming potential (GWP) of a kilogram of CO_2 (Forster, et al., 2007). As to C emissions replaced

Table 5.1 Selected key parameters modified in DAYCENT model for bioenergy sorghum study

Parameter	Definition	Value	Default
DMPST	Damping factor for calculating soil temperature by layer	0.005	0.003
PMXTMP	Effect of biomass on maximum surface temperature	-0.0048	-0.0032
PRDX(1)	Coefficient for calculating potential production	0.8	0.5
PPDF(1)	Optimum temperature for production (°C)	35	30
PPDF(2)	Maximum temperature for production (°C)	50	45
FRTC(2)	Fraction of C allocated to roots in mature plants	0.3	0.1
CKMRSPMX(2)	Maximum fraction of juvenile live fine root C that goes to maintenance respiration for crops	1.0	0.5
CKMRSPMX(3)	Maximum fraction of mature live fine root C that goes to maintenance respiration for crops	1.0	0.5
CGRESP(2)	Maximum fraction of juvenile fine root live C that goes to growth respiration for crops	1.0	0.5
CGRESP(3)	Maximum fraction of mature fine root live C that goes to growth respiration for crops	1.0	0.5

Table 5.2 Statistical tests between simulated and measured values of soil temperature, soil water content, aboveground biomass C, SOC, daily CO_2-C fluxes, daily N_2O-N fluxes, annual CO_2-C, and annual N_2O-N emissions for bioenergy sorghum study

Measurements	r^2	Slope	Intercept	RMSE*
		Calibration		
Soil temperature	0.88	0.72	8.34	3.12
Soil moisture	0.87	1.12	-0.01	0.03
Aboveground biomass C	0.58	0.80	27.94	165.63
SOC	0.67	0.75	639.95	130.46
Daily CO_2	0.53	0.43	1.08	2.63
Daily N_2O	0.73	0.55	-0.23	38.70
Annual CO_2	0.28	0.72	-22.36	347.81
Annual N_2O	0.93	0.80	-1529.00	3145.58
		Validation		
Soil temperature	0.91	0.78	6.61	3.64
Soil moisture	0.73	0.88	0.02	0.04
Aboveground biomass C	0.72	1.11	-36.66	118.92
SOC	0.43	0.76	601.79	242.11
Daily CO_2	0.57	0.34	0.95	3.16
Daily N_2O	0.36	0.19	10.42	61.60
Annual CO_2	0.76	1.51	-822.88	312.93
Annual N_2O	0.92	1.35	-4084.60	1984.52
		Overall		
Soil temperature	0.90	0.76	7.17	3.40
Soil moisture	0.80	1.01	0.01	0.03
Aboveground biomass C	0.56	0.81	60.26	147.44
SOC	0.51	0.75	639.20	145.64
Daily CO_2	0.53	0.38	1.03	2.91
Daily N_2O	0.51	0.35	6.48	51.51
Annual CO_2	0.49	1.08	-371.47	330.83
Annual N_2O	0.81	1.04	-2508.90	2629.92

* RMSE indicates root mean square error

by harvested biomass conversion, the protocol used by Adler, et al. (2007) was adopted, which was calculated using harvested biomass C/0.45/1,000,000*90%*381*6.75/10.3*671.3, where 0.45 was used to convert from C to yield, assuming 1 g C per 2.2 g dry matter (Hartman, et al., 2011), 1,000,000 was yield unit conversion from g to Mg, 90% was harvested biomass use ratio, 381 was theoretical ethanol yield per Mg of dry matter as corn stover, 6.75 and 10.3 were fuel economy ratios of fossil fuel to biofuel, which was 6.75 km L^{-1} ethanol divided by 10.3 km L^{-1} gasoline (Sheehan, et al., 2004), and 671.3 was CO_2e-C emission per liter of gasoline consumed.

5.3 Results and Discussion

5.3.1 Treatment Differences

Results showed higher irrigation increased biomass C yield, SOC, and N_2O emissions, with limited irrigation seeming to have advantages over non-irrigation and full-irrigation mainly due to its significant increase in sorghum yield and SOC compared to dryland and lower N_2O and only slightly lower yield compared to full-irrigation (Figure 5.1). Limited irrigation was shown to be the most effective irrigation strategy for bioenergy sorghum yield by Hao, et al. (2014) in a three-year study in the Texas High Plains. Biomass yields in their study ranged from 15 Mg ha^{-1} to 23 Mg ha^{-1}, 11 Mg ha^{-1} to 18 Mg ha^{-1}, and 8 Mg ha^{-1} to 13 Mg ha^{-1} at full and limited irrigation, and under dryland, respectively. Our simulations indicated average yields for full, limited, and non-irrigation were 14, 12, and 7 Mg ha^{-1}. Reasons why our data were at the lower ends of their ranges might be that averages in our study were taken from all management practices and counties. Low fertilization treatments and counties not suitable for bioenergy sorghum production lowered average yields compared with yields under adequate fertilization in their study which was located in a traditional high fertility production area of the High Plains. Another two-year field trial conducted in Alabama

