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Quantifying Crop Yield, Bioenergy Production And Greenhouse Gas Emissions From Cropland And Marginal Land Using A Model-Data Fusion Approach

Zhangcai Qin
Purdue University

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For the degree of Doctor of Philosophy

Is approved by the final examining committee:

Indrajeet Chaubey
Chair

Wallace E Tyner

Tony J Vyn

Qianlai Zhuang

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Approved by Major Professor(s): Qianlai Zhuang

Approved by: Indrajeet Chaubey 09/11/2013
Head of the Graduate Program Date

QUANTIFYING CROP YIELD, BIOENERGY PRODUCTION AND GREENHOUSE GAS EMISSIONS FROM CROPLAND AND MARGINAL LAND USING A MODEL-DATA FUSION APPROACH

A Dissertation

Submitted to the Faculty

of

Purdue University

by

Zhangcai Qin

In Partial Fulfillment of the

Requirements for the Degree

of

Doctor of Philosophy

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West Lafayette, Indiana

TO

My parents and my wife

献给

父母和妻子

ACKNOWLEDGEMENTS

Completion of this doctoral journey was only possible with the support of many who have shared my best and worst moments in the past three years. I owe my gratitude to all those people who have contributed to the production of this dissertation and supported my study at Purdue.

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“Wherever you go, go with all your heart.”

TABLE OF CONTENTS

Page

Page

APPENDICES

LIST OF TABLES

Appendix Table Page

LIST OF FIGURES

Figure Page

Figure Page

Appendix Figure Page

LIST OF ABBREVIATIONS

Some abbreviations frequently used in this study are listed in the following, and defined as showing below unless otherwise stated in the text.

AgTEM	the Agroecosystem model based on TEM
C	carbon
CO_2	carbon dioxide
CO_2eq	CO_2 equivalent
HBIO	harvestable biomass
GHG	greenhouse gas
GPP	gross primary production
GWP	global warming potential
GWP_i	global warming intensity
N	nitrogen
N_2O	nitrous oxide
NOX	nitrogen oxides
NCE	net carbon exchange
NPP	net primary production
TEM	the Terrestrial Ecosystem Model

ABSTRACT

Qin, Zhangcai. Ph.D., Purdue University, December 2013. Quantifying Crop Yield, Bioenergy Production and Greenhouse Gas Emissions from Cropland and Marginal Land using a Model-Data Fusion Approach. Major Professor: Qianlai Zhuang.

Bioenergy is becoming increasingly attractive to many countries, but has sparked an intensive debate regarding energy, economy, society and environment. Biofuels provide alternative energy to conventional fossil fuels. However, the environmental impact of producing and using biofuel is a major concern to our society. This study is dedicated to quantifying and evaluating biofuel production and potential climate change mitigation due to potential large-scale bioenergy expansion in the conterminous United States, using model-data fusion approaches.

Biofuel made from conventional (e.g., maize (*Zea mays* L.)) and cellulosic crops (e.g., switchgrass (*Panicum virgatum* L.) and *Miscanthus* (*Miscanthus* × *giganteus*)) provides alternative energy to fossil fuels and has been considered to mitigate greenhouse gas emissions. To estimate the large-scale carbon and nitrogen dynamics of these biofuel ecosystems, process-based models are needed. Here, we developed an agroecosystem model (AgTEM) based on the Terrestrial Ecosystem Model for these ecosystems. The model incorporated biogeochemical and ecophysiological processes including crop phenology, biomass allocation, nitrification and denitrification as well as agronomic

management of irrigation and fertilization. It was used to estimate crop yield, biomass, net carbon exchange, and nitrous oxide (N_2O) emissions at an ecosystem level. We found that AgTEM reproduces the observed annual net primary production and N_2O emissions of most sites, with over 85% of total variations explained by the model. Local sensitivity analysis indicated that the model sensitivity varies among different ecosystems. Net primary production of maize is sensitive to temperature, precipitation, cloudiness, fertilizer and irrigation and less sensitive to atmospheric carbon dioxide (CO_2) concentrations. In contrast, the net primary production of switchgrass and *Miscanthus* is most sensitive to temperature among all factors. The N_2O emissions are sensitive to management in maize ecosystems, and sensitive to climate factors in cellulosic ecosystems. The developed model should help advance our understanding of carbon and nitrogen dynamics of these biofuel ecosystems at both field and regional scales.

Next, we estimated the potential emissions of greenhouse gases from bioenergy ecosystems with AgTEM, assuming maize, switchgrass and *Miscanthus* will be grown on the current maize-producing areas in the conterminous United States. The modeling experiments suggested that, the maize ecosystem acts as a mild net carbon source while cellulosic ecosystems (i.e., switchgrass and *Miscanthus*) act as mild sinks. Nitrogen fertilizer use is an important factor affecting biomass production and N_2O emissions, especially in the maize ecosystem. To maintain high biomass productivity, the maize ecosystem emits much more greenhouse gases, including CO_2 and N_2O, than switchgrass and *Miscanthus* ecosystems, when high-rate nitrogen fertilizers are applied. For maize, the global warming potential amounts to 1-2 Mg CO_2eq ha^{-1} yr^{-1}, with a dominant contribution of over 90% from N_2O emissions. Cellulosic crops contribute to the global warming potential of less than 0.3 Mg CO_2eq ha^{-1} yr^{-1}. Among all three bioenergy crops, *Miscanthus* is the most biofuel productive and the least GHG intensive at a given cropland. Regional model simulations suggested that, substituting *Miscanthus* for maize to produce biofuel could potentially save land and reduce GHG emissions.

Since growing biomass from marginal lands is becoming an increasingly attractive choice for producing biofuel, we looked further into bioenergy potential and possible GHG emissions from bioenergy crops grown on marginal lands in the United States. Two broadly tested cellulosic crops, switchgrass and *Miscanthus*, were assumed to be grown on the abandoned land and mixed crop-vegetation land with marginal productivity. Production of biomass and biofuel as well as net carbon exchange and N_2O emissions were estimated in a spatially explicit manner, using AgTEM. Modeling experiments showed that, cellulosic crops, especially *Miscanthus*, could produce a considerable amount of biomass and thus ethanol. For every hectare of marginal land, switchgrass and *Miscanthus* could produce 1.4-2.3 kL and 4.1-6.9 kL ethanol, respectively. The actual amount of ethanol production depends on nitrogen fertilization rate and biofuel conversion efficiency. Switchgrass has high global warming intensity (100-190 g CO_2eq L^{-1} ethanol), in terms of GHG emissions per unit ethanol produced. *Miscanthus*, however, emits only 21-36 g CO_2eq to produce every liter of ethanol. To reach the mandated cellulosic ethanol target of 21 billion gallons by 2022 in the United States, growing *Miscanthus* on the marginal lands could save a large amount of land and reduce GHG emissions in comparison to growing switchgrass.

It should be noted that, ecosystem modeling may be useful for evaluating ecosystem services and environmental impacts, and the results could be informative for policy

making concerning energy, food security and sustainability. However, the modeling results are limited in terms of advising agricultural management practices, land use change and energy system analysis, due to modeling uncertainties, data unavailability, and simulation scale and boundary limitations. High-accuracy data assimilation, model improvement and life cycle assessment still await future study.

CHAPTER 1. INTRODUCTION

1.1 Bioenergy as Alternative Energy Source

With the rapid growth of the world population and economy, the energy requirement of the fossil-fuel-supported society has increased multifold globally during the last several decades and is expected to rise by 60% by year 2030 (Bessou *et al.*, 2011). The known reserves of fossil fuels are limited and concentrated in only certain regions of the world; cheap reserves will not be sufficient to fulfill the world's continuously growing energy demand. The overbearing dependence on conventional fuels such as coal, petroleum and natural gas has stimulated the world to search for alternative energy sources for an energy transition (IEA, 2012). More importantly, the fossil fuels have been reported to be the primary anthropogenic cause of carbon dioxide (CO_2) emission and climate warming (IPCC, 2007). With increasing political, economic and environmental concerns about climate change and energy security, the world has to rethink its fossil-fuel-based energy structure and consider accelerating the development of renewable energy (Kim *et al.*, 2009; Melillo *et al.*, 2009).

Bioenergy is expected to play an important role in the global energy mix in the foreseeable future. Bioenergy made available from materials derived from biological sources meets the dual purpose of enhancing energy security and mitigating climate change, and is likely a reliable alternative to petroleum fuels (Kim *et al.*, 2009; Beringer *et al.*, 2011). A number of countries have set voluntary or mandatory biofuel targets for substituting petroleum fuels with biofuels (Fagione *et al.*, 2010). Global biofuel production has increased dramatically in the last decade, especially in U.S. and Brazil (**Figure** 1.1) (Carriquiry *et al.*, 2011). For fuel ethanol in the U.S., production increased from less than 2 billion gallons in the early 2000s to 4 billion gallons in 2005, and 13 billion gallons in 2010 (RFA, 2012). According to the Energy Independence and Security Act of 2007 (US Congress, 2007), the United States is expected to produce 36 billion gallons (136 billion liters) of renewable fuels by 2022, including 21 billion gallons (79 billion liters) of cellulosic ethanol.

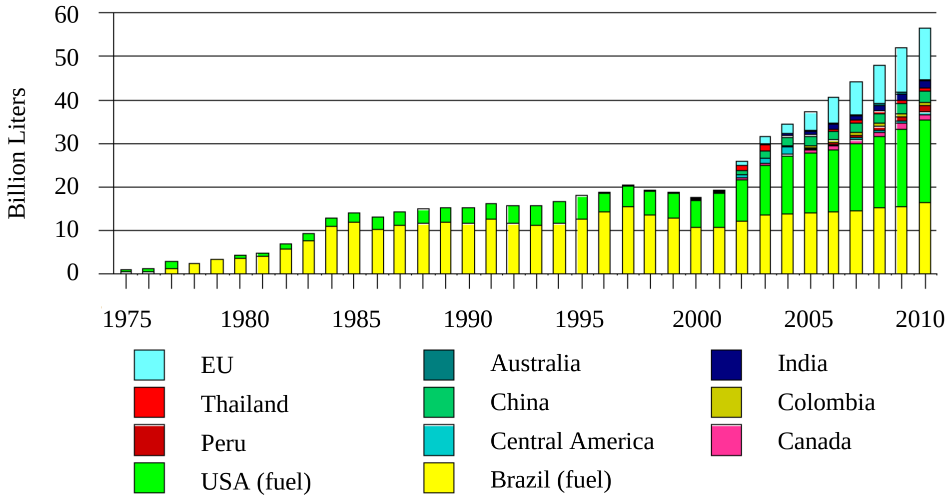

Figure 1.1 World ethanol production by country/region. Source: Berg, 2004.

However, the rapid growth of food-based biofuel is controversial, and issues of food security and potential ecological and environmental problems are often discussed. Currently, most biofuels are made from food crops like corn and soybeans. This raises major nutritional and ethical concerns, since growing crops for fuel consumes land, water and energy resources that could otherwise be used in food production for humans (Pimentel *et al.*, 2010). In the U.S., 13 million hectares of cropland is required to produce 37 million liters biofuel production in 2008 (Fargione *et al.*, 2010). That is about 7% of the 179 million hectares of national cropland (Nickerson *et al*., 2011). To meet the 2022 biofuel mandate, another 15% of the cropland will be used in the U.S. for biofuel production. Producing biofuel from food threatens food security not only in the U.S., but also in other countries, especially countries that have populations suffering from malnourishment (Pimentel *et al.*, 2010; Tilman *et al.*, 2009). Studies show that conventional food-based biofuels contribute to monoculture and deforestation, which jeopardizes ecological biodiversity and ecosystem services (Fargione *et al*., 2008; Searchinger *et al.*, 2008). Further, some biofuels are not competitive with existing fossil fuels, and may result in negative energy return and net greenhouse gas emissions (Searchinger *et al.*, 2008; Pimentel *et al.*, 2010). To date, conventional biofuels manufacture has important limitations (Evans, 2007) and the production may not be able to keep pace with fast growing industry needs and energy demand (Hill *et al.*, 2006; Hurt *et al.*, 2006). These problems limit further development of conventional biofuels.

Second-generation biofuels are expected to help solve these problems, and to provide a considerable proportion of the fuel supply sustainably, affordably, and with greater environmental benefits. These biofuels are derived from lignocellulosic crops, and the biomass feedstock encompasses a wide range of sources such as food crop stalks, forest residues, and grass. Food crops like corn and soybeans will then be consumed less for biofuel purposes. Tilman *et al.* (2006) reported that biofuels derived from well-managed energy crops provide more usable energy, higher greenhouse gas (GHG) reductions and less agrichemical pollution than conventional biofuels. Perennial energy crops like switchgrass (*Panicum virgatum* L.) require less water and nutrition input and produce much higher biomass per hectare for biofuel use than food crops (Hill *et al.*, 2006; Fargione *et al.*, 2010; Carriquiry *et al.*, 2011), and can be produced on degraded or abandoned agricultural land, eliminating the competition with food production for cropland, and without causing a loss of biodiversity via habitat destruction (Tilman *et al.*, 2006, 2009; Carriquiry *et al.*, 2011). Even though food-based biofuels currently eat up most of the bioenergy market, the majority of increased production after 2020 is expected to come from second-generation biofuels (IEA bioenergy, 2008; Fargione *et al.*, 2010). Further, the technologies required to process cellulosic feedstocks into bioenergy are expected to be available within the next 10-20 years (Ragauskas *et al.*, 2006; Beringer *et al.*, 2011).

1.2 Land Available for Bioenergy Production

1.2.1 Cropland

In the United States, only about 18% of total land area is used as cropland for crops, pasture and other purposes (Nickerson *et al*., 2011). Among the many crops, maize (*Zea mays* L.), wheat (*Triticum aestivum* L.) and soybeans (*Glycine max* (L.) Merr.) dominate the food production in the United States and use a majority proportion of the cropland area (**Figure** 1.2a); currently, maize grain and soybeans are served as major biofuel feedstocks. To meet the ambitious biofuel mandate by using only food crops, a large amount of land will be needed to support the demand of biomass feedstocks, under current food productivity and biofuel conversion efficiency (Fargione *et al*., 2010). Even though crop production has increased continuously during the last several decades (**Figure** 1.2b), only a very limited amount of produce, e.g., maize grain, can be actually used for biofuel production, due to many economic and societal concerns, such as food security, needs for livestock feed (Davis *et al*., 2012; Fargione *et al*., 2010). Extra land requirement due to bioenergy expansion may lead to land use or land cover change.

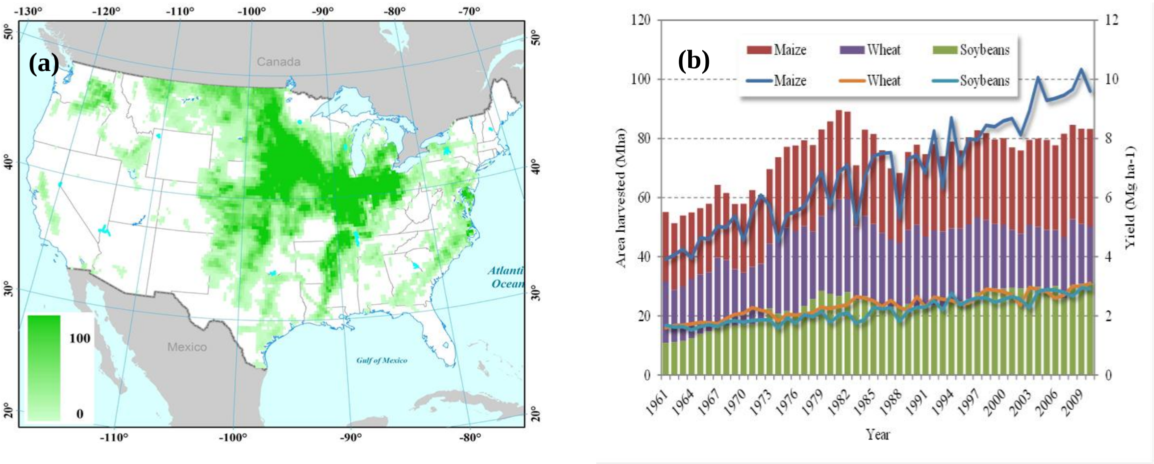

Figure 1.2 Cropland distribution, harvest area and grain yield of major commodities in the United States. (a) Distribution of croplands producing maize, wheat and soybeans, determined according to Monfreda *et al*., 2008; (b) Area harvested and grain yield of maize, wheat and soybeans in the United States (1961-2010), determined according to FAOSTAT, 2012.

Switching crops from food crops (e.g., maize) to more productive cellulosic crops (e.g., switchgrass, *Miscanthus* × *giganteus*) could be a promising option to increase biomass and biofuel productivity, while still using the same available croplands

(VanLoocke *et al*., 2012; Davis *et al*., 2012). Previous studies suggested that, by substituting *Miscanthus* for maize, about 40-60% of cropland could be saved to reach the United States bioenergy goal (Qin *et al.*, 2012; Heaton *et al*., 2008).

1.2.2 Other Lands

Besides crop switching, some other land types may also serve as alternative land sources for biomass production, such as abandoned and degraded land (**Figure** 1.3) (Wiegmann *et al*., 2008; Wicke, 2011). Abandoned agricultural land is land previously used for crop production or as pasture that has been abandoned and not converted to other uses (e.g., forest, urban areas) (Field *et al*., 2008); the agricultural activities have been stopped, due to economic, environmental or even political reasons (Wiegmann *et al*., 2008). Degraded land has experienced long-term loss of ecosystem function and services caused by disturbances from which the system cannot recover unaided (UNEP, 2007); it's mostly characterized by reduction of soil fertility and land productivity. Fallow land is temporarily suspended from cultivation to allow recovery of certain ecosystem services, e.g., soil fertility (Wicke, 2011); it's not normally used for agricultural activities. Wasteland is not favorable for growing crops due to its natural and biological conditions. Marginal land is an economic or a suitability term, often referring to lands that are not cost-effective for producing food under given poor conditions of soil fertility, cultivation techniques and other environmental factors (Wiegmann *et al*., 2008; Wicke, 2011). However, these lands, if well selected, may be usable for growing cellulosic crops with high efficiencies of using water and nutrient resources (Fargione *et al.*, 2010; Wicke, 2011).

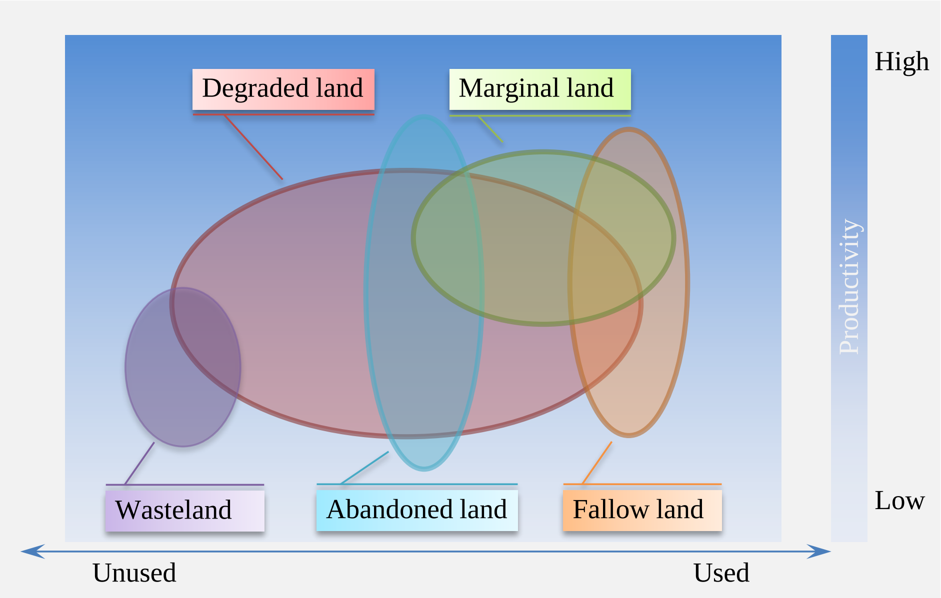

Figure 1.3 Relationships among different land types. The graph shows the relationships, and the size and domain do not necessarily reflect the actual extent of different land types. Adapted from Wicke (2011).

By characterizing marginality of land productivity according to land suitability, soil health and environmental degradation, previous studies identified marginal lands for various purposes at different spatial scales, from local to national and even global scales (e.g., Cai *et al*., 2011; Gopalakrishnan *et al*., 2011; Wicke, 2011). According to Cai *et al*. (2011), there is a total area of 320-1107 Mha of marginal lands around the world; the actual size may vary due to the coverage of land types (**Table** 1.1). Among them, 43-127 Mha of lands are distributed in the United States, including possible abandoned and degraded cropland (**Table** 1.1). If these lands were cultivated and used to grow cellulosic crops (e.g., switchgrass, *Miscanthus*), a considerable amount of biomass feedstocks could be harvested for biofuel production.

Table 1.1 Marginal lands estimated for potential biomass production in the United States and world

Scenario	Marginal lands	Land area (Mha)[*]	
		US	World
S1	Marginal mixed crop and vegetation land	43	320
S2	S1, plus abandoned and degraded cropland	68	702
S3	S2, plus marginal grassland, savanna and shrubland	127	1411
S4	S3, minus the land possibly used for pasturing	123	1107

[*] Data retrieved from Cai *et al*., 2011.