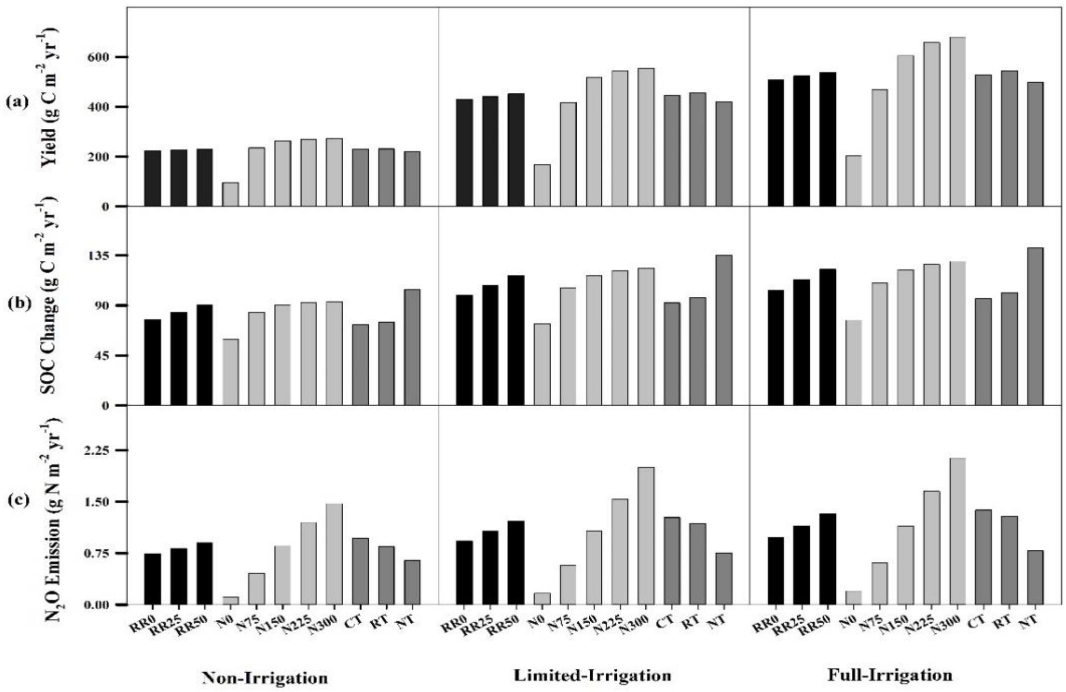

Figure 5.1 Annual aboveground biomass C (a), SOC change (b), and N_2O emission (c) under different residue return, N fertilization, and tillage intensity under three irrigation systems in 2016-2050 with bioenergy sorghum. RR, N, CT, RT, and NT represent the percentage of biomass returned, the amounts of fertilizer N added in kg ha^{-1}, conventional tillage, reduced tillage, and no-till, respectively

also demonstrated higher sorghum biomass with irrigation compared with dryland (Rocateli, et al., 2012).

The model also indicated that SOC increased as irrigation increased (Figure 5.1b). However, the rate of increase was not as high as that demonstrated for yield. One reason might be that increased yield from higher irrigation may have been more quickly decomposed under more favorable soil water conditions with greater irrigation. Irrigation increased biomass C assimilation, which often translates to more crop residues returned to the soil, including both aboveground dead material and root systems left after harvest (Wilhelm, et al., 2004). On the other hand, more belowground C allocation as a microbial energy source and more favorable soil moisture may have facilitated microbial decomposition, causing C loss as CO_2. A long-term study on the effects of irrigation on CO_2 emissions in soybean [*Glycine max* (L.) Merr.] production systems showed higher growing season CO_2 emissions under irrigated than under dryland management, especially during dry growing seasons (Smith and Brye, 2014). In the DAYCENT model, the potential decomposition rate is influenced by multiplicative functions of soil moisture and soil temperature. Microbial activity increases up to a point with increasing soil water content, which directly influences soil respiration (Franzluebbers, et al., 2001).

Higher N_2O emission with greater irrigation might be attributed to more beneficial soil water conditions for either nitrification or denitrification. Emissions of N_2O from cropped soils are most often a byproduct of nitrification or denitrification (Del Grosso, et al., 2000, Parton, et al., 2001, Parton, et al., 1996). In DAYCENT, N gas flux from nitrification is assumed to be a function of soil NH_4^+ concentration, soil water content, temperature, and pH. Denitrification is a function of soil NO_3^- (e^- acceptor) concentration, labile C (e^- donor) availability, water-filled pore space (WFPS), and soil physical properties related to texture that influence gas diffusivity. Denitrification prevails under anaerobic conditions, commonly associated with excessively wet soils, although very high CO_2 concentrations in microsites within the soil may be conducive to denitrification on a small scale. When WFPS in soil reaches more than 80%, denitrification is anticipated to be the dominant N_2O-producing process, while lower soil moisture levels would be more conducive to nitrification (Del Grosso, et al., 2011). In either case, increased soil water content could accelerate N gas fluxes.

Within an irrigation level, higher residue return and N fertilization increased all the selected indices (Figure 5.1a, b, c). Crop residues serve as important sources of SOC and various nutrients, protect topsoil from erosion, and modify soil water and temperature, thus offering potentially higher crop production (Wilhelm, et al., 1986). Research has shown that excessive biomass removal in forage and grain sorghum production systems decreased subsequent biomass yield (Powell and Hons, 1992). Additionally, agricultural residues favor SOC through increased soil aggregation, which further improves soil structure, increases soil water holding capacity, and improves soil aeration as well (Wilhelm, et al., 2004). Higher total and active organic C pools, as well as improved soil aggregation, were found at higher residue return rates in various cropping systems (Malhi and Lemke, 2007, Osborne, et al., 2014, Saffigna, et al., 1989). In contrast, SOC and nutrients were significantly decreased when all stover was removed in grain and forage sorghum production systems (Powell and Hons, 1991). As indicated by our simulations, residue return may also potentially increase soil microbial activity and GHG emissions (Saffigna, et al., 1989). Generally, CO_2 and N_2O were increased with residue returned because of enhanced microbial activity, nutrient cycling, and nitrification/denitrification (Huang, et al., 2004, Jin, et al., 2014, Saffigna, et al., 1989),

Nitrogen fertilization has a vital impact on C and nutrient cycling. As the main yield-determining macronutrient, N fertilizer is able to increase the production of various crops (Malhi and Lemke, 2007, Nyakatawa and Reddy, 2000, Sainju, et al., 2006).

Nitrogen fertilization increased SOC (Figure 5.1b), which may result mainly from increased net primary productivity (NPP). Nitrogen fertilization has been reported to result in higher total and aggregate-associated SOC levels over time in different cropping systems (Dou and Hons, 2006, Malhi and Lemke, 2007). However, N fertilization is also typically one of the largest factors contributing to GHG emissions, especially N_2O (Figure 5.1c). N_2O emissions from agriculture generally increase with increasing application of N fertilizers (Malhi and Lemke, 2007, Mosier, et al., 2006, Pelster, et al., 2011) and the positive role of N fertilization in facilitating production and sequestering C may be offset by N_2O emissions (Snyder, et al., 2009).

Lower tillage intensity lowered yield slightly, but significantly increased SOC and reduced N_2O emissions, which has also been demonstrated by other studies. Tillage destroys macroaggregates, exposing previously sequestered organic C to microbial activity. Numerous studies have shown that conservation tillage systems, especially NT, increased both total SOC and labile SOC as well as soil aggregation in comparison with conventional tillage (Dou and Hons, 2006, Dou, et al., 2008, Wright and Hons, 2005). Use of conservation tillage practices has been claimed as one of the most important approaches to reducing the rate of increase of atmospheric CO_2 by decreasing disturbance and decomposition of organic C in the soil (Follett, 2001). Additionally, parallel or lower N_2O emissions were observed in some cases in short-term NT systems (Malhi and Lemke, 2007, Pelster, et al., 2011). Six, et al. (2004) and Plaza-Bonilla, et al. (2014) suggested that N_2O emissions could be reduced by long-term NT, possibly due to an improvement of soil structure. This indication was in agreement with the meta-analysis conducted by van Kessel, et al. (2013). Our simulations showed the yield trend being reduced tillage with the highest yield, followed by conventional tillage and no till. This trend was not true for all cases, but depended on whether increased water holding capacity and retained mineral N by more residue left on soil surface under reduced tillage or no-till dominated crop growth. Increased soil moisture content with lower tillage intensity has been reported to increase seed germination and root growth, thus improving crop production (Nyakatawa and Reddy, 2000, Plaza-Bonilla, et al., 2014, Triplett, et al., 1996). However, litter left on the soil surface with reduced or no till could be decomposed by microorganisms and the subsequent mineralized N might either be utilized by crops, gasified or leached. According to our simulation design, it seemed tillage during the growing season was the most effective way to increase yield by releasing more residue N compared to no till and holding more soil water compared to conventional tillage.