1.3 Estimating Greenhouse Gas Emissions and Ecosystem Modeling

Among the many recent debates regarding environmental sustainability of bioenergy expansion, study of carbon (C) and nitrogen (N) dynamics and balances are of great importance for quantifying the consequences of greenhouse gas (GHG) emissions and potential GHG mitigation in growing bioenergy crops for biofuel feedstocks (Fargione *et al*., 2010; Mellilo *et al*., 2009). By far, a large number of field studies have looked into the possible emissions of major GHG such as CO_2, nitrous oxide (N_2O) and even methane (CH_4) from traditional food crops (e.g., maize) and most recently from cellulosic crops (e.g., switchgrass and *Miscanthus*). Site level experiments using maize or cellulosic crops indicated that, net CO_2 flux in terms of net ecosystem exchange (NEE) is positive, suggesting a net C sink; but the ecosystem C balance is close to neutral if accounting for crop harvest and residue return (e.g., Suyker *et al*., 2004; Verma *et al*., 2005; Skinner & Adler, 2010). Annual N_2O emissions in maize ecosystem range from less than 1 kg N ha^{-1}

to over 10 kg N ha^{-1} (e.g., Halvorson et al., 2006; Adviento-Borbe *et al*., 2007; Hoben *et al*., 2011; Omonode *et al*., 2011), with a positive relationship with N input (McSwiney & Robertson, 2005; Grassini & Cassman, 2012). Generally, cellulosic-crop ecosystems require less N fertilizer than maize, and therefore release relatively less N_2O emissions (Nikiema *et al*., 2011; Heaton *et al*., 2008). CH_4 emissions are negligible for many traditional food crops and cellulosic energy crops (Drewer *et al*., 2012).

To study regional or national GHG emissions due to bioenergy expansion, not only field experiments but also ecosystem modeling are needed for further investigating large-scale direct and indirect effects of land use changes caused by biofuel production. Unlike experiment-based empirical or statistical estimation, ecosystem models specifically describe underlying physiological, biophysical and biogeochemical processes that determine biomass formation, C and N dynamics, can be used to simulate plant biomass production, C balance and N_2O emissions (Surendran Nair *et al*., 2012; Thomas *et al*., 2013). Models designed for specific agroecosystem or those with modules including agroecosystems, such as Agro-IBIS (Kucharik, 2003), Agro-BGC (Di Vittorio *et al*., 2010), DAYCENT (Parton *et al*., 1998) and LPJml (Bondeau *et al*., 2007), were frequently used for the purpose of simulating greenhouse gas emissions in regional (Del Grosso *et al*., 2005) or global agricultural systems (e.g., Bondeau *et al*., 2007), and estimating possible direct and indirect effects of land use or land cover changes resulted from bioenergy development (e.g., Melillo *et al*., 2009).

However, many previous studies of indirect impacts focused primarily on the possible land use changes from natural ecosystems to bioenergy ecosystems, and less attention was paid to other potential land use or land cover changes such as previously mentioned crop switching and marginal land development. Our previous studies (Qin *et al*., 2011; 2012) and other investigations (Heaton *et al*., 2008; Fargione *et al*., 2010; Davis *et al*., 2012) suggested that, cropland and marginal lands could potentially be used for growing cellulosic bioenergy crops, and produce competitive biomass for biofuel use. Compared with ecosystems of traditional food crops (e.g., maize), these dominated by high land-use-efficiency and nutrient-use-efficiency cellulosic crops may essentially provide comparable or even higher biomass feedstocks while still produce less GHG emissions per unit biofuel (Tilman *et al*., 2009; Fargione *et al*., 2010). To investigate the large-scale GHG emissions and subsequent global warming potential in bioenergy ecosystems is critical for estimating overall environmental impacts of growing energy crops for biofuel use, e.g., evaluating life-cycle GHG balance. Ecosystem model designed for specific bioenergy crops can advance our understanding of C and N cycling in certain ecosystems and its applications at regional or global scales will contribute to estimations of biomass production, GHG emissions and related environmental impacts (Surendran Nair *et al*., 2012; Thomas et al., 2012).

1.4 Objectives and Outline of Thesis

1.4.1 Objectives and Research Questions

In this study, we aim to develop an ecosystem model (AgTEM) characterizing crop growth and agricultural activities with a focus on C and N cycling in the agroecosystem. The model will be used as a primary tool to address the following research questions:

1. Under given land, what are the ecosystem productivity (e.g., net primary production) and biofuel potential if certain bioenergy crops were grown? What is the impact of agricultural management on land productivity?
2. What is the difference of land use efficiencies among different bioenergy crops and different land types? How much land would be required to produce the mandated biofuel in the US under given crop × land?
3. How much GHG would be released from different agroecosystems of bioenergy crops? What is the change of global warming potential, if any, due to land use / land cover change associated with biofuel expansion?

1.4.2 Research Design and Outline of Thesis

In this study, two types of land, i.e., cropland and marginal lands, are proposed to be used for growing crops for energy purposes. One traditional food crop (i.e., maize) and two cellulosic crops (i.e., switchgrass and *Miscanthus*) are selected as bioenergy crops that could potentially produce biomass for biofuel use. As illustrated in **Figure** 1.4, input data describing ecosystem processes and quantifying biogeochemical cycles are used for model development, and those describing land use, site-level or regional climate, soil and vegetation conditions are used as forcing data for model simulations. The model AgTEM is designed for general land types and crops. It can be specifically parameterized and validated for maize, switchgrass and *Miscanthus*. Model outputs can be analyzed to address research questions.

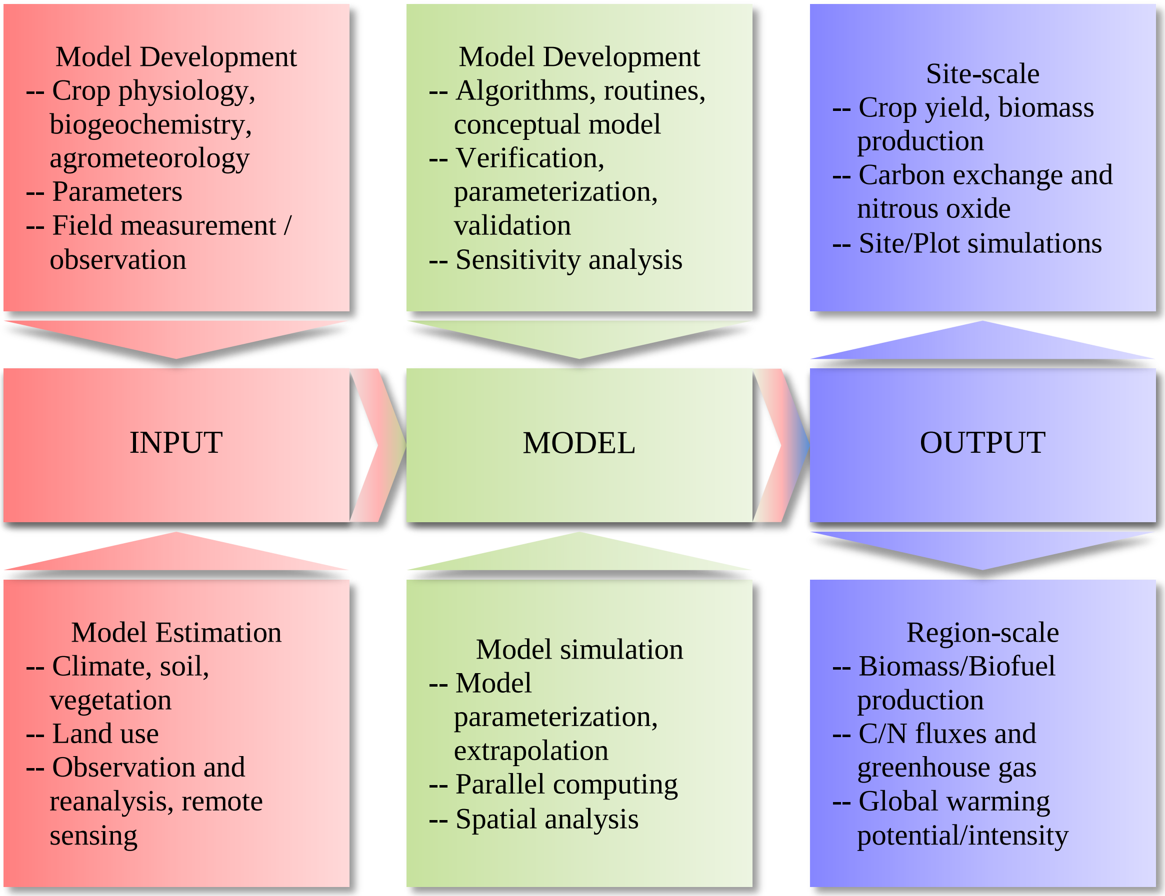

Figure 1.4 Schematic technology roadmap for modeling study in the dissertation. Two major components: model development (modeling) and model application (simulation). The model is used for site- and region-scale simulations. Arrows show flow of data or sequence of modeling steps.

In the dissertation, Chapter 1 introduces study background and clarifies some definitions related to land types and modeling. Model development including model conceptualization, formulation, verification, validation and sensitivity analysis is documented in Chapter 2. Research questions are addressed in Chapters 3 through 4.

Chapter 5 is for summarizing results, findings and uncertainties of the analyses and discussing potential future improvement and needs (**Figure** 1.5).

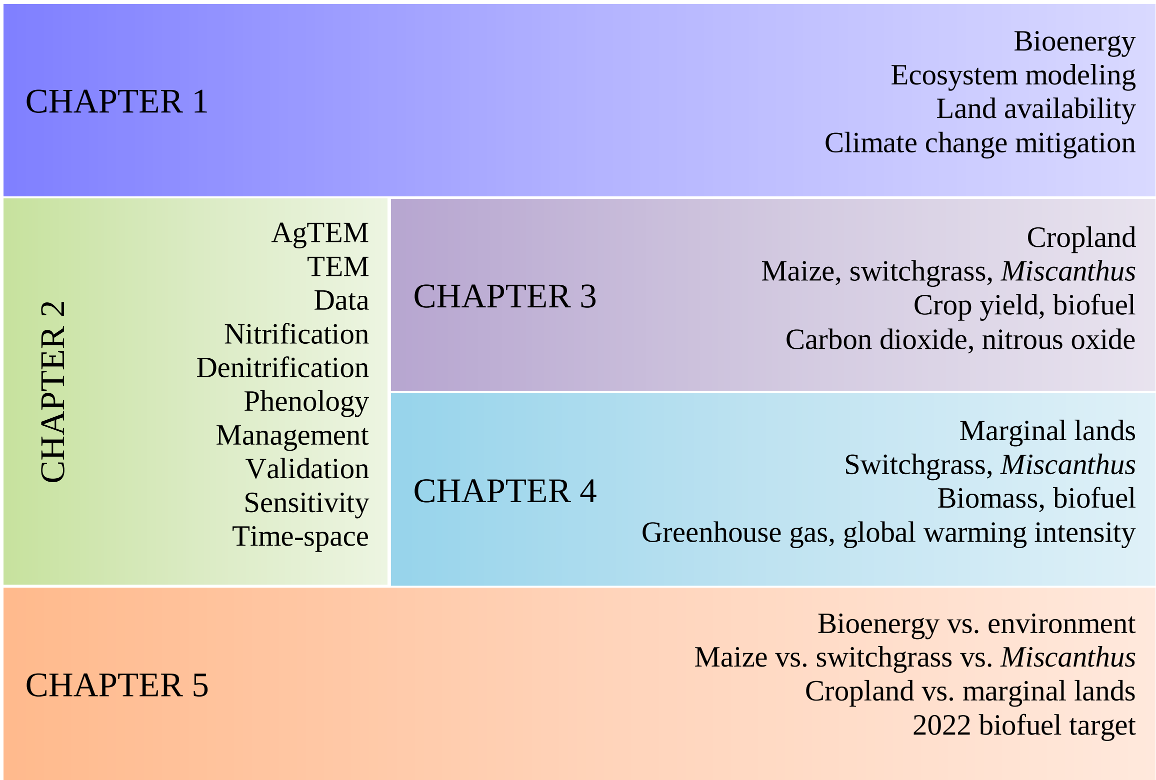

Figure 1.5 Thesis outline. Framework of chapters 1 through 5, with keywords describing major elements covered in each chapter.

1.5 Acknowledgement

This chapter has been partially published in Qin *et al*., 2011; 2012 (reprinted and adapted with permission).

CHAPTER 2. AGROECOSYSTEM MODEL DEVELOPMENT

2.1 Introduction

Bioenergy is becoming increasingly attractive to many countries, but has sparked an intensive debate regarding energy, economy, society and environment. Biofuels provide alternative energy to conventional fossil fuels. However, producing biofuels requires a large amount of biomass feedstocks, which may lead to land, water and nutrient competitions between bioenergy crops and grain crops (Tilman *et al.*, 2009; Pimentel *et al.*, 2010), causing problems such as food insecurity (Fargione *et al.*, 2010; Diffenbaugh *et al.*, 2012). In addition, the environmental impact of producing and using biofuel is another concern to our society. In particular, to what degree, biofuel feedstock producing, biofuel conversion, and biofuel use will mitigate the climate change has been a research focus (Farrell *et al.*, 2006; Searchinger *et al.*, 2008; Melillo *et al.*, 2009).

Biofuel crops can assimilate carbon dioxide (CO_2) from the atmosphere and accumulate C into biomass and soils. Using fossil fuels, however, releases CO_2. From the perspective of C cycling, biofuels deserve more credits for their C sequestration effect than fossil fuels (Tilman *et al.*, 2006; Clifton-Brown *et al.*, 2007). To date, many studies indicated that, substituting biofuels, especially using cellulosic crops, for fossil fuels (e.g., gasoline) would mitigate GHG emissions, and therefore benefit the environment (e.g., Farrell *et al.*, 2006; Bessou *et al.*, 2011). However, looking beyond agroecosystems and considering land availability and indirect land-use change impacts due to bioenergy expansion, the biofuel effects on the environment are not so clear. Besides using existing cropland to grow crops for bioenergy use, natural ecosystems (mainly forest and grassland) might be converted to biofuel crops to produce biomass feedstocks, which will inevitably cause land-use change. Studies have shown that by considering the GHG emissions caused by indirect land-use change, the C savings or C credit through developing biofuel is significantly reduced or even became negative (Searchinger *et al.*, 2008; Melillo *et al.*, 2009). The discrepancies among different studies are due to a number of uncertainty sources, including the definition of the process of interest, system boundaries of the life cycle of biofuel production, understanding of biogeochemical or physiological mechanisms, data assimilation, and methods applied. These uncertainties are unavoidable when complex systems and human behavior are included in the carbon sink and source analysis of biofuel development and use (Fargione *et al.*, 2010). The high degree of uncertainty highlights the necessity of further research on large-scale bioenergy development.

To estimate regional GHG emissions of land ecosystems, biogeochemical models that represent the C and N processes and dynamics under changing environmental conditions were used (McGuire *et al.*, 2001; Surendran Nair *et al.*, 2012). These models are either empirically- or mechanistically-based. By using data from field observations, empirical models represent relationships between a dependent variable (e.g., biomass yield, CO_2 emission) and independent variables regarding climate, soil and management (e.g., Heaton *et al.*, 2004; Jager *et al.*, 2010). This approach is relatively simple but also less accurate as it does not include the biogeochemical and physical processes of ecosystems.

In contrast, most process-based models used to quantify the C and N budget of bioenergy ecosystems have been derived from models originally developed for natural ecosystems (Kucharik, 2003; Bondeau *et al.*, 2007; Di Vittorio *et al.*, 2010). These models incorporated with agroecosystem processes can simulate biomass accumulation and allocation as well as C and N dynamics of agroecosytems. For example, Agro-IBIS was developed by taking advantage of the mechanistic nature of a well-tested model, the Integrated BIosphere Simulator (IBIS), which simulates interactions among soil, plant, and the atmosphere. The Agro-IBIS has been used to simulate maize yield (Kucharik, 2003) and cellulosic biomass production (Vanloocke *et al.*, 2010). Similarly, Agro-BGC is a modified version of the Biome-BGC ecosystem model, with processes added to simulate C4 perennial grass functionality and agricultural practices (Di Vittorio *et al.*, 2010). Another example is LPJml, a model for managed land. It was developed based on the well-established Lund–Potsdam–Jena–DGVM. The LPJml can simulate crop yield and C balance (Bondeau *et al.*, 2007). Some species-specific models, such as ALMANAC (Kiniry *et al.*, 1992, for switchgrass and *Miscanthus*), APSIM (Keating *et al.*, 1999, for sugarcane), MISCANMOD and MISCANFOR (Clifton-Brown *et al.*, 2004; Hastings *et al.*, 2009, for *Miscanthus*) were also developed to simulate crop growth. These models may have diverse structures and use different algorithms to describe the same biogeochemical process, but all of them can be used to simulate crop biomass production and some can also simulate C and N dynamics (e.g., Agro-BGC, LPJml).

The Terrestrial Ecosystem Model (TEM) is a global-scale biogeochemical model, among the most-used ecosystem models for estimating C, N and water dynamics of terrestrial ecosystems (e.g., McGuire *et al.*, 1992; Zhuang *et al.*, 2003; Zhuang *et al.*, 2013). Although many efforts were made towards modifying TEM for agricultural ecosystems, the crop physiology and agroecosystem processes have not been explicitly considered to date (McGuire *et al.*, 2001; Felzer *et al.*, 2004; Melillo *et al.*, 2009). Here we develop an agricultural version of TEM (AgTEM) to explicitly model the C and N dynamics of agroecosystems.

AgTEM mainly incorporated two sets of processes that are related to agricultural ecosystems: one is on C accumulation and allocation, and the other is on N cycling by introducing nitrification and denitrification processes in soils. In TEM, total C sequestered through photosynthesis is allocated into two major pools of vegetation and soil of natural ecosystems. For agricultural ecosystems, photosynthesis, phenological development and biomass allocation are crucial for determining ecosystem C fluxes and pools. In addition, agricultural management (e.g., fertilization and irrigation) affects crop development and therefore was considered in AgTEM. For agroecosystems, the N input from outside the ecosystem significantly affects crop N uptake, soil N availability, and the whole N cycle in a plant-soil-atmosphere system. Thus, special attention was paid to the N dynamics in crop soils and the interactions between soil and crop plants in AgTEM.

2.2 Materials and Methods

2.2.1 Overview

Based on TEM, this study developed an agricultural ecosystem model (AgTEM) to simulate the C and N dynamics of crop ecosystems. The site-level observational data of C and N fluxes and pools were used to test the model performance in simulating net primary production (NPP) and nitrous oxide (N_2O) emissions. The model sensitivity responding to major input variables was also analyzed. In a companion study, we examined potential N_2O emissions from bioenergy ecosystems using the model, as presented in Chapter 3 and Qin *et al*. (2013b). Below we first introduce the TEM model, and then detail how AgTEM is developed, followed by descriptions on model parameterization, validation and sensitivity analysis.

2.2.2 The Terrestrial Ecosystem Model

TEM estimates C and N fluxes and pool sizes of ecosystems at a monthly time step and a given spatial resolution (e.g., 0.5° latitude by 0.5° longitude) using spatially referenced information on climate, elevation, soil, vegetation and water availability as well as soil- and vegetation-specific parameters. TEM was first documented and applied for regional estimates in the early 1990s (Raich *et al.*, 1991; McGuire *et al.*, 1992), and several major improvements have been made during the past two decades as a result of advance of ecosystem understanding and available computing resources (e.g., McGuire *et al.*, 2001; Zhuang *et al.*, 2003; Felzer *et al.*, 2004). Equilibrium, as well as transient types of simulations were introduced to TEM in the late 1990s to early 2000s, and inherited thereafter in the later versions. New modules, such as splitting N pools, ozone effects and soil thermal and hydrological models were incorporated into TEM to better understand terrestrial C and N dynamics under changing environmental conditions (Zhuang *et al.*, 2002; Zhuang *et al.*, 2003; Felzer *et al.*, 2004; Felzer *et al.*, 2009).

Many efforts have been put into improving understanding of natural ecosystem processes. Managed ecosystems (e.g., agricultural cropland), however, were less studied using TEM. To understand the agricultural ecosystem C and N dynamics, some progress has been made towards modeling land-use change and cropping effects (McGuire *et al.*, 2001; Felzer *et al.*, 2004; Melillo *et al.*, 2009). However, a significant compromise in earlier versions of TEM for modeling agricultural ecosystems was that crop ecosystems were parameterized as grassland ecosystem (e.g., Felzer *et al.*, 2004) (**Table** 2.1). Nitrogen oxides (NO_X) emitted from agroecosystems, particularly in fertilized croplands, were not included or not mechanistically modeled in TEM (**Table** 2.1). In ecosystem models, NPP is the difference between gross primary production (GPP) and autotrophic respiration (R_A). It represents the biomass produced by plants and is used to estimate agricultural yield of the agroecosystem (Hicke *et al.*, 2004).

Table 2.1 Agricultural modules used in AgTEM and historical TEM versions

TEM version	Agricultural module	Vegetation / Crop type	Phenology	Soil N / N_2O	Notes and references
TEM4.1 and earlier	N/A*	Natural ecosystems, such as forest, grass, shrub; managed ecosystems N/A	Empirical model simulates relative changes in the photosynthetic capacity of mature vegetation	Soil N mineralization, assimilation; N_2O simulations N/A	Earlier TEM focused on natural ecosystems only; managed ecosystems were noticed but not incorporated (Raich *et al*., 1991; McGuire *et al*., 1992)
TEM4.2 w/ crop module	RAP approach† of Esser (1995) was included for "cultivated ecosystems"	Crop as a whole; model uses GRASS parameterization to describe the C and N dynamics of crops	Inherited from TEM4.1	Inherited from TEM4.1	Initial attempts were made to incorporate the effects of agriculture on terrestrial C and N dynamics (McGuire *et al*., 2001; Felzer *et al*., 2004)

Table 2.1 Continued.