5.3.2 Regional Distribution

For arable land in each county, potential yield was higher in eastern compared to western counties under dryland management mainly due to precipitation patterns in Texas (Figure 5.2a). Precipitation in Texas varies widely, generally increasing from west (arid) to east (humid). Water stress controls on primary production in the conterminous U.S. were evaluated in the biogeochemical model Biome-BGC and by the remote sensing-based model MOD17 by Mu, et al. (2007). Results showed that gross primary production (GPP) and leaf area index (LAI) decreased from east to west as water stress increased, which was the same pattern as indicated in our simulations. Differences were

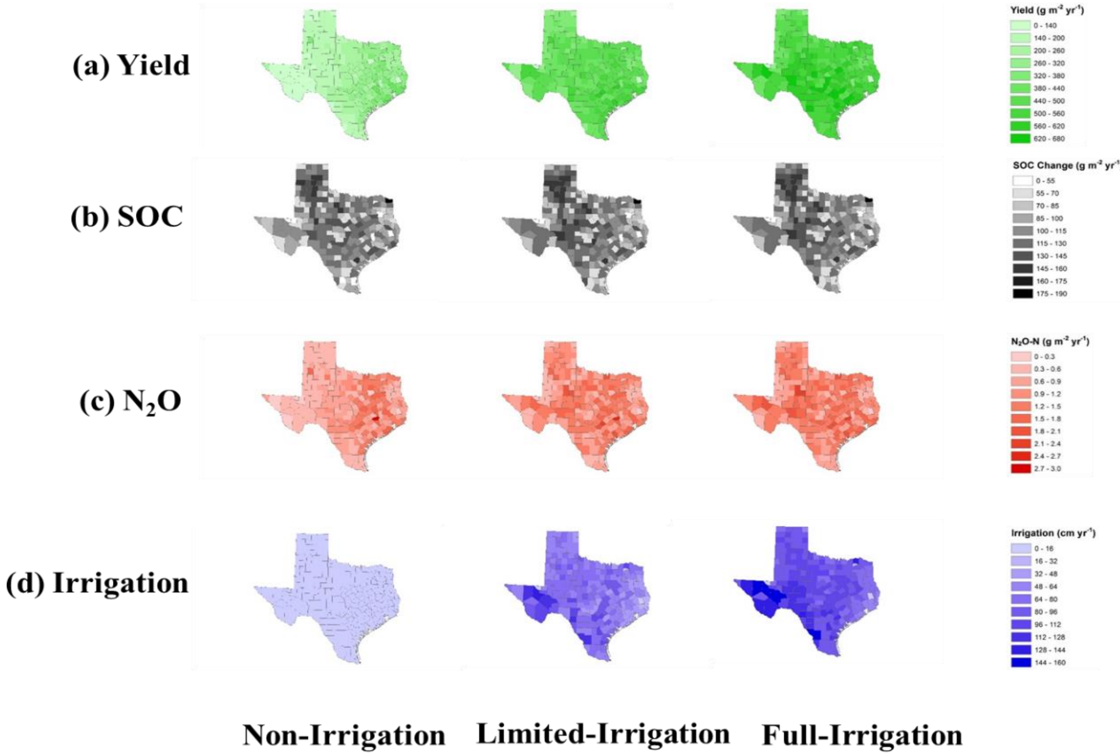

Figure 5.2 Annual aboveground biomass C (a), SOC change (b), N_2O emission (c), and irrigation amount per unit area (d) under different residue return, N fertilization, and tillage intensity under three irrigation systems in 2016-2050 with bioenergy sorghum

eliminated as irrigation level increased. However, more irrigation was acquired to achieve the same yield target in western compared to eastern Texas, mainly due to the greater water stress in western portions of Texas (Figure 5.2a).

Soil organic C change didn't show the same patterns as yield and N_2O (Figure 5.2b). Instead of responding to the west to east precipitation pattern, SOC change was more related to basic soil properties, such as texture, pH, and fertility. On one hand, organic C input might be decreased from the southeast to the northwest because of lower annual temperature and precipitation. On the other hand, however, satisfactory environmental factors for crop growth also favor microbial activity, which can offset the

C gain from additional crop litter. The long-term interaction of both created the pattern that we obtained from field investigations and model simulations. Growing season irrigation overall had a rather limited effect on long-term SOC change, indicating that annual temperature and fundamental soil properties likely had the greatest impact on SOC equilibrium. Irrigation in cm ha^{-1} to reach a certain yield goal increased from east to west due to declining annual precipitation (Figure 5.2d)

When arable land area in each county was accounted for, county-level yield, SOC sequestration, and N_2O emissions were concentrated in plain and prairie areas such as the High Plains, Rolling Plains, Rio Grande Plains, Blackland Prairie, and Coast Prairie (Figure 5.3a, b, c). Correspondingly, total irrigation amounts in these areas were also higher than those without much arable land (Figure 5.3d). Several of these areas are also classified as arid or semi-arid, again increasing total irrigation needed to achieve a target yield on a county basis. Arable land distribution is a result of a multiple-factor integration including climate, soil, geology, and landscape. Generally, areas with a considerable amount of arable land are those with flat or nearly level surfaces which encourages irrigation and mechanization without much erosion problem. At the same time, these areas are often located on fertile soils with some access to irrigation water. For example, groundwater from the Ogallala aquifer is the sole source of irrigation water in the Texas High Plains, while the Rio Grande Plains and Gulf Coast Prairie rely heavily on surface water (Wagner, 2012). Lark, et al. (2015) tracked crop-specific expansion pathways across the conterminous U.S. in 2008-2012 and the indicated potential biofuel crop conversion areas in Texas were highly consistent with areas with a

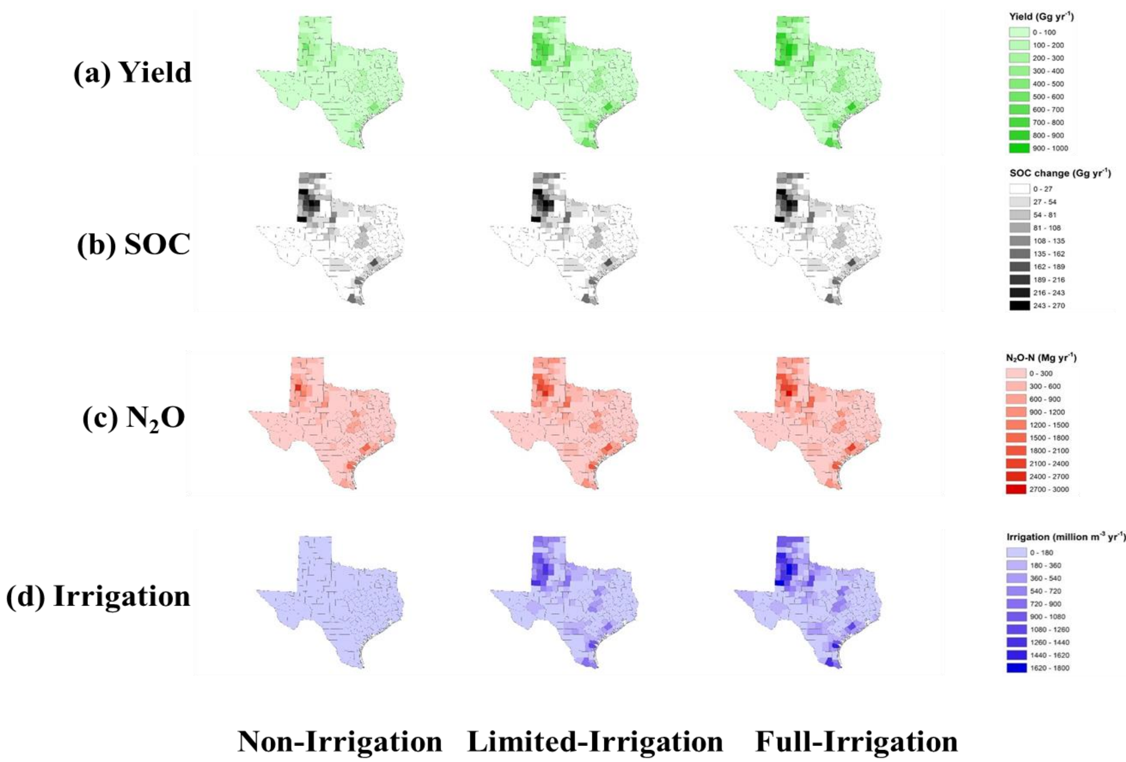

Figure 5.3 Annual aboveground biomass C (a), SOC change (b), N_2O emission (c), and irrigation amount per county (d) under different residue return, N fertilization, and tillage intensity under three irrigation systems in 2016-2050

high percentage of arable land. Additionally, as irrigation increased, corresponding higher yield, SOC change, and N_2O emissions occurred as have been discussed in previous sections.

5.3.3 Net greenhouse gas (GHG) Emissions

When determining net GHG emission (positive) or mitigation (negative), all studied irrigation levels were able to mitigate GHG emissions at the field level if best management practices were selected (minimum sum of SOC change and N_2O emission based on the prerequisite of increased SOC compared to initial year) without taking into account C emission replaced by harvested biomass conversion (Figure 5.4a). This screening criteria favored a combination of 50% residue return, no-till, and 75 kg N ha^{-1} fertilization in most cases. However, lower mitigation potential was indicated with higher irrigation, which was attributed to increased N_2O outweighing barely increased SOC sequestration. In addition, average yield in some areas might not be high enough to make the planting bioenergy sorghum feasible. When C emission replaced by harvested biomass conversion was considered (Figure 5.4b), however, a treatment combination of 0% residue return, no-till, and 150 kg N ha^{-1} fertilization was more favored. Higher biomass yield was attained by applying this combination and increased GHG mitigation potential with irrigation was demonstrated (Figure 5.4b). As a result, 0% residue return, no-till, and 150 kg N ha^{-1} fertilization under limited irrigation might be the best overall consideration for optimum management of bioenergy sorghum production.