TEM4.3	RAP approach improved; agricultural management discussed	Inherited from TEM4.2	GDD approach[‡], using single set of parameters for CROP	Inherited from TEM4.1	TEM4.3 was initially designed to simulate ozone effects on C fluxes, and practices such as irrigation and fertilization were discussed (Felzer *et al*., 2004); it's also used to simulate cellulosic biofuels (Melillo *et al*., 2009)
AgTEM1.0	Based on TEM4.2; similar RAP algorithms were used	Maize, switchgrass and *Miscanthus*; crop-specific model parameterization was adopted	Inherited from TEM4.2	Inherited from TEM4.1	First attempt to calibrate TEM for crop-specific C dynamics purposes; it was used for testing potential biomass production from bioenergy

Table 2.1 Continued.

					crops at ecosystem level (Qin *et al*., 2012)
AgTEM2.0 (current)	Agricultural version of TEM; agricultural management, such as irrigation, fertilization	Inherited from AgTEM1.0	GDD approach, using crop-specific parameters	Soil N mineralization, assimilation, nitrification, denitrification; N_2O simulations available	Daily version of AgTEM was designed to simulate C and N dynamics in agricultural ecosystems, especially applicable in bioenergy crop ecosystems

[*] N/A, not available.

[†] RAP approach indicated relative agricultural productivity, where agricultural productivity was simulated as a multiplier of the original natural vegetation.

[‡] GDD approach adopted growing degree days to simulate crop phenology development.

2.2.3 AgTEM Modeling

2.2.3.1 Overall Governance

AgTEM was developed to estimate C and N dynamics of bioenergy crop ecosystems (namely, maize, switchgrass and *Miscanthus*) at a daily time step and at any given spatial resolution. In AgTEM, the algorithms of modeling C and N fluxes and pool sizes are inherited from TEM. A majority of the algorithms describing ecosystem biogeochemical processes in TEM are still applicable in agroecosystems (**Table** 2.1). Similar to TEM, five differential equations were used to govern the dynamics of state variables and fluxes (Raich *et al.*, 1991):

$$\frac{dC_V}{dt} = GPP_t - R_{At} - L_{Ct}(-H_{Ct}) \tag{2.1}$$

$$\frac{dN_V}{dt} = NUPTAKE_t - L_{Nt}(-H_{Nt}) \tag{2.2}$$

$$\frac{dC_S}{dt} = L_{Ct} - R_{Ht}(+R_{Ct}) \tag{2.3}$$

$$\frac{dN_S}{dt} = L_{Nt} - NETNMIN_t(+R_{Nt}) \tag{2.4}$$

$$\frac{dN_{av}}{dt} = NINPUT_t + NETNMIN_t - NLOST_t - NUPTAKE_t \tag{2.5}$$

where C_V, N_V, C_S, N_S and N_{av} are pools of vegetation C, vegetation N, soil C, soil N and available N, respectively, determined by corresponding C and N fluxes (**Figure** A 1) (see acronyms in **Table** 2.2). The terms in parentheses of Eqns. (2.1) to (2.4) refer to biomass harvest (*H*) and return (*R*) in agroecosystems, which were not included in earlier version of TEM for natural ecosystems. In these equations, *t* refers to the time step used for

Table 2.2 Variables used in AgTEM to govern C and N fluxes and pools

Variable	Definition	Unit
State variables		
C_S	C in soil and detritus	g C m^{-2}
C_V	C in vegetation	g C m^{-2}
N_{av}	Available N in soil and detritus	g N m^{-2}
N_S	Organic N in soil and detritus	g N m^{-2}
N_V	N in vegetation	g N m^{-2}
Carbon fluxes		
E_P	Decomposition of harvested products	g C m^{-2} day^{-1}
GPP	Gross primary production	g C m^{-2} day^{-1}
H_C	C in harvested products	g C m^{-2} day^{-1}
L_C	C in litterfall	g C m^{-2} day^{-1}
NCE	Net carbon exchange	g C m^{-2} day^{-1}
NPP	Net primary production	g C m^{-2} day^{-1}
R_A	Autotrophic respiration	g C m^{-2} day^{-1}
R_C	C in returned biomass	g C m^{-2} day^{-1}
R_H	Heterotrophic respiration	g C m^{-2} day^{-1}
Nitrogen fluxes		
L_N	N in litterfall	g N m^{-2} day^{-1}
$NETNMIN$	Net rate of soil N mineralization	g N m^{-2} day^{-1}

Table 2.2 Continued.

NINPUT	N inputs from outside ecosystem	g N m^{-2} day^{-1}
NLOST	N losses from ecosystem	g N m^{-2} day^{-1}
NUPTAKE	N uptake by vegetation	g N m^{-2} day^{-1}
R_N	N in returned biomass	g N m^{-2} day^{-1}

computation. To assure stability in the integration over time, 4th-5th order Runge-Kutta integration procedure (Cheney & Kincaid, 1985) or the Euler method (Atkinson, 1989; Butcher, 2008) can be used for different time steps. In this and the companion studies (Qin *et al*., 2013), Euler method was used because of its lower computational cost. Other major modifications and new algorithms in AgTEM include temperature effects on GPP, crop phenological process and biomass accumulation, agricultural management, as well as soil N nitrification and denitrification (**Table** 2.1). Below we detail the development.

2.2.3.2 Biomass Simulation and Management Factoring

GPP. Temperature effects on GPP are modeled in TEM as a multiplier on potential GPP utilizing minimum temperature, maximum temperature and optimum temperature for plant photosynthesis (Raich *et al*., 1991). For each time step, the temperature multiplier on GPP (*TEMP*) is modeled as:

$$TEMP = \begin{cases} 0, & \left(T_{air} < T_{min}\right) \\ \dfrac{(T_{air} - T_{min})(T_{air} - T_{max})}{(T_{air} - T_{min})(T_{air} - T_{max}) - (T_{air} - T_{optmin})^2}, & \left(T_{min} < T_{air} < T_{optmin}\right) \\ 1.0, & \left(T_{optmin} < T_{air} < T_{optmax}\right) \\ \dfrac{(T_{air} - T_{min})(T_{air} - T_{max})}{(T_{air} - T_{min})(T_{air} - T_{max}) - (T_{air} - T_{optmax})^2}, & \left(T_{optmax} < T_{air} < T_{max}\right) \\ 0, & \left(T_{air} > T_{max}\right) \end{cases} \tag{2.6}$$

where T_{air}, T_{min}, T_{optmin}, T_{optmax} and T_{max} are parameters of transient, minimum, maximum, minimum optimum and maximum optimum air temperatures, respectively. These parameters are crop-specific in AgTEM (**Table** 2.3).

Phenology. In TEM, plant phenology was empirically simulated using the estimated evapotranspiration and photosynthetic capacity to describe relative changes of mature vegetation (Raich *et al.*, 1991). In AgTEM, however, crop phenology describing crop growth stages can either be imported from historical observational data, or modeled according to a crop's response to air temperature. Growing degree day (GDD), a measure of heat accumulation, is used to predict plant development rates (Felzer *et al.*, 2004; Deryng *et al.*, 2011). Cumulative GDD is modeled as a function of daily temperature:

$$GDD = \sum max\left(0, min\left(T_{air}, T_{ceil}\right) - T_{base}\right) \tag{2.7}$$

where T_{base} and T_{ceil} are base and ceiling temperature parameters, defined as lower and upper temperature thresholds for the process of interest, respectively. These parameters vary among species and possibly cultivars (McMaster & Wilhelm, 1997). In AgTEM (**Table** 2.4), GDD are used to predict crop emergence and maturity, using crop-specific threshold parameters.

Table 2.3 Minimum, maximum and optimum temperatures for plant photosynthesis

TEM version	Vegetation / Crop type	T_{min}	T_{optmin}	T_{optmax}	T_{max}*	Notes and references
		(°C)				
TEM	Grass	0	13.0	32.7	38.0	In early TEM (e.g., TEM4.2, 4.3), crops were parameterized under *grass* vegetation type (McGuire *et al*., 2001; Felzer *et al*., 2004)
AgTEM	Maize	0	15.0	31.0	41.0	In AgTEM2.0, crop-specific sets instead of single set parameters were used for different crop type (Bird *et al*., 1977; Kim & Reddy, 2004; Sage & Kubien, 2007)
	Switchgrass	0	13.0	33.0	41.0	
	Miscanthus	0	13.0	33.0	41.0	

*T_{min}, T_{optmin}, T_{optmax} and T_{max} are minimum, minimum optimum, maximum optimum and maximum temperatures, respectively.

Biomass allocation. During the growth period between crop emergence and maturity, plants use solar energy to capture atmospheric CO_2 through photosynthesis. The total net chemical energy captured by plant, or cumulative NPP, forms the total biomass of a given ecosystem. In agroecosystems, crop grain (e.g., maize) or biomass (e.g., switchgrass) can then be harvested and removed from the ecosystems. Part of the biomass leftover such as

Table 2.4 Parameters used to determine growing degree days and simulate crop phenology

Vegetation / Crop type	T_{base}	T_{ceil}[*]	GDD_{emg}	GDD_{mat}[†]	Notes and references
	(°C)		(°C day)		
Grass	--	--	--	--	Not incorporated in TEM4.2 and earlier version (McGuire *et al*., 2001)
Crop	5	--	300	2000	Used in modified TEM4.3 for simulating agricultural activities (Felzer *et al*., 2004)
Maize	10 (5-15) [‡]	30	120	1600	Used in AgTEM according to Bondeau *et al*. (2007) and Nielsen (2010)
Switchgrass	10 (10-12) [‡]	30	300	2300	Used in AgTEM according to models such as ALMANAC (Kiniry *et al.*, 1992)
Miscanthus	10	30	300	2500	Used in AgTEM according to models such as MISCANMOD

Table 2.4 Continued.

(Clifton-Brown *et al.*, 2004)

[*] T_{base} and T_{ceil} are base and threshold temperatures for calculating vegetation- and/or crop-specific GDDs, respectively.

[†] GDD_{emg} and GDD_{mat} are GDD heat unites required for crop emergence and maturity, respectively.

[‡] value used for each crop species, but subject to change for different varieties (as in parentheses).

residues and dead roots will be returned to the soil C and N cycling. In AgTEM, biomass of interest (*YLD*, e.g., yield of grain or harvestable biomass) is modeled empirically based on total NPP (NPP_{tot}) following Hicke & Lobell (2004) and Monfreda *et al.* (2008):

$$YLD = \frac{NPP_{tot}\delta_{hi}}{\delta_c D_{hi}} \tag{2.8}$$

where δ_{hi}, δ_c, D_{hi} are parameters for determining the proportion of NPP being harvested, the C content in the dry matter, and the dry proportion of *YLD*, respectively (**Table** 2.5). For the grain harvest of food crops (e.g., maize), δ_{hi} is a function of the harvest index and a ratio of aboveground-to-belowground biomass (R_{hi}):

$$\delta_{hi} = \left(1 - \frac{1}{R_{hi} + 1}\right) HI \tag{2.9}$$

where *HI* refers to the harvest index, measuring the proportion of total aboveground biological yield allocated to the economic yield of the crop (**Table** 2.5). R_{hi}, also known as "shoot-to-root ratio," indicates the biomass allocation to aboveground and belowground and is assumed to be constant for a specific crop (Hicke & Lobell, 2004). For crops used for biomass harvest purposes, *HI* needs to be slightly modified such that harvestable biomass instead of grain can be accounted for in Eqn. (2.9).

Table 2.5 Values of crop-specific parameters used for biomass harvest in AgTEM

Crop type	δ_c[*]	D_{hi}[†]	R_{hi}[‡]	*HI*[¶]	
				Grain	*Biomass*
Maize	0.45	0.85	0.85/0.15	0.53	--
Switchgrass	0.45	0.90	0.58/0.42	--	0.90
Miscanthus	0.45	0.90	0.71/0.29	--	0.90

[*] δ_c is the carbon content in the dry matter.

[†] D_{hi} is the dry proportion of *YLD*.

[‡] R_{hi} is parameterized as aboveground biomass/belowground biomass here.

[¶] *HI* refers to maize grain harvested (grain) or the proportion of aboveground biomass harvested (biomass); no biomass harvested for maize at site level and no grain available for switchgrass and *Miscanthus*. Data sources and references: Prince *et al.*, 2001; Hicke & Lobell, 2004; Mosier *et al.*, 2006; Meyer *et al.*, 2010.

The net carbon exchange between the terrestrial biosphere and the atmosphere is described with Eqn. (2.10) in AgTEM:

$$NCE = NPP - R_H - E_P \tag{2.10}$$

where the net carbon exchange (*NCE*) is the remaining C flux from NPP, after heterotrophic respiration (i.e., decomposition) (R_H) and decomposition (E_P) of products harvested from ecosystems for human use (e.g., harvested for *YLD*) (McGuire *et al.*, 2001). A positive NCE indicates ecosystem acting as a CO_2 sink whereas a negative NCE means that ecosystem is a CO_2 source.

Management. Agricultural management practices such as irrigation, fertilization, rotation and cultivar selection affect mass and energy input and output in agroecosystems. However, the original TEM designated for natural ecosystems has not considered these factors (e.g., McGuire *et al.*, 1992). Using the modified TEM to simulate agroecosystem has some difficulties in modeling C-N-management interactions and integrating time-varying spatially explicit data into regional simulations (e.g., Felzer *et al.*, 2004) (**Table 2.1**). In contrast, AgTEM includes two major management practices of irrigation and N fertilization. Besides precipitation percolation, irrigation is considered as an additional direct water input into the soils, which is modeled based on Zhuang *et al.* (2002). N fertilizer, mainly in the form of NH_4^+-N and NO_3^--N, enters soils, as nutrients to support crop biomass accumulation and soil microbial activities. The N fertilization implementation in AgTEM is modeled as N input from sources outside the ecosystem, affecting NPP, N dynamics and C-N interactions, which were described in Raich *et al.*, (1991) and McGuire *et al.* (1992). N fertilizers also affect nitrification and denitrification processes in AgTEM.

2.2.3.3 Nitrification and Denitrification

Atmospheric nitrogen enters agroecosystems mainly through atmospheric deposition (e.g., lightning and rainfall), synthetic N fertilizer application, manure application and litter fall. These N inputs are further mineralized into soil available N such as NH_4^+ and NO_3^-. The gaseous NO_X emissions from soils, mostly in forms of N_2, nitric oxide (NO) and N_2O, are mainly produced through nitrification and denitrification processes (**Figure** 2.1). Nitrification describes the process of the biological oxidation of ammonia with oxygen into nitrite and nitrate. Denitrification represents a process of nitrate reduction that eventually produces N_2 and N_2O (**Figure** 2.1).

In AgTEM, NO_X emissions are simulated according to the amount of soil inorganic N, determined by the micro-environment depending on temperature, soil pH, soil water content and soil biological activity (**Figure** A 2, A 3). Algorithms describing nitrification and denitrification processes from other studies (e.g., Bradbury *et al.*, 1993; Henault *et al.*, 2005) and models (EOSSE, Smith *et al.*, 2010; Bell *et al.*, 2012) were adapted. Three major NO_X fluxes (namely, N_2O, NO and also N_2) are included in AgTEM. NO_X (NOX) is the total NO and N_2O emissions from nitrification and N_2 and N_2O emissions from denitrification:

$$\left.\begin{array}{l} NH_4^+ \overset{NO_{ntf}}{\Rightarrow} N_2O_{\mathrm{ntf}} \\ NO_3^- \underset{N2_{dtf}}{\Rightarrow} N_2O_{\mathrm{dtf}} \end{array}\right| \Rightarrow N2O \,\Big|\Rightarrow NOX \tag{2.11}$$

where $N2O_{ntf}$, NO_{ntf}, $N2O_{dtf}$ and $N2_{dtf}$ indicate fluxes of N_2O from nitrification, NO from nitrification, N_2O from denitrification and N_2 from denitrification, respectively (**Table** A 1). Total N_2O fluxes ($N2O$) account for both $N2O_{ntf}$ and $N2O_{dtf}$ (more details on nitrification and denitrification modeling can be found in Appendix A).

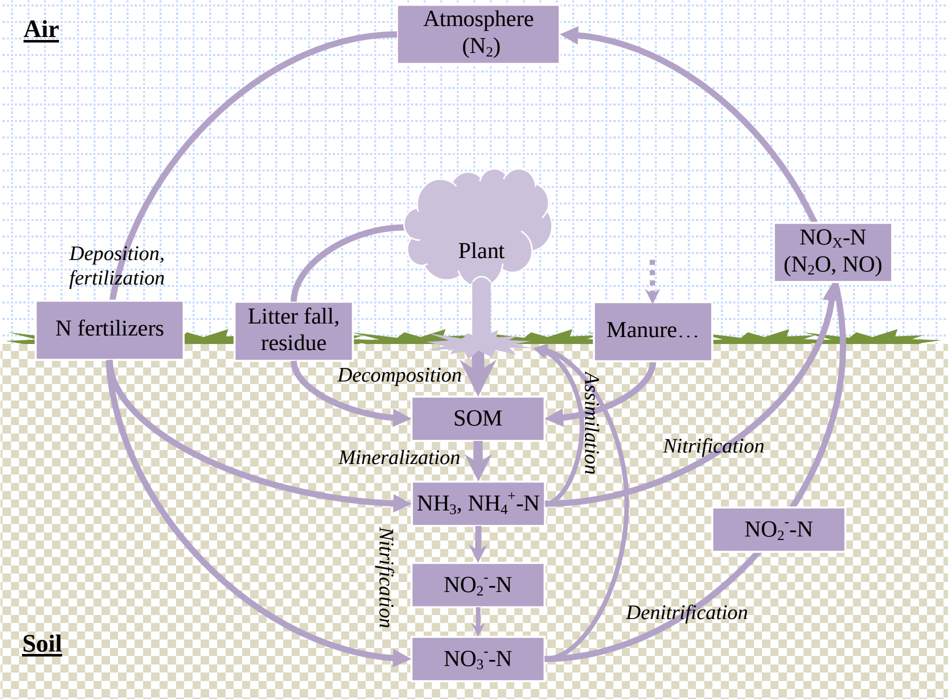

Figure 2.1 N cycling among the atmosphere, biosphere and pedosphere. Major processes were modeled in AgTEM. SOM, soil organic matter; N_2, nitrogen; NH_3, ammonia; NO_X, nitrogen oxides; N_2O, nitrous oxide; NO, nitric oxide.

2.2.4 Model Parameterization and Validation

There are a number of constant, vegetation-specific or soil-specific parameters in AgTEM. Most of them have been defined and determined in earlier studies (e.g. Raich *et al.*, 1991; McGuire *et al.*, 1992; Zhuang *et al.*, 2003). Some vegetation-specific parameters, such as those used to estimate C and N dynamics in maize, switchgrass and *Miscanthus* ecosystems, were determined via calibration of the model driven with climate data using observed data of C and N fluxes and pool sizes (Qin *et al.*, 2011; Qin *et al.*, 2012). To determine biomass allocation and biomass-yield conversion, crop-specific parameters used in Eqns. (2.8) and (2.9) were defined according to previous researches (**Table** 2.5). Most parameters used in soil N nitrification and denitrification can be found in earlier studies (**Table** A 2).

Validation investigates models' performance to reproduce the observations from a system within its domain of application (Rykiel, 1996). The model simulations are compared with observed data, and certain criteria are used to determine model performance (Smith *et al.*, 1997). In total, 29 field experiment sites, including 82 site-treatment (i.e., N input level) observational data sets, were organized for validating AgTEM across the United States. These sites cover three bioenergy ecosystems including maize, switchgrass and *Miscanthus* (**Table** 2.6). For maize, only continuous maize cropping systems were included in the validation. Data of biomass yield (e.g., maize grain, cellulosic biomass) and annual N_2O fluxes were used for model and data comparison. Site location, agricultural management, soil properties and daily climate conditions were used for model simulations. Site annual N_2O flux estimates were based on observations during the crop growing season, and accumulated through all growth stages. Possible N_2O fluxes from the non-growing season were not estimated. For site-level data collection and processing (e.g., NPP calculation) procedures, information can be found in earlier studies (Qin *et al.*, 2011; Qin *et al.*, 2012). The climate data of air temperature, precipitation, cloudiness were obtained from the ECMWF (European Centre for Medium-Range Weather Forecasts) Data Server (www.ecmwf.int). For each site-treatment, AgTEM was run for multiple years, using forcing data describing site location, elevation, climate, soil, vegetation and management. NPP, biomass of interest (i.e., maize

Table 2.6 Field experiments studying biomass production and N_2O emissions of bioenergy crops, used in this study

Bioenergy crop	Location	Collection period	Experimental treatment	Available observational data	References
Maize	Fort Collins, CO[†]	2002-2004	Three nitrogen levels (0 – 202/224 kg N ha^{-1}); maximum level differs for 2002 and 2003-2004	Grain yield, N_2O flux	Halvorson *et al.*, 2006; Mosier *et al.*, 2006
	Fort Collins, CO	2005-2006	Four nitrogen levels (0 – 246 kg N ha^{-1})	N_2O flux	Halvorson *et al.*, 2008
	Fort Collins, CO	2007-2008	Three nitrogen levels (0 – 246 kg N ha^{-1})	Grain yield, N_2O flux	Halvorson *et al.*, 2010
	West Lafayette, IN	2004-2006	One nitrogen level, changed from 222 kg N ha^{-1} in 2004-2005 to 260 kg N ha^{-1} in 2006	N_2O flux	Omonode *et al.*, 2011

Table 2.6 Continued.

Hickory Corners, MI	2001-2003	Nine nitrogen levels available, from 0 to 291 kg N ha^{-1}	Grain yield, N_2O flux	McSwiney & Robertson, 2005
Fairgrove, MI	2007-2008	Six nitrogen levels (0 – 225 kg N ha^{-1})	Grain yield, N_2O flux	Hoben *et al.*, 2011
Hickory Corners, MI	2007-2008	Six nitrogen levels (0 – 225 kg N ha^{-1})	Grain yield, N_2O flux	Hoben *et al.*, 2011
Mason, MI	2007	Six nitrogen levels (0 – 225 kg N ha^{-1})	Grain yield, N_2O flux	Hoben *et al.*, 2011
Reese, MI	2007-2008	Six nitrogen levels (0 – 225 kg N ha^{-1})	Grain yield, N_2O flux	Hoben *et al.*, 2011
Stockbridge, MI	2008	Six nitrogen levels (0 – 225 kg N ha^{-1})	N_2O flux	Hoben *et al.*, 2011
Lincoln, NE	2003-2005	Recommended and intensified management, each had three nitrogen levels (180 – 310 kg N ha^{-1})	Grain yield, N_2O flux	Adviento-Borbe *et al.*, 2007

Table 2.6 Continued.

	Rock Springs, PA	2006-2007	With only one nitrogen level (224 kg N ha^{-1})	Grain yield, N_2O flux	Adviento-Borbe *et al.*, 2010
Switchgrass	Chatham, MI[‡]	2009	Three nitrogen levels (0–112 kg N ha^{-1})	Harvested biomass, N_2O flux	Nikièma *et al.*, 2011
	Shabbona, IL	2004-2006	No nitrogen applied	Harvested biomass, limited[*]	Heaton *et al.*, 2008
	Simpson, IL	2004-2006	No nitrogen applied	Harvested biomass, limited	Heaton *et al.*, 2008
	Urbana, IL	2004-2006	No nitrogen applied	Harvested biomass, limited	Heaton *et al.*, 2008
	Manhattan, KS	2011	One nitrogen level (156 kg N ha^{-1})	N_2O flux	Propheter *et al.*, 2010; McGowan *et al.*, 2012

Table 2.6 Continued.

	Raleigh, NC	1999-2001	Four switchgrass cultivars were planted at eight sites (1-8); Nitrogen was applied to all plots at an annual rate of 100 kg N ha^{-1}, site 1	Harvested biomass	Fike *et al.*, 2006a; Fike *et al.*, 2006b
	Princeton, KY	1999-2001	Same as above, but for site 2	Harvested biomass	Fike *et al.*, 2006a; Fike *et al.*, 2006b
	Knoxville, TN	1999-2001	Same as above, but for site 3	Harvested biomass	Fike *et al.*, 2006a; Fike *et al.*, 2006b
	Jackson, TN	1999-2001	Same as above, but for site 4	Harvested biomass	Fike et al., 2006a; Fike et al., 2006b
	Blacksburg, VA	1999-2001	Same as above, but for site 5	Harvested biomass	Fike et al., 2006a; Fike et al., 2006b

Table 2.6 Continued.

	Blacksburg, VA	1999-2001	Same as above, but for site 6	Harvested biomass	Fike *et al.*, 2006a; Fike *et al.*, 2006b
	Orange, VA	1999-2001	Same as above, but for site 7	Harvested biomass	Fike *et al.*, 2006a; Fike *et al.*, 2006b
	Morgantown, WV	1999-2001	Same as above, but for site 8	Harvested biomass	Fike *et al.*, 2006a; Fike *et al.*, 2006b
Miscanthus	Urbana, IL¶	2010	Three nitrogen levels (0 –120 kg N ha^{-1})	Harvested biomass, N_2O flux	Behnke *et al.*, 2012
	Manhattan, KS	2011	One nitrogen level (156 kg N ha^{-1})	N_2O flux	Propheter *et al.*, 2010; McGowan *et al.*, 2012
	Shabbona, IL	2004-2006	No nitrogen applied	Harvested biomass	Heaton *et al.*, 2008
	Simpson, IL	2004-2006	No nitrogen applied	Harvested biomass	Heaton *et al.*, 2008

Table 2.6 Continued.

	Urbana, IL	2004-2006	No nitrogen applied		Harvested biomass	Heaton *et al.*, 2008

[*] No data for the first year.

[†] Maize site selected for model sensitivity analysis.

[‡] Switchgrass site selected for model sensitivity analysis.

[¶] *Miscanthus* site selected for model sensitivity analysis.

grain, harvestable biomass), and N_2O emission were analyzed. For all three crops, modeled *NPP* and N_2O were then compared with the observed data.

For comparison, the modeled data were plotted against observations, and a linear regression with a zero intercept was computed to estimate the slope and coefficient of determination (R^2). The closer the regression slope to 1, the better the model fits to the observed data. R^2 ($0 \leq R^2 \leq 1$) indicates the pattern of simulated and observed values (Smith *et al.*, 1997; Huang *et al.*, 2009). The root mean square error (RMSE) and model efficiency (EF) (Loague & Green, 1991) were also reported to show the discrepancies between simulations and observations.

We also estimated the N_2O emissions following the Intergovernmental Panel on Climate Change (IPCC) N-input approach (Tier 1) (De Klein *et al.*, 2006). The annual direct soil N_2O emissions were empirically calculated as a factor (0.01) of total N input into soils, including N from fertilizer, manure, water and residue. Water N was not accounted for in our study, partly because of its scarcity compared to other N sources and also due to a lack of data. Model performance was evaluated in a similar manner to AgTEM.

2.2.5 Model Sensitivity Analysis

A sensitivity analysis studies the response of the model to different sources of variance in input data (e.g., parameters, forcing data) (Loucks *et al.*, 2005). To study AgTEM sensitivity, three sites with the most accessible information, one for each ecosystem type (**Table** 2.6), were selected. Six major input variables representing the climate, management and CO_2 conditions were included in the sensitivity analysis. For a simplified general form of AgTEM (Eqn. 2.12), an output corresponding to change in input variables can be written as Eqn. (2.13):

$$Y = f\left(X_1, \ldots, X_6\right) \tag{2.12}$$

$$\mathrm{E}\left(Y_i^j\right) = E_{X_i}\left(Y|X_i^0\right) \tag{2.13}$$

where X_i denotes the *i-th* input variables, and X_1 to X_6 are daily air temperature (*TAIR*), daily precipitation (*PREC*), daily cloudiness (*CLDS*), daily N fertilizer application (*FTLZ*), daily irrigation (*IRGT*) and annual atmospheric CO_2 concentrations (*KCO2*), respectively. Y indicates the model output whose sensitivity to environment will be evaluated, and here j can refer to NPP and N_2O fluxes in AgTEM. Y_i corresponds to input X_i. As for Eqn. (2.13), $(Y|X_i^0)$ is the model simulation under changing variable X_i while other variables are fixed (X_i^0). Therefore, the change of model output due to a given changing input can be expressed as:

$$V\left(Y_i\right) = \frac{E\left(Y_i\right)}{E\left(Y_0\right)} - 1 \tag{2.14}$$

where $V(Y_i)$ is the change of output Y responding to changing input X_i, relative to a reference scenario where all input variables are fixed (as in Y_0). In the study, all input forcing data collected for each site was used for the reference scenario. In particular, the N fertilizer application rate in the reference scenario was set as 134 kg N ha^{-1} for maize and 56 kg N ha^{-1} for switchgrass and *Miscanthus*. A certain perturbation was exerted to the forcing data to represent input changes:

$$\boldsymbol{X}^T\boldsymbol{C} = \left(TAIR \quad PREC \quad CLDS \quad FTLZ \quad IRGT \quad KCO2\right)^T \left(\mathbf{-1} \quad \mathbf{0} \quad +\mathbf{1}\right) \tag{2.15}$$

As in Eqn. (2.15), for each variable X, negative (**-1**) and positive (+**1**) changes (***C***) were added on to the reference (**0**) forcing data to calculate output sensitivity to increases and decreases of inputs, respectively. For each model simulation regarding the changing variable X, NPP and N_2O outputs were analyzed, and a decadal average $V(Y)$ was reported to demonstrate the magnitude of sensitivity for a given Y.

2.3 Results

2.3.1 Site-level Biomass Production and Nitrous Oxide Emissions

The field experiment sites (i.e., maize, switchgrass and *Miscanthus*) selected for model validation spread across a majority portion of the maize-producing areas in the conterminous United States, covering a variety of climate zones such as semiarid steppe climate, humid continental climate and humid subtropical climate (**Figure** 2.2a). Of the 82 site-treatment datasets collected from 29 sites, 65 of them contain N_2O observational data (maize: 57, switchgrass: 4, *Miscanthus*: 4), and 62 have NPP data (maize: 45, switchgrass: 10, *Miscanthus*: 7). These data were used as dependent variables for comparisons between model simulations and observations. N input at the site-level ranges from 0 to 310 kg N ha^{-1} for maize and 0 to 156 kg N ha^{-1} for switchgrass and *Miscanthus* (**Table** 2.6), representing a wide diversity of N treatments.

AgTEM simulations of crop NPP are consistent with the observations (**Figure** 2.2b). The observed NPP of maize has an average of 680 g C m^{-2}, with a range from 287 to 1400 g C m^{-2}. Crop productivity tends to increase with increasing N application. Observed NPP of switchgrass and *Miscanthus* are relatively higher than maize, about 850 and 1400 g C m^{-2}, respectively. But the biomass production is not necessarily related to

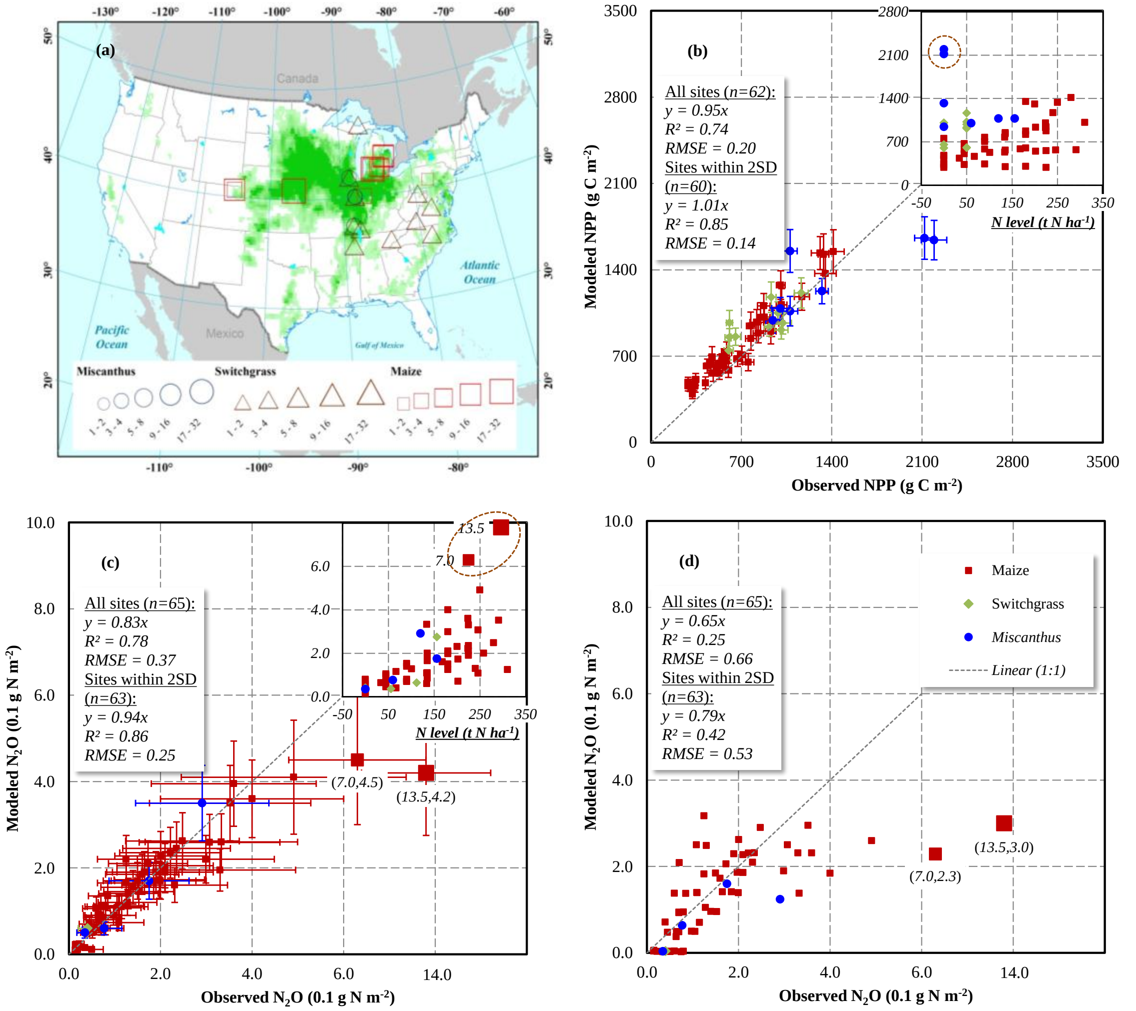

Figure 2.2 Modeled vs. observed NPP and N_2O emissions in bioenergy ecosystems at site-level. (a) Maize, switchgrass and *Miscanthus* sites cover a majority of the maize-producing areas (shadowed in deep green) across the conterminous United States (Monfreda *et al.*, 2008); (b) AgTEM modeled vs. observed NPP, with illustration of NPP change over N input level in the upper right inset; (c) AgTEM modeled vs. observed N_2O, with illustration of N_2O change over N input level in the upper right inset; (d) IPCC modeled vs. observed N_2O. Error bar indicates standard deviation.

the N input level. For all sites (n=62), the regression between modeled and observed NPP yields an R^2 of 0.74 with a slope of 0.95 ($P<0.001$). However, two observations (**Figure**

2.2b, circled) evidently deviate from the 1:1 line, showing an underestimation in AgTEM. These two observations of *Miscanthus* from central and southern Illinois show an extremely high biomass production (Heaton *et al.*, 2008), with an average annual NPP flux of about 2150 g C m^{-2}, about three times the average NPP of the rest of the 60 observations. The peak biomass production may be because of favorable climate, management and proper harvest time during the experiment time (Heaton *et al.*, 2008). To better illustrate the model performance at the majority of sites, observations beyond the range of (mean ± 2SD (standard deviation)) were removed for the comparison. For these sites within 2SD, the indices indicate that fitness of simulations is improved. The slope of regression approximates 1, with a R^2 of 0.85; the *RMSE* decreases from 0.20 to 0.14 and *EF* increases from 0.83 to 0.88 (**Figure** 2.2b).

N_2O fluxes from maize, switchgrass and *Miscanthus* were modeled using both AgTEM and an IPCC empirical model. Observations from maize ecosystems show that N_2O emitted from croplands with high N application rates are mostly larger than those with lower N input levels (**Figure** 2.2c). As for all sites (n=65), the average N_2O flux is 1.8 kg N ha^{-1} (1 kg N ha^{-1} = 0.1 g N m^{-2}), with the maximum flux reaching 13.5 kg N ha^{-1} observed in a continuous maize field in Indiana (Omonode *et al.*, 2011). Normally, N fertilizers are not applied to switchgrass and *Miscanthus*, and the highest N application rate tested in the field experiments is 156 kg N ha^{-1}. N_2O emissions from soils of these cellulosic crops are comparable with those from maize cropland under similar N input levels (**Figure** 2.2c). The model simulations using AgTEM well estimate the N_2O change, at least for fluxes within a reasonable range (e.g., less than 5.0 kg N ha^{-1}). The comparison between modeled and observed N_2O results in a slope of 0.83 and R^2 of 0.78, for all sites. By moving two maize observations outside the 2SD range (**Figure** 2.2c, circled), one from Stockbridge, MI (Hoben *et al.*, 2011) and the other from West Lafayette, IN (Omonode *et al.*, 2011), the regression generates a higher slope of 0.94 with a greater R^2 of 0.86. The *RMSE* declined from 0.37 to 0.25, and *EF* slightly improved from 0.81 to 0.88. The discrepancies between modeled and observed fluxes are partly explained by high soil organic matter content (Hoben *et al.*, 2011). Possible maize residues and residual mineral N gains from N fixation by the previous crop (Omonode *et al.*, 2011) contributed to N_2O emissions, while AgTEM did not capture these changes.

The IPCC approach relates N_2O emissions solely to N input, such as N fertilizer and residue, but fails to consider environmental factors that also significantly affect N dynamics (Grassini & Cassman, 2012). In our study, the predictions from the IPCC model capture a proportion of the observations, with more persuasive indices supporting the fitness for sites within 2SD than for all available sites (**Figure** 2.2d). However, high variances still existed; the *RMSE* and *EF* were 0.66 and 0.41 respectively for all sites (n=65), and 0.53 and 0.46 respectively for limited sites (n=63). The emission factor of 0.01 may not fit all ecosystems. Based on the observations collected in this study, the emission factor of N_2O for maize is 0.010 (R^2=0.44, P<0.001, n=63) or 0.013 (R^2=0.33, P<0.001, n=65); for switchgrass it is 0.013 (R^2=0.62, P=0.2, n=4) and for *Miscanthus* it is 0.016 (R^2=0.56, P=0.2, n=4).

Compared with the IPCC empirical model in most cases, AgTEM is a better tool to estimate N_2O fluxes from maize, switchgrass and *Miscanthus* ecosystems. The IPCC approach is a good substitute when process-based models are not used due to lacking data or when the estimation accuracy requirement is not high. AgTEM will work under more complicated circumstances, especially when N_2O accounting has higher accuracy requirement while the environment conditions are complex. For example, regional, national or even global large-scale estimates require process-based modeling for better accounting for the complex climate-soil-atmosphere interactions (Bondeau *et al.*, 2007; Del Grosso *et al.*, 2010).

2.3.2 Model Sensitivity to Environment and Management Factors

A sensitivity analysis quantifies the impact of changes in input data on model outputs. Usually, only a subset of input variables dominates outputs in process-based models (Loucks *et al.*, 2005). To identify those input variables, AgTEM simulations were conducted by varying six input variables at three separate locations, one site for each type of crop. The sensitivity of NPP and N_2O in terms of percentage change relative to the reference simulation is reported separately for maize, switchgrass and *Miscanthus*.

In AgTEM, climate, soil and CO_2 conditions, and agricultural management including irrigation and fertilization which determine photosynthesis and autotrophic respiration will ultimately affect NPP. The sensitivity analysis shows that the perturbations to input variables affect NPP for all three crops. However, the magnitudes of sensitivity differ among variables and crops (**Figure** 2.3). For all crops, KCO2, TAIR, PREC, FTLZ and IRGT (except no IRGT available for cellulosic crops) have positive effects on NPP, where a positive change of input results in a positive change of output, while CLDS has a negative effect on NPP. All crops are comparably sensitive to CO_2 and air temperature, but cellulosic crops (i.e., switchgrass and *Miscanthus*) are much less sensitive than maize to precipitation, cloudiness and fertilizer application (**Figure** 2.3). In maize ecosystems, NPP is most sensitive to air temperature, where about 20% of the NPP increase was due to a 10% temperature increase and a 16% NPP decrease was due to a 10% temperature decrease, and least sensitive to CO_2, where only about a 7% NPP change was due to a 10% CO_2 input change (**Figure** 2.3a). In switchgrass and *Miscanthus* ecosystems, air temperature is still the dominant factor affecting NPP, and a 10% input change caused a 20% NPP change. However, NPP responses are much less noticeable in response to changes in precipitation, cloudiness and fertilization, only a 1-5% change resulted from a 10% input change (**Figure** 2.3b, 2.3c).

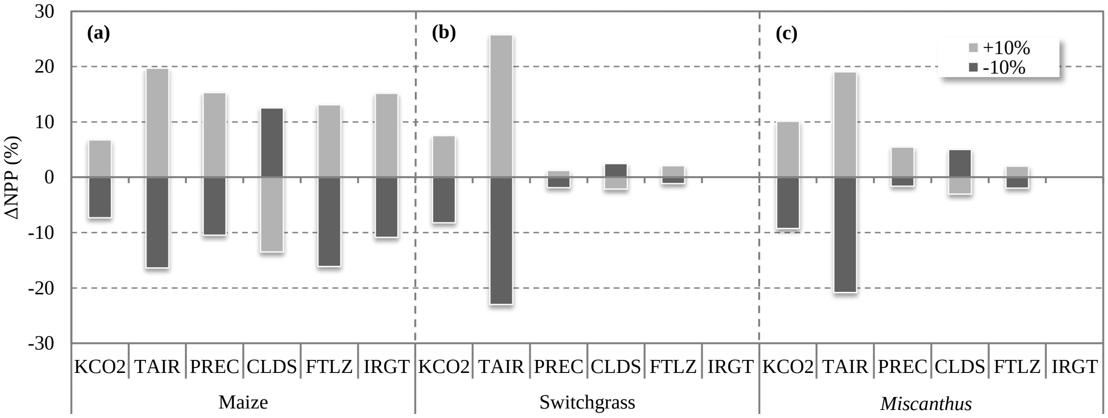

Figure 2.3 Sensitivity of NPP responding to model input (±10% change) in different ecosystems. Estimates were made for (a) maize at site Fort Collins, CO, (b) switchgrass at site Chatham, MI and (c) *Miscanthus* at site Urbana, IL. KCO2, atmospheric CO_2 concentration; TAIR, temperature; PREC, precipitation; CLDS, cloudiness; FTLZ, fertilizer amount; IRGT, irrigation amount.

These responses may be partly explained by the fact that environmental and management factors directly or indirectly affect the plant photosynthesis and respiration.