When accounting for arable land area in each county, net GHG emissions were again concentrated in areas with the most arable land, no matter if C emissions replaced by harvested biomass conversion were counted or not (Figure 5.5a, b). According to the simulation results comparing treatments, effects of irrigation were the most significant on yield, followed by N_2O, and then SOC change. Higher net GHG mitigation potential may exist when higher irrigation intensity is applied when accounting for C emissions substituted for by more harvested biomass conversion for biofuel production, while the trend was the opposite on a field level when only SOC and N_2O were considered. Predictably, higher GHG mitigation potential will be achieved when biofuel conversion efficiency is improved.

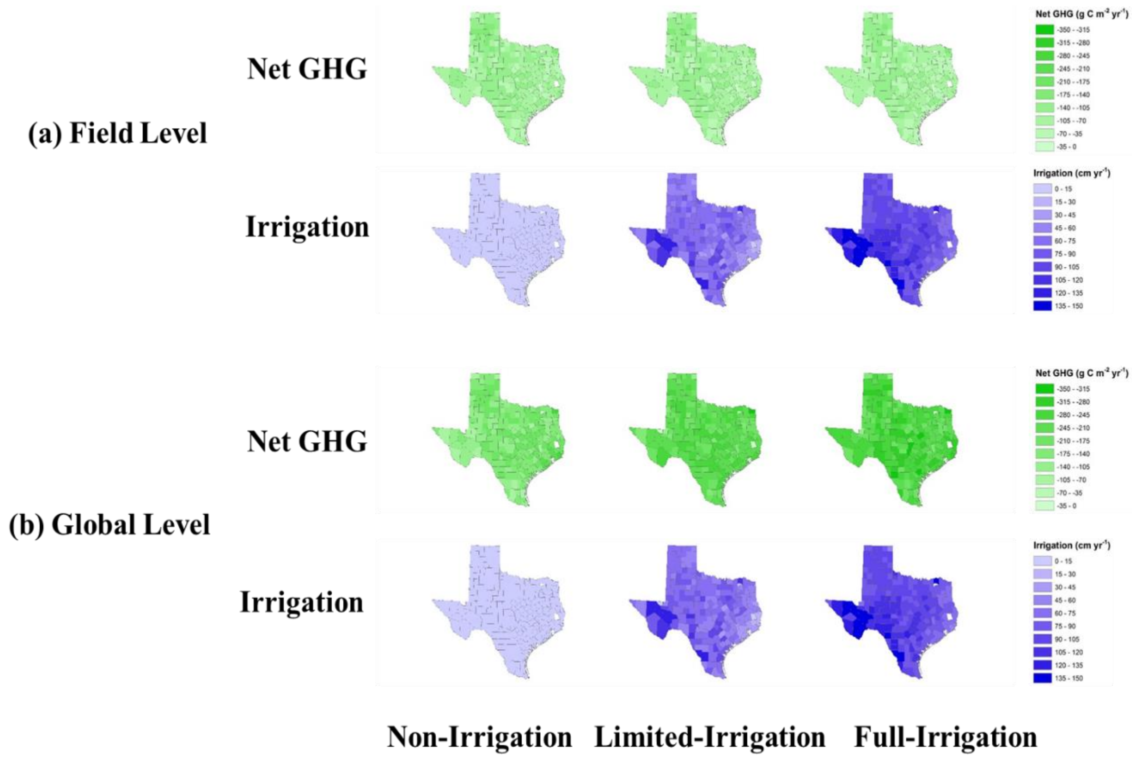

Figure 5.4 Annual net GHG emissions and irrigation amounts when accounting for C mitigation with harvested biomass conversion (global level) and without (field level) per unit area under best residue return, N fertilization, and tillage intensity combinations under three irrigation systems in 2016-2050 with bioenergy sorghum

5.3.4 Uncertainty Analysis

According to the model calibration and validation in our field trial, there were several shortcomings where the model may not capture the outputs satisfactorily. First, the model does not include a mechanism for soil water holding capacity increase by incorporating litter. This deficiency might affect yield differences among different residue return levels, especially when the returned residue would be transferred to subsoil through tillage practices (Wang, et al., 2017). Second, the model's sensitivity for the effect of soil moisture content on SOC decomposition may not match well enough