The atmospheric CO_2 positively affects GPP production via photosynthesis. Elevated CO_2 significantly increases leaf photosynthetic CO_2 uptake rate (Leakey *et al.*, 2004; Oliver *et al.*, 2009). Higher temperature means a longer growth period and higher GDD, which may benefit crops, especially those grown in the relatively colder areas. An example is the selected switchgrass site in the central Upper Peninsula of Michigan, U.S.A. (46.55º N, 86.92 º W, 266.1m a.s.l.) (Nikièma *et al.*, 2011). Abundant but not excessive precipitation can protect crops from drought, providing sufficient water for evaporation and transpiration. Lower cloudiness allows more solar radiation to be absorbed by plants, and therefore more energy to be stored in vegetation. Favorable management practices could always benefit crop production, e.g., irrigation for water inputs and fertilization for nutrient inputs. However, switchgrass and *Miscanthus* seemed to benefit less from increased water and nutrient inputs or less harmed due to less input (**Figure** 2.3b, 2.3c). This is because that these biofuel crops have a relatively higher efficiency for using solar radiation, water and nutrients (e.g., N) compared with maize. Studies reported that switchgrass and *Miscanthus* could intercept large proportions of the photosynthetically active radiation (Heaton *et al.*, 2008), use much less irrigation than food crops (Fargione *et al.,* 2010), and have no or only slight responses to N fertilization (Lewandowski *et al.*, 2003).

Among the six factors, CO_2 generally has the least impact on N_2O output in AgTEM among all three ecosystems (**Figure** 2.4). N_2O output is negatively related to CO_2 input; less than a 0.5% N_2O flux change was estimated in response to a 10% CO_2 change. For maize ecosystems, the model is more sensitive to fertilization and irrigation, and less responsive to climate factors (**Figure** 2.4a). For switchgrass and *Miscanthus* ecosystems, the model shows a much higher sensitivity to climate factors than management. A 4-9% change in N_2O is observed as a result of a 10% change of temperature or precipitation, and a 2-3.5% N_2O change has occurred in response to a cloudiness change (**Figure** 2.4b, 2.4c). Low N input level (56 kg N ha^{-1}) partly explains the insensitivity of modeling response to fertilization.

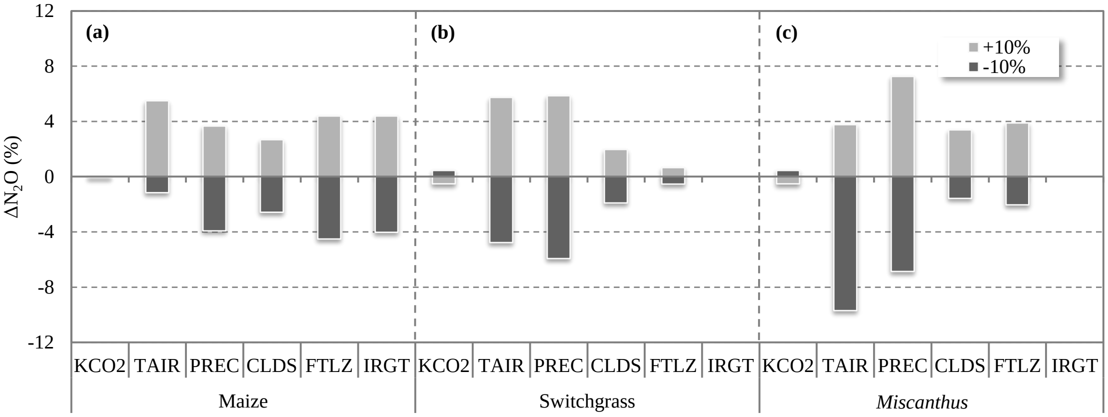

Figure 2.4 Sensitivity of N_2O responding to model input (±10% change) in different ecosystems. Estimates were made for (a) maize at site Fort Collins, CO, (b) switchgrass at site Chatham, MI and (c) *Miscanthus* at site Urbana, IL. Abbreviations are same as in **Figure** 2.3.

Additional tests using ±20% input change confirmed the pattern of local responses of NPP (**Figure** A 4) and N_2O (**Figure** A 5) to input perturbations. However, the relative output changes vary among different input variables and ecosystems. It should be noted that the local sensitivity analysis here is not for quantifying the regional impacts of input on outputs. The sensitivity results may change due to change of input data and the sites for conducting the analysis. A global sensitivity analysis at regional levels would be needed to allow full exploration of the input space, accounting for high-dimensionality, interactions, and spatial heterogeneity. However, the global sensitivity analysis requires more information to build probability distributions for the input variables and parameters and expects higher computational complexity (Tang & Zhuang, 2009).

2.4 Discussion

2.4.1 Impacts of N Input on Biomass Production and N_2O Emissions

Nitrogen, an indispensable nutrient for plants, is often the limiting factor for both crop growth and N_2O production. Generally, crop yields and NPP depend on N availability; higher productivity normally requires considerable N inputs, especially for soils with poor nutrient contents (Millar *et al.*, 2010). Many earlier recommendations on crop N application were made based on a positive N-yield relationship (e.g., Stanford, 1973). However, later N response trials and observations questioned the poor N-yield relationship because crop yield may not necessarily increase at excessive N input levels (Nafziger *et al.*, 2004; Millar *et al.*, 2010). N input may enhance crop growth at lower N levels, but may reach a crop yield threshold when the N application is sufficient (Nafziger *et al.*, 2004). For example in the three-year trials in Michigan, McSwiney & Robertson (2005) observed that maize grain yields increased in response to N additions from 0 to 101 kg N ha^{-1}, but then leveled off when more N was added.

When N availability exceeds the needs by plant and competing biota, N_2O emissions can be substantial and exhibit exponential responses to the magnitude of N inputs. It has been found in this study (**Figure** 2.2c) and others (McSwiney & Robertson, 2005; Hoben *et al*., 2011) that the relationship between N_2O flux and N input is nonlinear, with a lower emission rate at relatively low N application levels, and a much higher rate when N input increases. N_2O emissions are often simulated as an exponential function of the N input rate with empirical models (McSwiney & Robertson, 2005; Van Groenigen *et al.*, 2010), instead of simply applying a linear model like the IPCC tier 1 approach (De Klein *et al.*, 2006). That is, with increasing N, the marginal gain of crop yields decreases while the marginal N_2O emissions increase. The recommended rate of N application can only be reached at such a point that the marginal benefit from crop production balances marginal loss or cost via resource input (e.g., N fertilization) and environment pollution (e.g., GHG emissions). More attention should be paid to environmentally or ecologically optimum N rates from the perspective of ecosystem services (Millar *et al.*, 2010; Chen *et al.*, 2011a; Davis *et al.*, 2012).

2.4.2 Approximation and Simulation in Modeling

Agroecosystem models and crop models share expanding common interests, yet they also have their own specialties. Both groups facilitate the application of models in a system approach to quantifying crop ecosystem dynamics. Both provide a framework to integrate knowledge about soil, climate, plant and management to transfer the understanding from one location to another, from site to region, supporting decision making with less time and resources required for analyzing complex systems (Raich *et al.*, 1991; Jones *et al.*, 2003; Loucks *et al.*, 2005). However, crop models are mostly used in the agriculture sector to help understand the impacts of environment factors and especially management practices on crop growth and therefore crop yield (grain-based) or biomass (non-grain or not interested in grain), and to provide recommendations on agricultural management or hazard protection. Model simulations focus on finer resolutions, for instance, at site- or field- scale for a specific crop type (e.g., CERES-Maize for maize, Hodges *et al.*, 1987) or for specific purposes (e.g., AquaCrop for water management, Steduto *et al.*, 2009). In contrast, agroecosystem models have usually been used to understand the impacts of natural (e.g., climate) or anthropogenic activities (e.g., cropping) on ecosystem dynamics (e.g., McGuire *et al.*, 2001; Felzer *et al.*, 2009). Crop yields or biomass production is part of the C cycle. The spatial scale can be region, nation and even globe (Bondeau *et al.*, 2007).

In our study, AgTEM models the C and N dynamics for agroecosystems with vegetation-specific parameters for each species or crop type. The model structure and algorithms used to describe the biogeochemical and physical processes (e.g., photosynthesis, biomass allocation) are similar, with only minor changes for specific crops. For example, maize has an extra C pool (grain) while switchgrass and *Miscanthus* do not have one. Vegetation-specific parameters calibrated with observational data were used to capture the magnitude of differences among crops. Some of these parameters can be found from either experiment-based models or crop models (e.g., **Table** 2.3, 2.4). Management practices such as irrigation and fertilization were considered in AgTEM, and grain and biomass harvest were estimated.

In the validation and sensitivity analyses, we used the annual total value at multiple sites instead of daily fluxes from a single site to evaluate the NPP and N_2O fluxes. We also combined estimates of three species, maize, switchgrass and *Miscanthus,* instead of making separate calculations. In the agroecosystem model, biomass (e.g., grain) is estimated based on NPP, a large-scale and long-term average quantity considering both natural and anthropogenic effects. In comparison with crop models, crop yields are small-scale and short-term results of G×E×M (gene/species × environment × management) interactions. Therefore, using agroecosystem models to estimate small-scale C and N dynamics of crop ecosystems, by calibrating parameters to capture short-term (e.g., day-by-day) fluxes, might result in high uncertain ecosystem dynamics (Bell *et al.*, 2012). In addition, observational data might not be in agreement between experiments or repeated samples as a result of measurement uncertainty such as ground disturbance, investigator biases, method divergences and laboratory requirement differences (Müller & Hoper, 2004; Kessel *et al.*, 2013). In this study, for example, the N_2O experiments collected gas samples at different time intervals during various time courses (e.g., McSwiney & Robertson, 2005; Omonode *et al.*, 2011) at weekly (Parkin & Hatfield, 2010), biweekly (Nikièma *et al.*, 2011) or irregular (Hoben *et al.*, 2011) time steps. Frequency, timing and quantity of N fertilization may affect daily N_2O fluxes significantly (Mosier, 1994), and the N_2O variations could be principally due to the degree of coincidence of fertilizer application and major rainfall events (Dobbie *et al.*, 1999). It is therefore useful to use seasonal or annual total N_2O emissions from several years' data from a certain ecosystem in a variable climate to obtain a robust estimate of mean N_2O fluxes (Dobbie *et al.*, 1999).

2.4.3 Estimation Uncertainties and Future Needs

The discrepancies between modeled and observed NPP and N_2O come from several sources of uncertainties. Imperfect representation of processes (structural uncertainty) and limited knowledge of parameter value (parameter uncertainty) in a model constitute model uncertainty (Loucks *et al.*, 2005). In addition, AgTEM only considers irrigation and fertilization in terms of agricultural management. Tillage, crop rotation, crop straw management that affect the biomass and N_2O emissions (Halvorson *et al.*, 2008; Liu *et al.*, 2011), however, were not considered. This is partly because of the difficulty to quantify the spatial variability of human activities due to a lack of consistent evidence (Millar *et al.*, 2010), and no spatially explicit data concerning these management practices are available for regional simulations (Felzer *et al.*, 2004). Input data are another source of uncertainty. First, the observational data could be biased due to experimental uncertainty. Compared with maize, there are less data for switchgrass and *Miscanthus* for model validation. More observational data will help to parameterize and validate AgTEM at locations under different environmental conditions (e.g., Europe and China). The forcing data for model simulations were collected from various sources, thus may not represent local environmental conditions. For example, the temperature and precipitation data used in AgTEM were obtained from the ECMWF reanalysis database. The data may be suitable for regional estimation, but not accurate for site-level simulations (Dee *et al.*, 2011). Thus, local climate, soil and vegetation data at the site are desirable.

Uncertainty cannot be removed but can be narrowed, and the model can be improved. From the perspective of observation, better estimates can be achieved via dedication to cross-site experimental research that are of considerable long period with appropriate time intervals during sufficient time courses (e.g., N_2O), covering various climate and management (Dalal *et al.*, 2003). The ecosystem C budget quantification can be improved using eddy flux data (e.g., Chen *et al.*, 2011b). In this study, however, the NCE data of crop ecosystems are not available. Among the many Ameriflux sites (http://ameriflux.ornl.gov/), only a very limited number of sites cover croplands (IGBP) with ecosystem C balance data (e.g., NEE, net ecosystem exchange). There are only two sites listed (Rosemount G21 Conventional Management Corn Soybean Rotation / US-Ro1, Minnesota; Mead Irrigated Rotation / US-Ne2, Nebraska) covering maize croplands that can be potentially used for AgTEM. However, the observed fluxes at these sites measure the maize-soybean rotation system, which did not well represent continuous maize ecosystems. Thus, Ameriflux data was not used in this study. Continuous efforts in the maize-, switchgrass- and *Miscanthus*-based ecosystem flux measurements, together with agronomic observations (e.g., yield, management) (e.g., Suyker *et al.*, 2004) should be made to improve the model performance.

Our understanding about the underlying ecophysiological and biogeochemical processes shapes the way we interpret and model agroecosystems. Improved observational data will help calibrate and validate models. The AgTEM, as well as many other agroecosystem models can be improved using more data. These models can be appropriately extrapolated to regional scales when they are well calibrated and validated (e.g., McGuire *et al.*, 2001; Bondeau *et al.*, 2007). The developed AgTEM can be used to quantify C and N dynamics of maize, switchgrass and *Miscanthus* ecosystems at regional scales.

2.5 Conclusion

Based on the Terrestrial Ecosystem Model, we developed an agroecosystem model (AgTEM) to incorporate significant biogeochemical and ecophysiological processes such as crop phenology, biomass allocation, nitrification and denitrification, and agronomic management of irrigation and fertilization. The model can be used to simulate ecosystem carbon and nitrogen dynamics and therefore to estimate regional crop yield/biomass and carbon balance, as well as nitrous oxide emissions. AgTEM was validated against field experimental data, and tested for model output sensitivity. Results showed that species-specific parameterized AgTEM can well reproduce the site-level net primary productivity and nitrous oxide fluxes in selected bioenergy-related ecosystems (i.e., maize, switchgrass and *Miscanthus*). Model outputs of biomass production and nitrous oxide emission are sensitive to atmospheric CO_2 concentration, temperature, precipitation, cloudiness, fertilizer application and irrigation, although with different magnitudes of importance varying among different crop types. The AgTEM can be potentially used for regional estimates of C and N balance in validated bioenergy ecosystems. However, further efforts are still in need to improve model performance and expand model output domain.

2.6 Acknowledgement

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CHAPTER 3. POTENTIAL GREENHOUSE GAS EMISSIONS AND GLOBAL WARMING INTENSITY FROM CROPLAND

3.1 Introduction

Increasing concerns about energy security and environmental sustainability have prompted development of renewable energy. Currently, global energy supplies are dominated by fossil fuels, with very limited renewable sources. In 2010, the world total primary energy supply amounted to over 12 000 Mtoe yr^{-1} (Mtoe, million ton of oil equivalent), which is more than double the supply in 1973. More than 80% of energy supplies come from fossil fuels including oil (32.4%), coal/peat (27.3%) and natural gas (21.4%) (IEA, 2012). The increasing use of fossil fuels has directly led to increasing greenhouse gas (GHG) emissions. The IPCC reported that greenhouse gas emissions have increased by an average rate of 1.6% yr^{-1} over the last three decades, with growing carbon dioxide (CO_2) emissions from the use of fossil fuels at a rate of 1.9% yr^{-1} (Rogner *et al.*, 2007). The total annual CO_2 emissions have approximated to 30 gigatonnes in 2008, and still keep increasing (UN, 2012). As of the year 2010, only a very small proportion of the world energy supply came from renewable energy sources like hydropower (2.3%). Energy from biofuels and biomass including those traditionally used for cooking and heating in the underdeveloped areas, however, account for about 10% of the world total energy supply, making it by far the most important renewable energy source (IEA, 2012).

In the United States, bioenergy production is receiving great attention from industry, government and the scientific community. Ethanol production increased from 19 billion liters during the 1980s to 45 billion liters during the 1990s, and 174 billion liters during the 2000s. In 2011 alone, the annual production reached 52.6 billion liters, 2.6 times the total production of the entire 1980s, or 1.14 times of the 1990s (RFA, 2012). As a comparison, the consumption of gasoline was about 500 billion liters in 2011 (EIA, 2012). The ethanol plant and production capacity have expanded enormously since the early 2000s. The United States is one of the world's largest energy producers and consumers in terms of fossil fuels as well as biofuels (IEA, 2012). Over 60% of world fuel ethanol is now produced in the United States (2011) (RFA, 2012). According to the Energy Independence and Security Act of 2007 (US Congress, 2007), 136 billion liters (36 billion gallons) of renewable fuels, including 79 billion liters (21 billion gallons) of cellulosic ethanol, are expected to be produced annually by 2022. The fast bioenergy expansion increases societal, economic and scientific concerns about food security, land availability and carbon (C) mitigation.

In the United States, most of the current biofuels are made from food crops, such as maize grain and soybeans (*Glycine max* (L.) Merr.). Although the production of food crops has increased during the last several decades, due to crop variety improvement, technology advances, management optimization and other factors, most food grain was used for human consumption, livestock feed or other industrial uses. Only a limited proportion of the food crops, for instance, about 30% of maize grain (2009) (USDA, 2010), can be used for biofuel. The traditional crop grain alone cannot support the ambitious bioenergy goal without massive crop area expansion or a dramatic increase of grain productivity. Additionally, the competitive consumption of resources such as land, water, and nutrients by biofuel crops could threaten food crops and therefore food security (Fargione *et al.*, 2010; Diffenbaugh *et al.*, 2012). From the perspective of climate change mitigation, the crop-based biofuel may increase GHG emissions due to the impacts of indirect land-use change from natural ecosystems to croplands to meet the increasing demand for land. Nitrogen (N) fertilizer application may also contribute to the GHG emissions when used in producing biofuel feedstocks (Searchinger *et al.*, 2008; Melillo *et al.*, 2009). Crutzen *et al.* (2008) reported that, the production of commonly used biofuels, including bioethanol from maize, depending on plant N uptake efficiency, can contribute even more to global warming by N_2O emissions than mitigation by fossil fuel savings. N fertilizer contributes significantly to maize yield and yet produces the majority of N_2O emissions from the ecosystem (McSwiney & Robertson, 2005; Hoben *et al.*, 2011).

Cellulosic crops were introduced and tested in Europe (e.g., Clifton-Brown *et al.*, 2004; Fischer *et al.*, 2010) and the United States (e.g., Fike *et al.*, 2006b; Heaton *et al.*, 2008) for their higher productivity in producing biofuel biomass and higher environmental stress resistance relative to food crops. Two major cellulosic crops, switchgrass and *Miscanthus*, were selected as potential energy crops to substitute for maize grain for producing ethanol. Switchgrass is a perennial, warm-season lignocellulosic crop native to North America, with an annual yield ranging from 5 to 20 Mg dry matter (DM) ha^{-1} (Wright & Turhollow, 2010). *Miscanthus* is a genus of several species of perennial grasses, mostly native to subtropical and tropical regions of Asia, and introduced to the United States recently as an energy crop (Stewart *et al.*, 2009). Its yield normally ranges from 20 to 30 Mg DM ha^{-1}, with a maximum yield at 60 Mg DM ha^{-1} (Heaton *et al.*, 2008). These cellulosic crops are favored for their high efficiencies in making use of resources like land and nutrients. They require no or very limited amount of N fertilizer, while maize normally needs continuous N and other forms of fertilizer application to support growth (Lewandowski *et al.*, 2003; Fargione *et al.*, 2010). Relative to maize, cellulosic crops could potentially reduce N fertilization, and therefore mitigate N_2O emissions, and still provide competitive biomass feedstocks for biofuel production.

Compared with maize, the cellulosic crops may better serve as biofuel feedstocks in terms of GHG mitigation. Since most CO_2 absorbed by a plant via photosynthesis will eventually be emitted to atmosphere through biomass decomposition (e.g., litterfall or residues) or biofuel burning in case where plant is used for energy, the net C sequestered by the ecosystem is mostly located in soils. Field observations suggest that perennial energy crops could potentially sequester additional C into soils especially if established on former cropland. The ecosystems of cellulosic crops like switchgrass or *Miscanthus* have a generally larger soil C pool than the conventional annual crops (Kahle *et al.*, 2001; Dondini *et al*., 2010; Don *et al.*, 2012). Assuming national cropland switched from maize to cellulosic crops, Qin *et al.* (2012) estimated that the average soil C density in switchgrass and *Miscanthus* increased two thirds of that in maize. For cropland, the N_2O-N emitted is about 1 percent of the N fertilizer applied (De Klein *et al.*, 2006). Assuming that maize normally received 100-200 kg N ha^{-1} fertilizer each year, the N_2O emissions from 30 Mha maize-producing areas in the United States could reach 30-60 Gg N_2O-N per year. Earlier estimates indicated that annual N_2O emissions from all crop and pasture lands ranged within 0.9-1.2 Tg N in 1990 (Li *et al.*, 1996), and were about 201 Gg N from soils of major commodity crops in 2007 (Del Grosso *et al.*, 2010). Switchgrass and

Miscanthus may not necessarily have a lower N_2O emission factor relative to maize (Qin *et al*., 2013), but they normally require much less N fertilizer (Lewandowski *et al.*, 2003; Heaton *et al*., 2004; Clair *et al*., 2008); therefore, the per hectare N_2O emissions could be lower. According to these field tests, cellulosic crops seem to be a promising alternative to maize, due to their high productivity of biomass feedstocks (e.g., Fike *et al.*, 2006b; Heaton *et al.*, 2008; Wright & Turhollow, 2010), and relatively low GHG emissions (e.g., Lewandowski *et al.*, 2003; Heaton *et al*., 2004; Clair *et al*., 2008).

Special attention should be given to extrapolating site-level understanding to regional scales. The spatial heterogeneity of climate and soil conditions may not allow a simple site-to-region extrapolation without considering environmental changes. For example, the N_2O emission factor may be applicable for some sites with a certain range of N fertilization, but not for some other sites, and especially not for those with high N application rates (McSwiney *et al.*, 2005; Hoben *et al.*, 2011). Ecosystem modeling, on the contrary, is capable of addressing the problem of spatial heterogeneity. With spatially explicit data, models can simulate C and N dynamics using information describing climate, soil and vegetation characteristics (Fargione *et al.*, 2010; Davis *et al.*, 2012). But the model should still be cautiously selected and tested. General ecosystem models, especially those originally designed for natural ecosystems, may not work well in simulating a specific bioenergy-related agroecosystem without crop-specific calibration. Here we parameterize and validate an agroecosystem model for specific crops to assess possible GHG emissions due to a potential large-scale expansion of bioenergy development in the United States. Specifically, we analyze the biomass and biofuel production and GHG emissions in bioenergy-related ecosystems, by assuming maize, switchgrass and *Miscanthus* could be grown on the current maize-producing areas in the conterminous United States. By using an agroecosystem- based biogeochemical model, we (1) simulate spatially explicit C and N dynamics of each ecosystem; (2) estimate C balance (i.e., net CO_2 emissions) and N_2O emissions during the crop growth and harvest periods; and (3) examine the potential GHG emissions and global warming intensity due to bioenergy expansion.

3.2 Materials and Methods

3.2.1 Model Description

AgTEM is a process-based biogeochemical model to simulate C and N dynamics in agroecosystems at a daily time step using spatially explicit data of climate, vegetation, topography, and soils (Qin *et al*. 2013a). AgTEM inherits the model structure from TEM (e.g., Raich *et al.*, 1991; McGuire *et al.*, 1992; Zhuang *et al.*, 2003), with additional biogeochemical and ecophysiological processes incorporated to assess C and N fluxes and pools. Agricultural management is also considered (Qin *et al*. 2013). Among many variables describing C and N cycling, two of them related to C are frequently used in ecosystem modeling studies. One is net primary production (NPP) to estimate crop biomass production. The other is net carbon exchange (NCE) to evaluate the net C balance at the ecosystem scale. NPP can be further used to assess crop grain (e.g., for maize) and harvestable biomass (e.g., for cellulosic crops) production, and eventually to calculate potential biofuel production from various biomass feedstocks. NCE accounts for the net C sink or source considering photosynthesis (e.g., aboveground- and belowground biomass accumulation), growth and maintenance respiration, soil respiration and biomass harvest. A positive NCE indicates a net CO_2 sink whereas a negative value indicates a net CO_2 source. Nitrogen fluxes, including nitrous oxide (N_2O), are also estimated considering both nitrification and denitrification processes in soils (Qin *et al*. 2013).

AgTEM is a generic agroecosystem model with vegetation-specific parameters characterizing specific crop structures and processes. Most parameters used in this study have been either predefined (e.g., Raich *et al.*, 1991; McGuire *et al.*, 1992; Zhuang et al., 2003) or calibrated for specific crops (e.g., Qin et al., 2011; Qin et al., 2012; Zhuang et al., 2013) in previous studies. The AgTEM version used here has been validated against observations from maize, switchgrass and *Miscanthus* ecosystems. More information regarding AgTEM can be found in Chapter 2 and Qin *et al*. (2013a).

3.2.2 Regional Simulations on Crop Biomass and GHG Fluxes

We assume that conventional grain crop, maize, and two cellulosic crops, switchgrass and *Miscanthus* will be grown separately as potential energy crops on currently available maize-producing areas in the conterminous United States (**Figure** 3.1). Using spatially referenced data on location, climate, soil and vegetation, the AgTEM was applied to simulate crop growth and C and N dynamics for each of these three cropping scenarios (i.e., maize, switchgrass and *Miscanthus*). Spatial analyses were then conducted at both grid- and national-levels to assess biomass production and GHG emissions.

Spatial forcing data describing climate, CO_2, soils, vegetation conditions and agricultural management were collected and organized at a 0.25° latitude × 0.25° longitude resolution for the study area. Specifically, climate data including the air temperature, precipitation and cloudiness were obtained from the ECMWF (European Centre for Medium-Range Weather Forecasts) Data Server (www.ecmwf.int) and organized at a temporal resolution of one day from 1989 to 2008. CO_2 data were derived from averaged annual atmospheric CO_2 concentrations collected from the NOAA Mauna Loa CO_2 record (www.esrl.noaa.gov/gmd/ccgg/trends/). The original elevation data were derived from the Shuttle Radar Topography Mission (SRTM) (Farr *et al.*, 2007) and soil texture data were based on the Food and Agriculture Organization/Civil Service Reform Committee (FAO/CSRC) digitization of the FAO/UNESCO soil map of the World (1971). Vegetation data describing the current maize crop distribution (2000) in the conterminous United States (**Figure** 3.1) were extracted from a global crop harvest area database (Monfreda *et al.*, 2008). For agricultural management, data indicating irrigation and fertilization were included in the simulations. Irrigation data were obtained from the average irrigation data in the USGS county-level database of estimated use of water in the United States (2005) (Kenny *et al.*, 2009). Since no data were available concerning the spatial heterogeneity of the N fertilization rate among different bioenergy crops, we selected the fixed N input as forcing data. However, to be more realistic, several different levels of N rate were assumed in simulations to examine crop response to N input. For maize, four N input levels were set at 0 (N0), 67 (N1), 134 (N2) and 246 g N ha^{-1} yr^{-1} (N3) according to field experiments (Mosier *et al.*, 2006; Halvorson *et al.*, 2008; Halvorson *et al.*, 2010). Switchgrass and *Miscanthus* require less N inputs, with normal rates of 50-60 g N ha^{-1} yr^{-1} in many experimental tests (Fike *et al.*, 2006b; Behnke *et al.*, 2012). We set two levels at 0 (N0) and 67 g N ha^{-1} yr^{-1} (N1) to be comparable with maize.

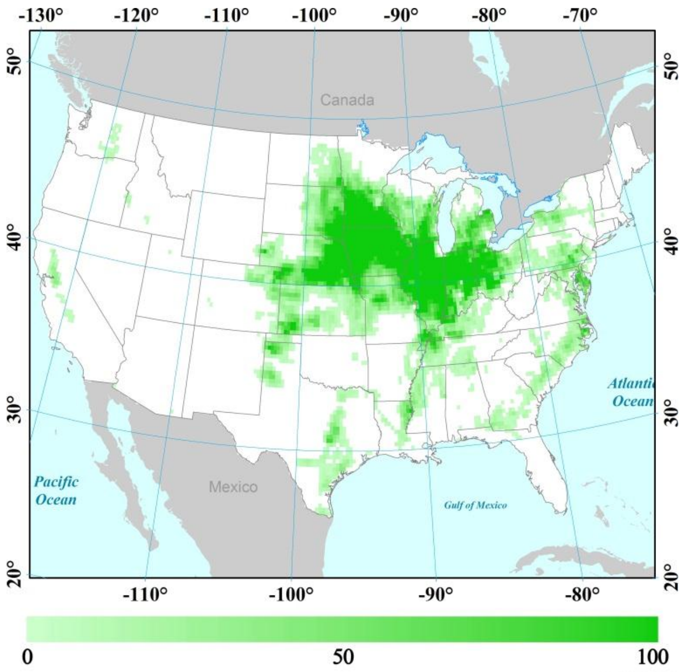

Figure 3.1 Maize cropland in the conterminous United States in the year 2000. Value shows the harvested area as the proportion of each grid cell (%). Data are derived from Monfreda *et al.* (2008).

To conduct regional simulations separately for maize, switchgrass and *Miscanthus*, we ran AgTEM grid-by-grid to estimate spatial C and N dynamics at a daily time step from 1989 to 2008. For each land cover scenario under certain N input levels, we first ran AgTEM to equilibrium using the first year data to determine the initial conditions, and then spun-up the model for 100 years repeatedly using the first 10 years' data to reach equilibrium. Finally the transient simulations from 1989 to 2008 were conducted to estimate changes of C and N fluxes and pools. Spatial analyses for both grid-level and national level were presented as average of the 1990s.

3.2.3 Evaluation of Biofuel Production, GHG Emissions and Global Warming Intensity

Bioethanol produced from biomass feedstocks, either maize grain or cellulosic biomass, is determined by the biomass-to-biofuel conversion efficiency, which varies between feedstock types and may also change due to technology advances. For maize, both grain and biomass can be used as feedstocks, but for switchgrass and *Miscanthus*, only biomass is usable (**Table** 3.1, *HI* of grain is unavailable or set to zero). Currently, conversion technology for conventional biofuels is relatively well established. For example, about 416 liter (L) of ethanol can be produced from each ton (1t = 1 Mg) of maize grain (Lynd *et al*., 2008). But technology of biomass conversion to second-generation biofuel is still new, and the conversion efficiency is relatively low, only two thirds of that for maize grain (**Table** 3.1). However, the conversion efficiency could be improved due to future technology advances, especially for cellulosic biomass. It is expected that, under improved efficiencies, cellulosic biomass could yield 40% more ethanol per unit feedstock than current production, while maize grain may increase only 2% in productivity (**Table** 3.1), making cellulosic crops very competitive to maize grain (Lynd *et al.*, 2008; Fargione *et al.*, 2010). In this study, we estimated biofuel productivity using both current and potential conversion efficiencies.

CO_2 and N_2O are two major GHG in agroecosystems contributing to climate change (Bondeau *et al.*, 2007; Smith *et al.*, 2012). The net production of these GHG was assessed separately, as the C or N balance at ecosystem scales. The contribution of GHG to climate warming was evaluated as global warming potential (GWP), which measures relative amounts of heat trapped by greenhouse gas in the atmosphere. The GWP of N_2O, in this study, was calculated in units of CO_2 equivalents (CO_2eq) over a 100-year time horizon assuming that one unit of N_2O mass is equivalent to 298 units of CO_2 (Forster *et al.*, 2007). For each ecosystem, the combined GWP for CO_2 and N_2O emissions was calculated as sum of contributions from NCE and N_2O produced in nitrification and denitrification (N2O):

$$GWP_{tot} = \underbrace{-NCE \times \frac{44}{12}}_{GWP_{CO2}} + \underbrace{298 \times N2O \times \frac{44}{28}}_{GWP_{N2O}} \qquad (3.1)$$

where GWP_{tot}, GWP_{CO2} and GWP_{N2O} are GWP for total GHG, CO_2 and N_2O, respectively. Positive GWP indicates a net GHG source, and a negative value refers to a net GHG sink of any particular ecosystem.

Table 3.1 Parameters used to estimate biomass harvest and biofuel production

	HI^*		$C_{bio,crt}^{\dagger}$		$C_{bio,ptn}^{\ddagger}$	
	Grain	Biomass	Grain	Biomass	Grain	Biomass
Maize	0.53	0.14	416	282	424	399
Cellulosic crop	--	0.90	--	282	--	399

[*] *HI*, harvest index as defined in Qin *et al.*, 2013, dimensionless.

[†] $C_{bio,crt}$ and [‡] $C_{bio,ptn}$ are current and potential biomass-to-biofuel conversion efficiencies, respectively, L ethanol Mg^{-1} biomass. Cellulosic crops refer to switchgrass and *Miscanthus* in the study. References and data sources: Hicke et al., 2004; Lynd et al., 2008; Fargione et al., 2010; Meyer *et al.*, 2010; Payne, 2010.

In order to relate agricultural practices to GWP, many studies used the term greenhouse gas intensity or global warming intensity by dividing GWP by crop yield (e.g., grain yield for maize) (Grassini & Cassman, 2012; Linquist *et al.*, 2012). Instead of relating GWP to crop yield, we applied a similar approach to address the contribution of GHG relative to biofuel yield. As in Eqn. (3.2), GWP_i is the global warming intensity in terms of total GWP for CO_2 and N_2O relative to biofuel produced (YLD_{bio}). For maize, switchgrass and *Miscanthus* studied here, the biofuel is referred to ethanol and the units for GWP_i are kg CO_2eq L^{-1} E. A positive GWP_i value indicates a net source of CO_2 equivalents per unit of ethanol yield and a negative value indicates net sinks of GHG to the ecosystem.

$$GWP_i = \frac{GWP_{tot}}{YLD_{bio}} \tag{3.2}$$

3.3 Results

3.3.1 Role of N Fertilization in Biomass and Biofuel Production

To examine the response of crop growth to N fertilization, we use grain and biomass production estimated with the model at four N input levels of N0, N1, N2 and N3 (**Table** 3.2, **Figure** B 1a). The national NPP results suggest that, maize is most sensitive to N rates among these bioenergy crops, and cellulosic crops, especially *Miscanthus,* are relatively less sensitive to changing N input. Maize is capable of producing 326 g C m^{-2} of NPP each year without N application, and additional 1.1-2.0 g C m^{-2} for each kg N fertilizer added. When the N rate is relatively high (e.g., N3 of 246 kg N ha^{-1} yr^{-1}) such that crop growth may no longer be limited by N, maize can reach a national average NPP

Table 3.2 Model estimated annual net primary production (NPP), crop grain yield and harvestable biomass yield of bioenergy crops, in the conterminous United States

N input[*]	NPP (g C m^{-2} yr^{-1})			Harvest (Mg DM ha^{-1} yr^{-1}) [†]			
	Maize	Switch-grass	*Miscan-thus*	Maize grain	Maize biomass[‡]	Switch-grass	*Miscan-thus*
N0	326 (38)	473 (56)	1440 (119)	3.3 (0.4)	0.9 (0.1)	5.5 (0.6)	20.5 (2.0)
N1	403 (42)	681 (59)	1482 (153)	4.0 (0.4)	1.1 (0.1)	7.9 (0.7)	21.1 (2.2)
N2	552 (52)	--	--	5.5 (0.5)	1.5 (0.1)	--	--
N3	702 (79)	--	--	7.0 (0.8)	1.9 (0.2)	--	--

[*] N0, N1, N2 and N3 are N input levels at 0, 67, 134 and 246 kg N ha^{-1} yr^{-1}, respectively; same hereafter in all tables and figures. Values presented are 10-yr mean (SD, standard deviation) of the 1990s and may not total precisely due to rounding; same in **Table** 3.3 and 3.4.

[†] DM, dry matter.

[‡] About 30% of total aboveground biomass (excluding grain) were harvested, and the rest were returned to soil for soil fertility sustainability (Payne, 2010).

of 702 g C m^{-2} yr^{-1}. Switchgrass responds positively to N addition at low N input levels, and reaches its relatively high production level at N1. *Miscanthus*, however, does not respond to N addition at a significant level; its productivity is relatively stable with or without N application (**Table** 3.2, **Figure** B 1a). According to the fertilizer consumption and use for maize (USDA, 2012), the N application rate in the United States varies among regions, roughly ranging from 70-180 kg N ha^{-1} yr^{-1} in the 1990s, which is in between our estimates of N levels at N2 and N3. The model estimated crop NPP of 552-702 g C m^{-2} yr^{-1} with fertilizer input between N2 and N3 is comparable with NPP from national statistical data (FAOSTAT, 2012) of 540-730 g C m^{-2} yr^{-1} in the 1990s. The estimated biomass production of switchgrass at N1 and *Miscanthus* at N0 is also close to field observations (Fike *et al.*, 2006b; Heaton *et al.*, 2008; McIsaac *et al.*, 2010; Nikièma *et al.*, 2011). Our study suggests that the modeled N fertilization levels of N2-N3 for maize, N1 for switchgrass and N0 for *Miscanthus* may be reasonable to inform the current productivity of these biofuel crops in the United States.

Cellulosic crops generally have higher biomass production than maize. For example, with 67 kg N ha^{-1} N application, switchgrass produces 70% higher NPP than maize and *Miscanthus* produces twice as much NPP as switchgrass (**Table** 3.2). However, considering potential maize production from N addition, switchgrass may not necessarily be more productive than maize. *Miscanthus* can produce over 20 Mg of dry matter for each hectare of land, which is about twice as much as switchgrass or maize could produce at their highest productivity (**Table** 3.2). In terms of biofuel production, conversion efficiency is another factor determining the difference in productivity among crops. Maize, with relatively low biomass production, may produce considerable biofuel, compared with switchgrass; maize grain produces more unit-land-based ethanol than cellulosic biomass does. With an increasing N input, maize-based biofuel yield increases.

Maize has the highest biofuel production at N3, producing about 2.7 and 3.5 kL ethanol per hectare of land, under current and potential conversion technologies, respectively (**Figure** 3.2). Compared with maize, switchgrass is comparably productive when they are both grown under low N levels (i.e., N0, N1). Because of its high biomass production, *Miscanthus* is still the most productive crop for biofuel among the three crops. Without N application, *Miscanthus* can produce 5.8-8.2 kL ethanol ha^{-1}, depending on conversion technology. For *Miscanthus*, N fertilization does not affect its biofuel production as much as that for maize (**Figure** 3.2).

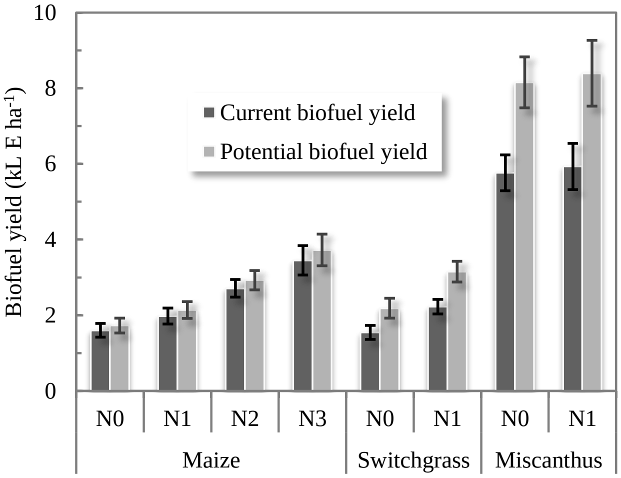

Figure 3.2 Estimated biofuel produced from the maize, switchgrass and *Miscanthus* ecosystems. Estimates are made for both grain and harvestable biomass for maize, and for harvestable biomass for switchgrass and *Miscanthus*. Error bar indicates standard deviation.

3.3.2 Ecosystem C Balance in the Bioenergy Ecosystems

Ecosystem C balance, accounting for net CO_2 exchange between the atmosphere and ecosystems, varies temporally and spatially under changing environment, such as climate and soil conditions. The annual NCE of any specific site/grid could be either negative or positive and its interannual variability depends on environmental factors (McGuire *et al.*, 2001). The average NCE across multiple years is mainly determined by management and land-use change, instead of natural causes such as interannual climate variations (**Figure** 3.3). Generally, by growing maize and harvesting grain and biomass for biofuel use, the regional NCE tends to be negative in the Midwest areas where most maize is produced, and mostly positive in the southern regions (**Figure** 3.3). That is, intensive maize cropping tends to result in a C source. With increasing use of N fertilizer, the spatial NCE changes dramatically. In many areas, C sinks weaken. For instance, as N rate increases from N0 to N1, the NCE of many areas in Kansas and Missouri states decreases from over 40 g C m^{-2} yr^{-1} (**Figure** 3.3a) to less than 20 g C m^{-2} yr^{-1} (**Figure** 3.3b). Some C sink areas even become net sources. For example, the NCE of Texas is above 80 g C m^{-2} yr^{-1} at zero N rate (**Figure** 3.3a), and decreases to -10 to -40 g C m^{-2} yr^{-1} when N rate increases to N3 (**Figure** 3.3d). In contrast with the maize ecosystem, cellulosic crop ecosystems sequester more C than they release in intensively cropped areas. For switchgrass, most areas act as or near C neutral, with 0 to ±5 g C m^{-2} yr^{-1} of NCE, when there is no N application (**Figure** 3.4a). With the N rate increase to N1, the NCE-positive areas are strengthened and become relatively stronger C sinks (**Figure** 3.4b). For *Miscanthus*, the N application does not impact the C balance significantly. In the crop intensive areas, the NCE is mostly above 20 g C m^{-2} yr^{-1}, and even reaches 160 g C m^{-2}

yr^{-1} in some scattered areas in the Midwest (**Figure** 3.4c). With additional N fertilizer application, only part of southern regions lower than 35°N (e.g., Texas and Mississippi states) changes from a C sink to a source (**Figure** 3.4c, 3.4d).