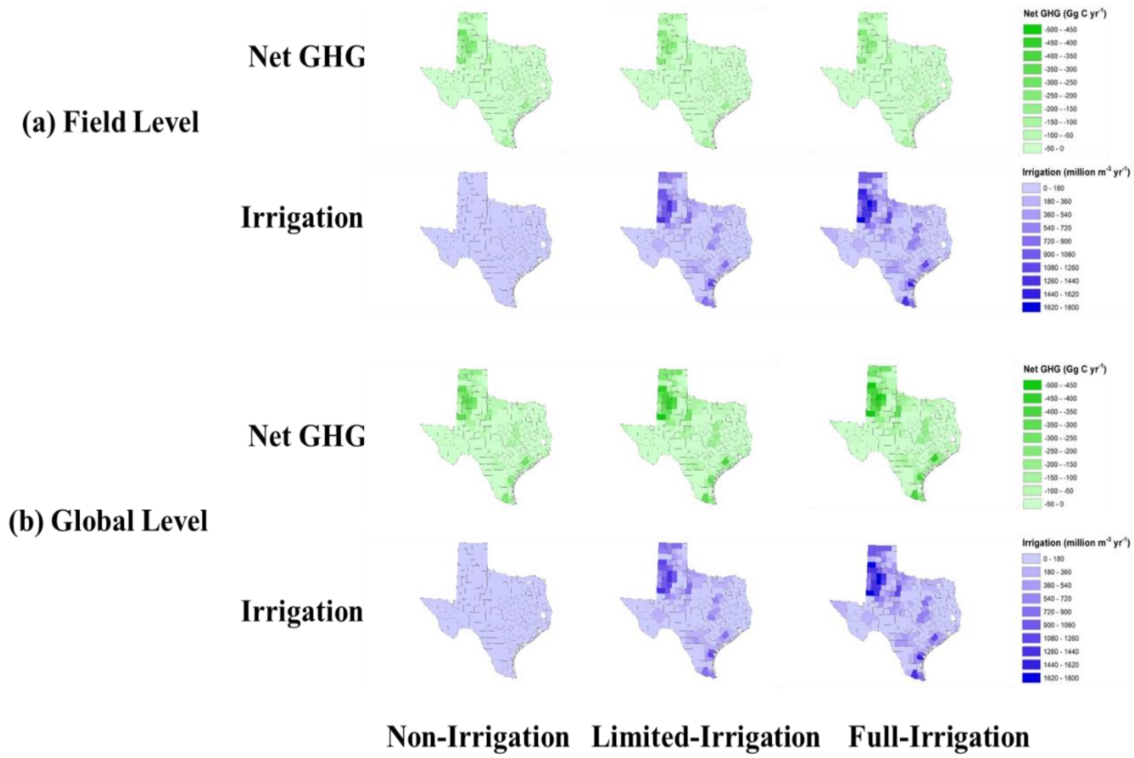

Figure 5.5 Annual net GHG emissions and irrigation amounts when accounting for C mitigation with harvested biomass conversion (global level) and without (field level) per county under best residue return, N fertilization, and tillage intensity combinations under three irrigation systems in 2016-2050 with bioenergy sorghum

what actually occurred in the field, possibly resulting in too conservative seasonal SOC change. It has been shown by other studies that SOC change produced by the model was smaller compared to observations (Campbell, et al., 2014, Paustian, et al., 1992). Third, DAYCENT does not have SOC distribution throughout the soil profile, only to 20-cm depth. This near surface effect would potentially overlook SOC decomposition from deeper in the soil profile, which may supply mineral N for plant growth and also release GHGs. This effect could be especially important under insufficient N fertilization and intensive water input either through precipitation or irrigation, particularly when the simulation bias could be potentially larger if the decomposition effect of soil moisture on SOC were taken into account. Additionally, other field factors would also affect actual field measurements which were not included in the model, such as pest infestation, soil compaction, etc.

Other than the potential model mechanism shortcomings, there were also other factors that may decrease the model's accuracy. One would be field data collection, especially for GHG emissions such as N_2O. Like many other studies, N_2O fluxes used for model verification in our study were sporadic and variable. Additionally, N_2O flux was determined weekly during growing seasons, but less frequently during fallow seasons due to labor, funding, and time shortages. The complexity of N gas fluxes and difficulty of data collection could involuntarily affect model verification. A second factor would be the regional data collection, especially for soil properties. Different than site simulation, regional simulation needs resolution and representative data selection. Soil properties may vary spatially from the representative point we selected for each county. Precipitation amount and distribution could also vary from the selected point, especially in summer. However, county level simulations should give a general pattern and an overall evaluation of the effects of conversion from conventional crops to bioenergy sorghum on biomass yield, soil C dynamics and GHG emissions.

5.4 Conclusions

Statewide county level simulations to study the effects of different field management practices and irrigation levels on bioenergy sorghum production showed that higher irrigation increased yield, SOC, and N_2O emissions, with limited irrigation appearing to have advantages over non-irrigation and full-irrigation. Within an irrigation level, higher biomass return and N fertilization increased yield, SOC, and N_2O emissions. Lower tillage intensity increased SOC and reduced N_2O emission, while the yield trend was reduced tillage having the highest yield, followed by conventional tillage and no till. For the arable land in each county, potential yield and N_2O emissions were higher in eastern compared to western Texas under non-irrigation, but these differences were eliminated as irrigation level increased. Soil organic C didn't show the same pattern as yield and N_2O. When accounting for arable land area in each county, higher yield, SOC sequestration, and N_2O emissions were concentrated in plain and prairie areas when irrigation was adequate. For net GHG emission, the treatment combination of 50% residue return, no-till, and 75 kg N ha^{-1} fertilization was generally lowest when not taking into account C emission replaced by harvested biomass conversion. However, average yield with this treatment might not be high enough to make bioenergy sorghum production feasible. A treatment combination of 0% residue return, no-till, and 150 kg N ha^{-1} had greater GHG mitigation potential when C emission replaced by harvested biomass conversion was considered. Higher yield was attained with this treatment and irrigation, increasing the positive effect on GHG mitigation potential. As a result, 0% residue return, no-till, and 150 kg N ha^{-1} fertilization under limited irrigation might be the best combination for optimum management of bioenergy sorghum production.