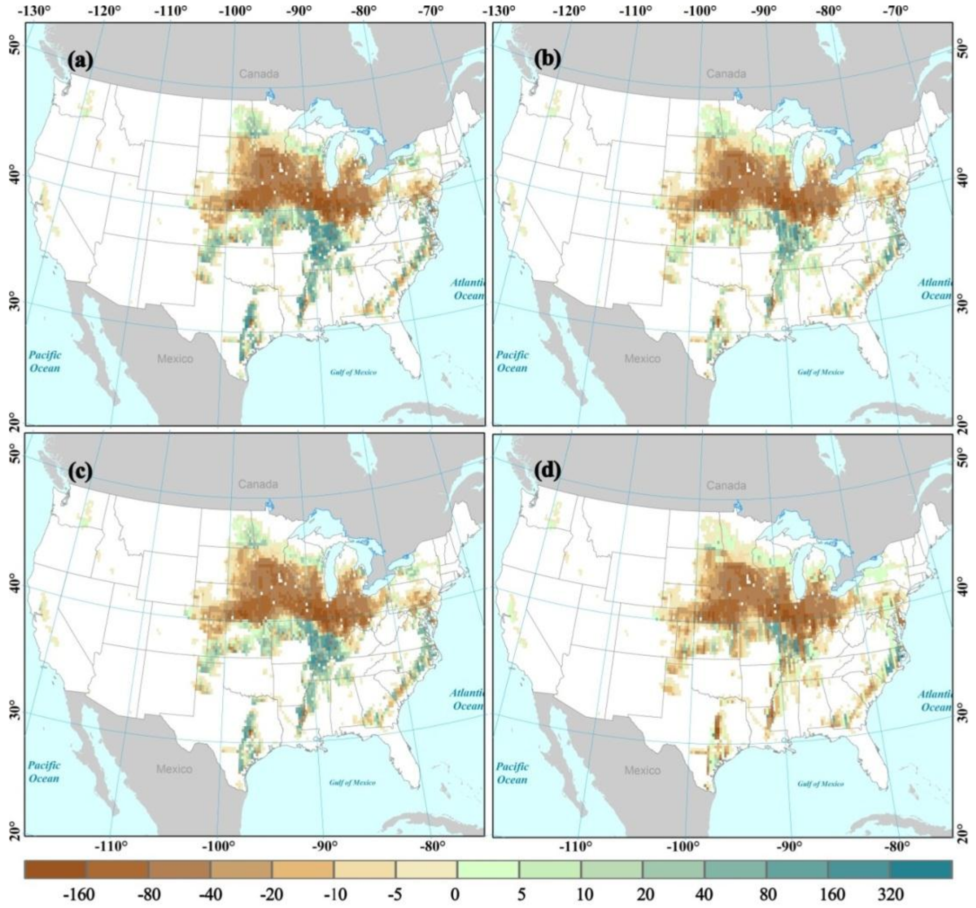

Figure 3.3 Annual net carbon exchange estimated for maize produced in the conterminous United States. The NCE fluxes (g C m^{-2} yr^{-1}) at different N input levels (a) N0, (b) N1, (c) N2 and (d) N3 are presented as averages of the 1990s. A positive NCE indicates a net CO_2 sink whereas a negative value indicates a net CO_2 source. Value presented are weighted by cropland area; same hereafter in **Figure** 3.4-3.6, unless otherwise stated.

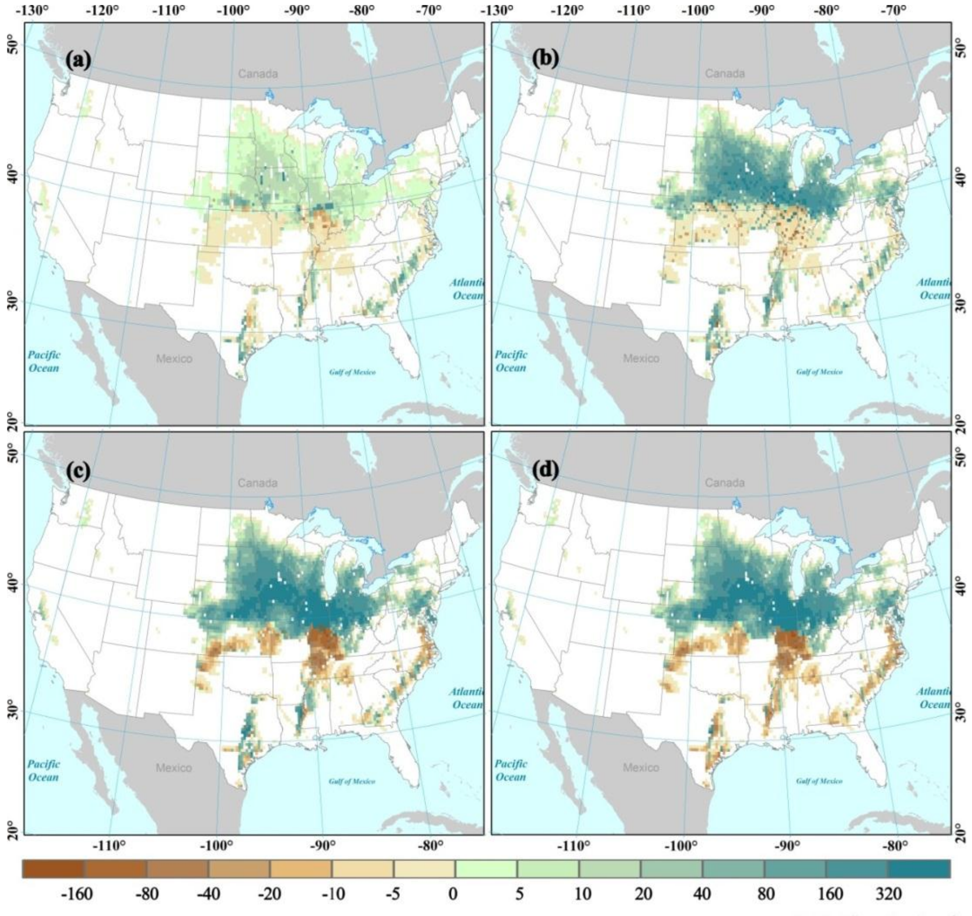

Figure 3.4 Annual net carbon exchange estimated for switchgrass and *Miscanthus* produced in the conterminous United States. The NCE fluxes (g C m^{-2} yr^{-1}) are presented for switchgrass at N input levels (a) N0 and (b) N1 and for *Miscanthus* at (c) N0 and (d) N1. A positive NCE indicates a net CO_2 sink whereas a negative value indicates a net CO_2 source.

Nationally, cellulosic crop-based ecosystems act as a net C sink and maize-based ecosystems as a net C source (**Table** 3.3). Maize ecosystems emit C at an average of 0.9-2.3 g C m^{-2} yr^{-1} or a total of 0.3-0.7 Tg C each year, depending on the actual N inputs. Switchgrass has an annual NCE of 0.8 g C m^{-2} without N application or 5.4 g C m^{-2} with moderate N input. *Miscanthus* holds a relatively high NCE of over 10 g C m^{-2} yr^{-1}, regardless of N fertilization. If growing *Miscanthus* on all currently available maize cropland areas, the C sink would reach more than 3 Tg C each year.

Table 3.3 Estimated average and total net carbon exchange (NCE) at different N input levels in the conterminous United States

N input	Average NCE (g C m^{-2} yr^{-1})			Total NCE (Tg C yr^{-1})		
	Maize	Switch-grass	*Miscanthus*	Maize	Switch-grass	*Miscanthus*
N0	-0.88 (0.09)	0.81 (0.09)	10.71 (1.20)	-0.27 (0.03)	0.25 (0.03)	3.31 (0.38)
N1	-1.46 (0.16)	5.38 (0.60)	10.42 (1.12)	-0.45 (0.05)	1.66 (0.18)	3.22 (0.35)
N2	-1.90 (0.20)	--	--	-0.59 (0.06)	--	--
N3	-2.34 (0.28)	--	--	-0.72 (0.08)	--	--

3.3.3 Potential N_2O Emissions from Bioenergy Ecosystems

Maize ecosystems release enormous amounts of N_2O, especially for regions with intensive cropping and high N fertilization rates. As a reference, the scenarios with no N application (N0) indicate background emissions of N_2O. For maize, the background N_2O is mostly 0.01-0.07 g N m^{-2} yr^{-1} as weighted by cropland area. The central Midwest has relatively higher N_2O fluxes because more maize is produced in these areas (**Figure** 3.5a).

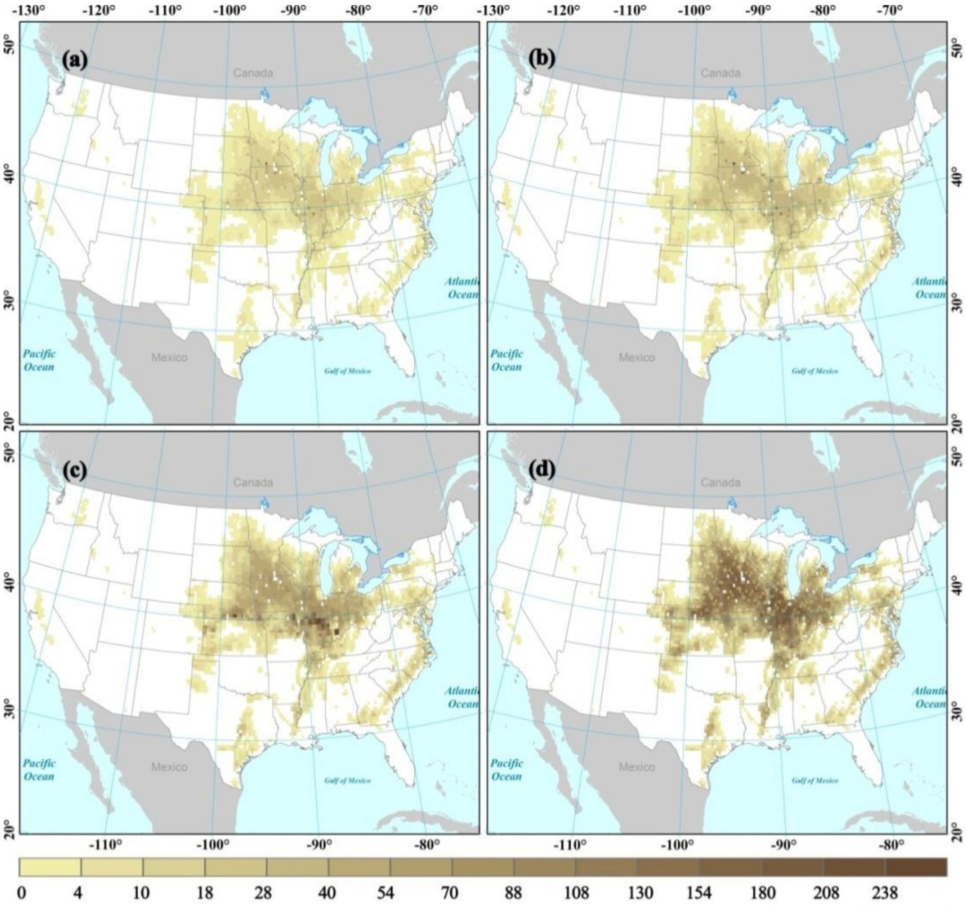

Figure 3.5 Annual N_2O fluxes estimated for maize produced in the conterminous United States. Same N input levels as in **Figure** 3.3. Unit: 10^{-3} g N m^{-2} yr^{-1}.

Over the maize-producing areas, the average N_2O emissions are 0.06 g N m^{-2} yr^{-1} with a large variance of 0.01 g N m^{-2} yr^{-1} due to interannual variation and spatial heterogeneity (**Table** 3.4). With increasing use of N fertilizer, the N_2O emissions increase dramatically, especially in areas with already high N_2O fluxes. Nationally, the average annual N_2O flux is 0.1 g N m^{-2} at the N1 level (**Figure** 3.5b), and increases by 124% when N fertilizer doubled (**Figure** 3.5c). When maize is grown under the highest N input scenario (N3),

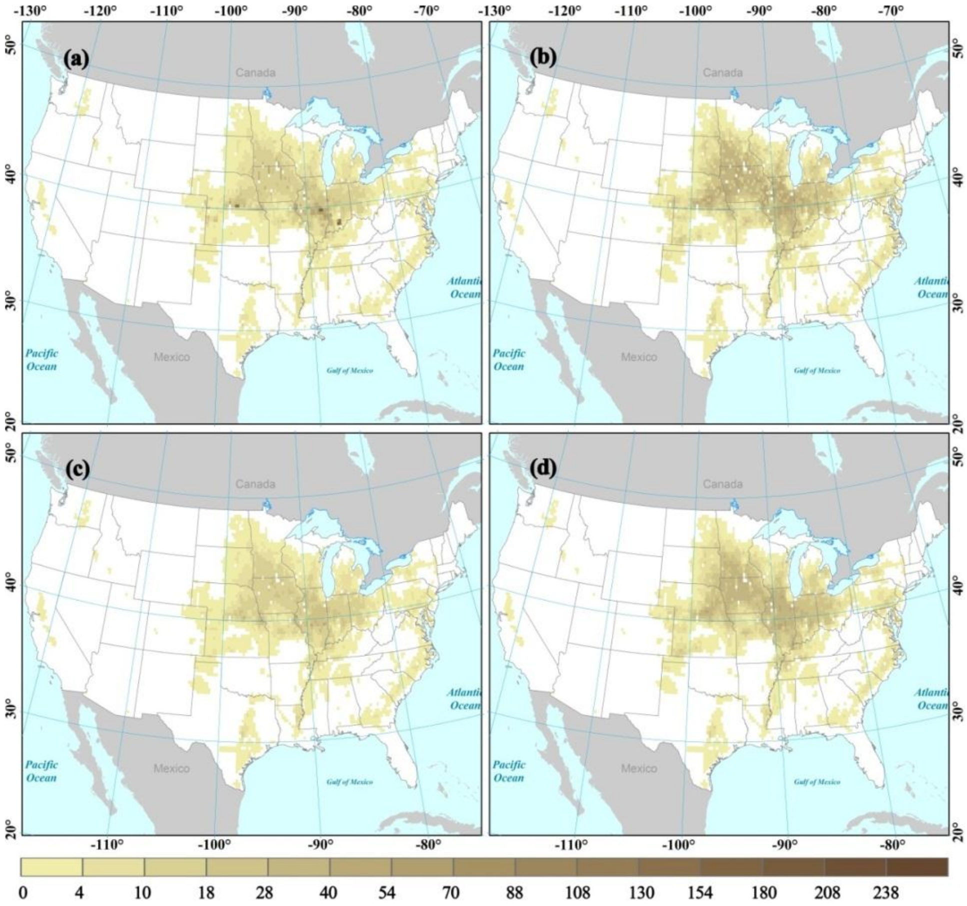

Figure 3.6 Annual N_2O fluxes estimated for switchgrass and *Miscanthus* produced in the conterminous United States. Same N input levels for switchgrass and *Miscanthus* as in **Figure** 3.4. Unit: 10^{-3} g N m^{-2} yr^{-1}.

N_2O emissions could reach a national average of 0.45 (±0.1) g N m^{-2} yr^{-1}, about 7.5 times that of the reference scenario (**Table** 3.4).

Similar to maize ecosystems, ecosystems of cellulosic crops also release N_2O. However, the total amount of N_2O emissions can decrease due to reduced use of N fertilizer. Spatially, the annual N_2O fluxes of cellulosic crops share a common pattern with maize, with higher emissions in the intensively cropped areas than areas with only small proportion of cropping (**Figure** 3.6). Nationally, switchgrass and *Miscanthus* have comparable N_2O fluxes with maize, about 0.05-0.11 g N m^{-2} each year depending on crop type and N applied (**Table** 3.4). The N_2O emission intensities, in terms of N_2O emissions per unit of land at the same N application rate, of switchgrass (**Figure** 3.6a, 3.6b) and *Miscanthus* (**Figure** 3.6c, 3.6d) are close to that of maize (**Figure** 3.5a, 3.5b). However, in order to maintain a reasonably high yield, maize requires much more N input than switchgrass and *Miscanthus*, and the additional use of N fertilizer significantly increases N_2O emissions.

Table 3.4 Estimated average N_2O fluxes and total N_2O emissions at different N input levels in the conterminous United States

N input	Average N_2O flux (g N m^{-2} yr^{-1})			Total N_2O emissions (Gg N yr^{-1})		
	Maize	Switchgrass	*Miscanthus*	Maize	Switchgrass	*Miscanthus*
N0	0.06	0.05	0.05	18.4	17.0	15.8
	(0.01)	(0.01)	(0.02)	(3.7)	(3.4)	(3.2)
N1	0.10	0.11	0.09	29.5	33.4	28.8
	(0.02)	(0.02)	(0.01)	(5.9)	(6.7)	(5.8)
N2	0.22	--	--	66.4	--	--
	(0.04)			(13.3)		
N3	0.45	--	--	138.0	--	--
	(0.09)			(27.6)		

Growing switchgrass and *Miscanthus* could remarkably reduce N_2O emissions, which would otherwise be emitted by growing maize at the national level. At N2-N3 input levels, the total N_2O emissions would reach 66-138 Gg N, which is about 1/3 to 2/3 of the total soil N_2O emissions from major commodity crops in 2007 (201 GgN) (Del Grosso *et al.*, 2010). However, if maize is replaced with cellulosic crops, the N_2O emissions will be greatly reduced (**Table** 3.4). Growing switchgrass across the United States results in N_2O emissions of 33 Gg N at the most. If *Miscanthus* is substituted for maize, the total N_2O emissions will be even less (16 Gg N) when N is not applied, and yet the biomass production will not be greatly affected.

3.3.4 GHG Emissions and Global Warming Intensity

GHG emissions, especially N_2O emissions caused mainly by N fertilizer use, directly contribute to global warming potentials (Mosier *et al.*, 2006; Adviento-Borbe *et al.*, 2007). By summing up contributions from both NCE and N_2O sources, we separately estimated the total GWP for the three ecosystems considering plant growth throughout the growing stage, crop harvest, and management practices (**Figure** 3.7a). Over currently available maize-producing areas in the United States, maize ecosystems in general act as net sources for both CO_2 and N_2O. N_2O emissions, in particular, dominate the GWP in maize, contributing over 90% of CO_2eq per unit land. With increasing N input, the proportion of GWP from N_2O also increases. At the reference scenario N0, the total GWP is about 0.3 Mg CO_2eq ha^{-1} yr^{-1}, but when the N input increases to relatively high levels (e.g., N2, N3), the total GWP would be enhanced significantly, reaching 1.1-2.2 Mg CO_2eq ha^{-1} yr^{-1} (**Figure** B 1b), close to an earlier estimate with a global average GWP of

1.4 (±0.4) Mg CO_2eq ha^{-1} yr^{-1} for the maize ecosystem (Linquist *et al.*, 2012). For cellulosic crops, the ecosystem NCE is positive and therefore offsets the GWP caused by N_2O emissions. In the switchgrass ecosystem, the total GWP is 0.2 Mg CO_2eq ha^{-1} yr^{-1} at the N0 level and 0.3 Mg CO_2eq ha^{-1} yr^{-1} at the N1 level (**Figure** B 1b). For the *Miscanthus* ecosystem, at the N0 level, the GWP of CO_2 overweighs GWP of N_2O, resulting in a net GWP of -0.2 Mg CO_2eq ha^{-1} yr^{-1} (**Figure** B 1b). Growing *Miscanthus* without N application could eventually mitigate global warming. Even with N application, the net GWP in *Miscanthus* is still much lower than in maize.

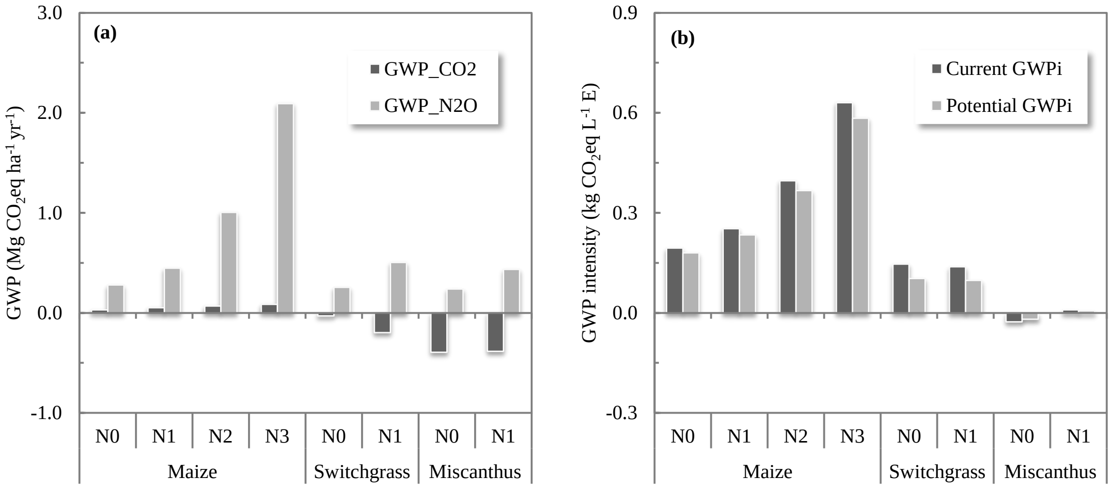

Figure 3.7 National average global warming potential and global warming intensity by developing maize, switchgrass and *Miscanthus* for bioenergy purpose. (a) Global warming potential (GWP) is for CO_2 and N_2O at different N input levels, and (b) global warming intensity (GWP_i) is GWP per unit biofuel produced under current or potential biomass-biofuel conversion efficiencies.

Taking biofuel productivity into consideration, *GWPi* measures the relative GWP with respect to ethanol production (**Figure** 3.7b). Our estimates over the United States indicate that, maize has the highest GWPi at all N levels, ranging from 0.2 kg CO_2eq L^{-1} E at the N0 level to 0.6 kg CO_2eq L^{-1} E at the N3 level. GWPi increases with increasing N input, suggesting that the marginal rate of GHG emission outpaces that of ethanol production when the N level changes. However, in switchgrass ecosystems, the GWPi at N1 is slightly lower than at N0 because the biofuel production increases greatly due to N application. By growing *Miscanthus* to produce biofuel, for each liter ethanol produced, the ecosystem generates 19-27 g CO_2eq of GHG "credit" by sequestering C into agroecosystems if no N applied. The ecosystem will release only 6-9 g CO_2eq of GHG if N is applied. This suggests that, substituting cellulosic crops for maize could make a great difference in reducing GHG emissions and therefore mitigating GWP. To produce one liter of ethanol under current technology, using switchgrass instead of maize would reduce 200-500 g CO_2eq of GHG emissions, and using *Miscanthus* would reduce an additional 100 g CO_2eq. Among the three bioenergy crops, *Miscanthus* produces the highest amount of biofuel and emits the lowest GHG using the same cropland.