CHAPTER VI

SUMMARY

The DAYCENT model simulated soil temperature satisfactorily well, reflecting the temperature difference caused by residue return and N fertilization, with both observed and simulated results showing higher average soil temperature in treatments with lower N fertilization and residue return, and lower average soil temperature in treatments with higher N fertilization and residue return. The model simulated soil moisture peaks caused by precipitation and irrigation events quite well. However, simulated soil water differences among treatments were small. DAYCENT does not reflect the improvement of water holding capacity by soil incorporated plant litter, which could have been another reason why biomass produced in the 50% residue return treatment was higher than that with 0% residue return, besides the higher nutrient level in the 50% residue return treatment. DAYCENT performed fairly well in simulating aboveground biomass C when sufficient N fertilization was applied. However, the model tended to underestimate yield when N fertilization was insufficient. Both observed and simulated results indicated greater SOC with higher N fertilization and residue return and lower SOC with lower fertilization and residue return. However, the model was not sensitive enough in simulating observed temporal SOC changes, especially when growing seasons were shorter and fallowed soil was left exposed to high temperatures and precipitation. The model performance in simulating GHG fluxes demonstrated a pattern similar to aboveground biomass C, with better performance when sufficient N was applied and a less accurate fit when more N was required in the system. DAYCENT only simulates SOC at 0-20 cm depth, which neglects SOC mineralization and N availability in deeper soil layers, and thus may underestimate crop yield and GHG fluxes when insufficient N was applied. Overall, DAYCENT was able to simulate observations of soil temperature, soil water content, aboveground biomass C, SOC, daily GHG fluxes, and annual GHG emissions reasonably well and captured variations caused by field management and seasonal changes. Thus, model outputs were deemed reliable for LCA of net GHG emissions under different field management practices when considering all C inputs and outputs from bioenergy sorghum production to bioethanol combustion.

Life cycle analysis of net GHG fluxes were conducted by combining DAYCENT model results with fossil fuel used to produce farm inputs and operate field machinery as well as other required information. Of all C sinks, displaced fossil fuel during bioethanol conversion and production was the largest one, followed by SOC sequestration and CH_4 oxidation. Of all studied C sources, N_2O was the largest one, followed by energy requirements for N fertilizer manufacture and field machinery operations. Compared to residue return and tillage, N fertilization was the largest contributor to high biomass yield, thereby resulting in high GHG mitigation by displacing fossil fuel C emissions. However, a high percentage of residue return might offset this mitigation potential, especially in fertilized treatments, because of less biomass available for conversion to biofuel. Treatments without N fertilization were most at risk of losing SOC unless residue return and reduced tillage practices were used. Nitrous oxide emissions were much higher in treatments with N fertilization, even with residue return and reduced tillage intensity. Most treatments tended to show net C sequestration, except that with N fertilization and residue return, mainly due to higher N_2O emissions and lower displaced fossil fuel C emissions.

Statewide county level simulations to study the effects of different field management practices and irrigation levels on bioenergy sorghum production showed that higher irrigation increased yield, SOC, and N_2O emissions, with limited irrigation appearing to have advantages over non-irrigation and full-irrigation. Within an irrigation level, higher biomass return and N fertilization increased yield, SOC, and N_2O emissions. Lower tillage intensity increased SOC and reduced N_2O emission, while the yield trend was reduced tillage having the highest yield, followed by conventional tillage and no till. For the arable land in each county, potential yield and N_2O emissions were higher in eastern compared to western Texas under non-irrigation, but these differences were eliminated as irrigation level increased. Soil organic C didn't show the same pattern as yield and N_2O. When accounting for arable land area in each county, higher yield, SOC sequestration, and N_2O emissions were concentrated in plains and prairie areas when irrigation was adequate. For net GHG emissions, the treatment combination of 50% residue return, no-till, and 75 kg N ha^{-1} fertilization was generally lowest when not accounting for C emission replaced by harvested biomass conversion. However, average yield with this treatment might not be high enough to make bioenergy sorghum production feasible. A treatment combination of 0% residue return, no-till, and 150 kg N ha^{-1} had greater GHG mitigation potential when C emission replaced by harvested biomass conversion was considered. Higher yield was attained with this treatment and irrigation, increasing the positive effect on GHG mitigation potential. As a result, 0%

residue return, no-till, and 150 kg N ha^{-1} fertilization under limited irrigation might be the best combination for optimum management of bioenergy sorghum production.

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