3.4 Discussion

3.4.1 Advantages and Disadvantages of Cellulosic Crops

Cellulosic crops, especially *Miscanthus*, can produce a comparable amount of biomass and yet release much less GHG than maize. High solar radiation interception and conversion of cellulosic crops is one of the most important characteristics contributing to their high productivity (Heaton *et al.*, 2008). *Miscanthus*'s larger leaf area and longer duration outweighs maize in terms of the full potential of C4 photosynthetic productivity (Dohleman & Long, 2009). Even using the same NADP-malic enzyme C4 pathway, *Miscanthus* can maintain high photosynthetic quantum yields and biomass productivity in relatively unfavorable climate (e.g., low temperature) where maize growth is highly limited (Naidu *et al.*, 2003). In addition, switchgrass and *Miscanthus* are tolerant to marginal soils, due to their relatively low demand of nutrient and highly efficient use of water. In fact, irrigation and fertilization are less frequently applied to switchgrass and *Miscanthus* than to maize (Lewandowski *et al.*, 2003; Fike *et al.*, 2006a; Stewart *et al.*, 2009). This makes switchgrass and *Miscanthus* promising bioenergy crops in areas beyond current cropland area, especially those with less favorable climate and soil conditions for food crops.

One major difference between maize crop and cellulosic crops is that maize is an annual plant and survives for just one growing season, while switchgrass and *Miscanthus* are perennial plants. Maize is grown and eventually harvested and part of its biomass (e.g., residues) is left to maintain soil fertility (e.g., soil C). From the perspective of long-term C cycling, in the maize ecosystems, CO_2 sequestered from atmosphere is eventually released through respiration, decomposition, harvest and burning, leaving only a small proportion of C stored in soils (Verma *et al.*, 2005; West *et al.* 2010). Perennial plants, however, accumulate C into their roots in addition to soils, and the vegetation C pools could also contribute to the ecosystem C sink (Stewart *et al.*, 2009). The GHG emissions from agroecosystems are mostly from N_2O fluxes caused by excessive use of N fertilizer. Switchgrass and *Miscanthus* release the amount of N2O similar to maize at a given N input (**Table** 3.4), but the formers require much less N than maize to produce the same or even high amounts of biomass. This makes these cellulosic crops favorable in reducing N_2O emissions while having the same amount of biomass. This may also partly explain the observations that the emission factor for switchgrass and *Miscanthus* is close to, if not larger than, that for maize (Qin *et al.* 2013a).

However, it should be noted that large-scale commercialization and long-term ecological sustainability are still issues for growing cellulosic crops. For example, the widely studied *Miscanthus* × *giganteus* is a primary hybrid being selected as a potential energy crop, but its mass propagation may involve high costs (Stewart *et al.*, 2009). Growing cellulosic crops on cropland may compete with food crops for land, water and nutrient resources, and jeopardize food security (Fargione *et al.*, 2010). Indirect land-use change due to bioenergy expansion may also impact ecological biodiversity and ecosystem services (Tilman *et al.*, 2009; Dale et al., 2010). Large-scale cropping may lead to monoculture and destroy habitat of other species; additional use of labor and transport due to massive biomass production and harvest may cause indirect emissions of GHG (e.g., Hill *et al.*, 2009).

3.4.2 Global Warming Potential under 2022 Bioenergy Goal

To evaluate the economics of producing biomass-based ethanol to achieve the 2022 biofuel mandate, we calculated the demand of biomass and land, and also potential GHG emissions as a consequence of growing bioenergy crops (**Table** 3.5, **Figure** B 1c, d). Given currently available technologies, we need to use 191 Tg maize grain to produce the 79 billion liters of cellulosic ethanol, about 27-35 Mha cropland will be needed to support the crop biomass production. That is, if by applying low-N management, the current maize cropland (31 Mha) is insufficient to meet the biofuel production goal, or by using high-N input, 88% of the maize cropland would be needed for biofuel purposes. Using

Table 3.5 Resources needed and GHG produced to reach the 2022 bioenergy goal

	Under current technology			Under potential technology		
Feedstock	Biomass (Tg DM)	Land (Mha)	GHG (Tg CO_2eq)	Biomass (Tg DM)	Land (Mha)	GHG (Tg CO_2eq)
Low-N fertilizer application[*]						
Maize grain	191	34.6	37.2	187	33.9	36.5
Maize total[†]	205	29.3	31.5	190	27.1	29.2
Switchgrass	282	51.4	11.7	199	36.3	8.2
Miscanthus	282	13.8	-2.1	199	9.7	-1.5
High-N fertilizer application[*]						
Maize grain	191	27.2	59.2	187	26.7	58.1
Maize total[†]	205	23.0	50.1	190	21.3	46.4
Switchgrass	282	35.7	11.0	199	25.2	7.8
Miscanthus	282	13.4	0.7	199	9.5	0.5

[*] Low-N scenarios are N2, N0 and N0 for maize, switchgrass and *Miscanthus*, respectively; and high-N scenarios are N3, N1 and N1 for maize, switchgrass and *Miscanthus*, respectively. Estimates were made for 2022 biofuel target of 79 billion liters of cellulosic ethanol.

[†] Maize total accounts for both grain and biomass harvested.

both maize grain and biomass would still need 23-29 Mha of cropland. If *Miscanthus* were available, a total of 282 Tg of biomass would be needed to produce the mandated ethanol, but only 13-14 Mha cropland would be needed. More than half of current cropland could be saved if *Miscanthus* replaced maize as a biofuel crop. With potentially higher biomass-to-biofuel conversion efficiencies, 21-34 Mha of cropland would still be needed for maize-based ethanol production; N application rate and feedstock type determine the actual share of land for fuel use. However, due to significant advancement of conversion efficiency (**Table** 3.1), by growing *Miscanthus*, less than 10 Mha of cropland would be sufficient, which is only about one third of the currently available maize cropland.

Miscanthus ranks as the lowest GWP contributor among all three crops (**Table** 3.5, **Figure** B 1d). To produce 79 billion liters of ethanol, using maize for biomass feedstocks releases 37-59 Tg CO_2eq of GHG, accounting for 0.7-1.2% of the average national CO_2 emissions produced each year in the 1990s from the burning of fossil fuels and cement manufacture (5.2 Pg CO_2) (UN, 2012). Increasing N use could somewhat improve crop productivity and therefore decrease the land use, but accelerates GHG emissions. In contrast with maize, the *Miscanthus* ecosystem releases a small amount of GHG and even acts as a sink for GHG if no N applied. Substituting *Miscanthus* for maize could reduce GHG emissions equivalent to the annual anthropogenic emissions produced by a small country (e.g., Norway, Denmark) (UN, 2012). Among the three potential bioenergy crops, switchgrass offers significant GHG savings but has the least biofuel productivity and therefore used the largest amount of cropland (**Table** 3.5). It may not be economically reasonable to substitute switchgrass for maize when grown on cropland.

3.4.3 What Other Options Do We Have for Bioenergy Development?

Land availability is a primary factor limiting biomass-based biofuel production. There is a total land area of nearly 0.92 billion hectares in the United States (2007), of which most are forestland, grassland and rangeland (57%), and only a small portion (18%) is used as cropland for crops, pasture or other purposes (Nickerson *et al.*, 2011). Considering possible economic, societal and environmental problems such as food insecurity (Fargione *et al.*, 2010), indirect land-use change and associated C emissions (Searchinger *et al.*, 2008; Melillo *et al.*, 2009), using food grain to produce biofuel or switching productive food-based cropland to biofuel-based cropland is not a sustainable option for long-term energy supply from biofuel. Thus, the less productive land, or marginal land, seems to be a promising alternative for growing bioenergy crops. Marginal land usually has little or no potential for profit, and often has poor soil or other undesirable characteristics for growing food crops, but some marginal land can be further developed for growing cellulosic crops which require relatively less nutrients and water than food crops (Fargione *et al.*, 2010; Qin *et al.*, 2011; Gelfand *et al.*, 2013). By classifying the land productivity according to soil productivity, topography, climate regimes and other indicators, Cai *et al*. (2011) estimated a total of 43-123 Mha of land with marginal productivity in the United States. Other possible land sources including abandoned agricultural lands (Campbell *et al*., 2008), degraded grassland (Wicke *et al*., 2011) and Conservation Reserve Program grassland (Lee *et al*., 2013) may also contribute to the production of biomass. With crop-specific selection, these lands may potentially serve as land sources for planting cellulosic crops. Under these circumstances, *Miscanthus* or even switchgrass could be much more productive and environmentally sustainable than maize.

Using maize grain to produce ethanol could still reduce the GHG emissions by breeding a high-yield maize hybrid and improving agricultural management. An estimate based on on-farm data indicated that high-yield maize may receive large N fertilizer and irrigation water inputs, but could achieve higher grain and net energy yields (i.e., energy produced per unit land) and lower GHG intensity in terms of GHG emissions per unit maize yield than the regularly reported US maize system (Grassini & Cassman, 2012). Management practices, such as rotation (Halvorson *et al.*, 2008), tillage (Halvorson *et al.*, 2006; Omonode *et al.*, 2011), irrigation and residue return (Liu *et al.*, 2011) could directly or indirectly affect the ecosystem C balance and N_2O emissions (Venterea *et al.*, 2012). Fertilizer N type, timing, placement, as well as N rate, may also affect N_2O emissions (Bouwman *et al.*, 2002; Millar *et al.*, 2010). Nitrification inhibitor (e.g., nitrapyrin) has been reported to be effective in prohibiting NO_3^- from accumulating in the soil (Bronson *et al.*, 1992), reducing N_2O emissions (Zaman *et al.*, 2009). By improving management practices, the existing maize-based biofuel cropland may eventually be able to reduce its GHG emissions.

It is worth noting that, the actual N rate for maximum biomass production may vary over space, depending on local plant uptake, soil N availability and N loss. It is possible that some locations may still respond to N levels higher than what we set in this study. Switchgrass, for instance, shows significant responses to N application (e.g., **Table** 3.2). Its biomass potential should be further investigated using long-term experiments with different N application levels. GHG emissions estimated in this study refer to the processes among crop growing stages in the ecosystem. Other processes outside ecosystem, such as fertilizer production, manufacturing, transportation, were not explicitly included. To account for these processes along the biofuel's life "from-cradle-to-grave", we suggest to couple ecosystem modeling results with life cycle assessment (LCA) to assess the efficiency and GHG impact of energy systems (Hillier *et al.*, 2009; Davis *et al.*, 2009).

3.4.4 Uncertainties and Future Needs

Agricultural management makes agroecosystem a more complicated system than the natural ecosystems. AgTEM incorporates major management factors, fertilization and irrigation, but other management practices, which may be also important, were not specifically considered due to inconsistent evidence, insufficient understanding (e.g., N type, N timing) (Millar *et al.*, 2010) and data unavailability (e.g., rotation, planting density) (Felzer *et al.*, 2004). This uncertain model structure and complex management could result in estimation uncertainty. In addition, model parameters and forcing data could also contribute to uncertainty (Chen & Zhuang, 2012; Qin *et al.*, 2013). Thus, future study should consider improving the management module in AgTEM. The further uncertainty and sensitivity analysis at large scales should also improve our modeling capability (Qin *et al.*, 2013).

It should also be noted that, ecosystem modeling may be useful for evaluating ecosystem services and environmental impacts, and the results could be informative for policy making concerning energy, food security and sustainability. However, the information derived from multiple-year and large-scale simulations may not be accurate. It should be cautious when using regional estimates to inform site-level practical cropping or agricultural management. Crop models, designed with the specific purpose of advising management practices (e.g., water management, Steduto *et al.*, 2009), together with spatially-explicit high-resolution data, should be more useful for directing agricultural management and practice.

3.5 Conclusion

N fertilizer application stimulates biomass production of maize, but also contributes to the GHG emissions from maize ecosystem. Cellulosic crops, especially *Miscanthus* have no or only moderate productivity response to N fertilization. The maize ecosystem as a whole acts as C source in the United States, while cellulosic crop-based ecosystems act as C sinks; however, the size of C fluxes is very limited compared with the NPP produced. All three ecosystems release an increasing amount of N_2O with increasing use of N fertilizer; the size of separate N_2O fluxes for maize, switchgrass and *Miscanthus* is similar at same N input level. However, to maintain high biomass production, maize in particular requires the highest N input and produces the greatest N_2O emissions. Among all three bioenergy crops considered for growth on cropland, *Miscanthus* is the most biofuel-productive and least GHG-intensive in terms of biofuel production and GHG emissions at a given cropland, respectively. Therefore, substituting *Miscanthus* for maize to producing biofuel could potentially save land and reduce GHG emissions.

3.6 Acknowledgement

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CHAPTER 4. BIOMASS PRODUCTIVITY AND CLIMATE CHANGE MITIGATION IN MARGINAL LANDS

4.1 Introduction

Bioenergy, an important renewable energy produced from biological materials, is becoming an increasingly attractive energy choice in the context of economic development, energy security and climate change. On the one hand, with increasing world population and rapidly growing regional and global economy, conventional fossil fuel-based energy alone is not likely to provide essential and sufficient support to the functioning of modern economies due to limited supply, high or volatile fossil fuel prices and concerns about national energy independence (Field *et al.*, 2008; Hill *et al.*, 2009). On the other hand, the society is increasingly aware of the destructive impacts of conventional energy use on the environment and climate change, and is looking for alternative sources of energy that are renewable and sustainable (Tilman *et al.*, 2009; Fargione *et al.*, 2010). Biofuels, compared with fossil fuels, could potentially support state energy goals, increase domestic energy supplies to reduce dependence on foreign oil and its potential disruptions, and yet reduces GHG emissions and other air pollutants (USDOE, 2011). In the US, only about 10% of total primary energy consumption is from renewable energy sources, but biomass-derived energy makes up about half of the total renewable energy (EIA, 2012). Compared with some other renewable energy alternatives (e.g., wind, solar power), bioenergy may be one of the most viable options to adopt in the near term (USEPA, 2009).

In order to meet ambitious mandate targets for biofuel production (US Congress, 2007), large amount of lands will be needed to grow energy crops for biomass feedstocks Among lands that can be used for production of biofuel feedstocks, marginal lands were often introduced as the last land option for energy cropping purpose, considering that switching food crops to biofuel crops to produce biomass on currently available croplands may raise concerns about food insecurity, unsustainable environment and other ethical and nutritional issues (Field *et al.*, 2008; Tilman *et al.*, 2009; Fargione *et al.*, 2010; Gramig *et al.*, 2013), while converting lands occupied by natural ecosystems (e.g., forest) to biofuel cropland could inevitably cause environmental and ecological problems such as deforestation, biodiversity loss, habitat fragmentation and land-use change induced GHG emissions (Searchinger *et al.*, 2008; Melillo *et al.*, 2009; Dauber *et al.*, 2010). Marginal land refers to those lands where a cost-effective production is not possible under given environmental conditions, cultivation techniques, agricultural management as well as other economic and legal conditions (Wiegmann *et al.*, 2008; Gopalakrishnan *et al.*, 2011), including lands such as idle or fallow cropland, abandoned or degraded cropland, and abandoned pastureland (Cai *et al.*, 2011; Gopalakrishnan *et al.*, 2011). Compared with cropland, marginal land normally has lower inherent agricultural productivity, due to its less fertile soils and often less favorable water, climate and possibly other environmental conditions. However, certain energy crops with high resource-use-efficiencies are still capable of growing on these lands where traditional food crops cannot survive (Fargione *et al.*, 2010; Gelfand *et al.*, 2013). For example, some perennial cellulosic crops, such as switchgrass and *Miscanthus*, could provide abundant biomass but require relatively less commercial fertilizer inputs than food crops

(Lewandowski *et al.*, 2003; Heaton *et al.*, 2004; Stewart *et al.*, 2009). These crops therefore, if well cultivated, could be used to grow biomass feedstock and produce cellulosic ethanol by using the less favored marginal lands, to avoid competing with food crops for cropland.

Field experiments suggested that cellulosic energy crops or herbaceous vegetation, once well established, could produce considerable biomass feedstocks and have a direct GHG emissions mitigation capacity that rivals that of conventional food crops. Switchgrass and *Miscanthus*, for example, can produce comparable or even higher biomass than the traditional biofuel crop – maize (Fike *et al.*, 2006; Heaton *et al.*, 2008; Nikièma *et al.*, 2011). These perennial cellulosic crops normally have high conversion efficiency of photosynthetically active radiation and are able to enhance carbon (C) accumulation in a wide range of soil and climate conditions (Heaton *et al.*, 2008). A considerable amount of C is assimilated and stored in the belowground biomass and soils, which fosters benefits for carbon dioxide (CO_2) sequestration (Don *et al.*, 2012; Monti *et al.*, 2012). In addition, cellulosic crops generally require only a very limited amount of nutrients (e.g., nitrogen fertilizer) due to their high nutrient-use efficiency, and therefore could possibly reduce fertilization induced nitrous oxide (N_2O) emissions (Lewandowski *et al.*, 2003; Monti *et al.*, 2012). Soil methane (CH_4) fluxes were negligible in these ecosystems (Drewer *et al.*, 2012). Gelfand *et al*. (2013) recently also reported in their comparative experiments that, if grown on marginal lands, successional herbaceous crops, such as alfalfa and poplar, could still produce “sizeable amounts of biomass” and meanwhile mitigate GHG emissions due to significant C sequestration in soils and large quantity of N_2O reduction.

However, biomass productivity and GHG emissions regarding large-scale bioenergy expansion on marginal lands are rarely studied (Gelfand *et al.*, 2013). During the past several decades, modeling was used extensively to study regional or global scale C, nitrogen (N) dynamics and GHG emissions of both natural (e.g., forest, grassland) and managed ecosystems (e.g., cropland) (Raich *et al.*, 1991; Smith *et al.*, 1997; Bondeau *et al.*, 2007; Huang *et al.*, 2009). More recently, models were increasingly used to assess agroecosystems related to bioenergy crops, either by incorporating agricultural modules into natural ecosystem models, e.g., Agro-BGC(Di Vittorio *et al.*, 2010) and LPJml (Bondeau *et al.*, 2007), or by developing crop-specific models, e.g., ALMANAC (Kiniry *et al.*, 1992) and MISCANMOD (Clifton-Brown *et al.*, 2004). These models can be applied to a large region to estimate biomass production or/and GHG emissions (Thomas *et al.*, 2012). As most previous modeling studies concentrated on the land-use change due to conversion of natural ecosystems to agroecosystems, or crop switch from food crops to energy crops on cropland (Fargione *et al.*, 2008; Searchinger *et al.*, 2008; Melillo *et al.*, 2009), another land use scenario of growing energy crops on marginal lands was also important but less studied (Qin *et al.*, 2011; Gelfand *et al.*, 2013). Accompanying with the biomass production, GHG emissions produced from or mitigated by marginal lands could significantly affect the total GHG budget in the lifecycle assessment of biofuel production, and therefore additional effort should be made to study potential C and N dynamics and GHG fluxes of these biofuel ecosystems.

Here we use a model-data fusion approach to conduct such a study assuming switchgrass and *Miscanthus* grown on the marginal lands in the conterminous US. The spatial estimates are made for biomass production, net carbon balance, N_2O emissions and therefore the total GHG emissions. Biofuel productivity, land use and global warming potential are further analyzed at regional scales to meet the US national biofuel mandate by year 2022.

4.2 Materials and Methods

4.2.1 Energy Crops

Switchgrass and *Miscanthus* were recently introduced to the US as energy crops for biomass production purpose due to their considerable productivity and stress tolerance to unfavorable environment (McLaughlin *et al.*, 2005; Heaton *et al.*, 2008). Switchgrass is a perennial cellulosic crop native to North America, with biomass productivity of 5-20 Mg (1 Mg = 1t) dry matter (DM) per hectare land. It was selected as “model” species and tested across the conterminous US (Wright *et al.*, 2010). *Miscanthus*, however, refers to a genus of several perennial grass species mostly native to the subtropical and tropical areas of Asia (Stewart *et al.*, 2009). Its yield could normally reach 20 to 30 Mg DM ha^{-1} if well cultivated (Heaton *et al.*, 2008). In this study, these two crops are assumed to be grown on marginal lands in the US to produce biofuel feedstocks.

4.2.2 Model Description

AgTEM is a biogeochemical model designed for agroecosystems, by incorporating ecophysiological, biogeochemical and management related processes into the framework of the Terrestrial Ecosystem Model (TEM; Raich *et al.*, 1991; McGuire *et al.*, 1992; Zhuang *et al.*, 2003, 2010). The model can be used to simulate C and N dynamics of agroecosystems at a daily time step, by using spatially explicit forcing data describing climate, soil, vegetation and agronomic conditions (Qin *et al.*, 2013a).

In AgTEM, all algorithms related to C and N fluxes and pools are governed by five equations describing changes of ecosystem states regarding vegetation and soil. Carbon cycling in the agroecosystems is modeled as following (Eqn. 4.1): atmospheric CO_2 is preliminarily assimilated by plants through photosynthesis and stored in the vegetation. In the model, net primary production (NPP) is the rate at which the plants produce net useful chemical energy. It is the difference between the rate at which the plant produces useful chemical energy (GPP, gross primary production) and the rate at which some of that energy is used during autotrophic respiration. NPP represents the total biomass of the ecosystem produced, which is partly harvested as harvestable biomass (HBIO), partly used during heterotrophic respiration and partly allocated to soil organic carbon (SOC) and belowground biomass (as in perennial crops). The C in HBIO is eventually released as CO_2 through biofuel production and use. The net C balance in the ecosystem is modeled as net carbon exchange (NCE) which accounts for all C fluxes into or out of the system. A positive NCE indicates a net ecosystem CO_2 sink while a negative value indicates a CO_2 source (Qin *et al.*, 2013a).

$$CO_2 \Rightarrow GPP \overset{CO_2\uparrow}{\Rightarrow} \underbrace{NPP \overset{CO_2\uparrow}{\Rightarrow} \left\{ \begin{array}{l} HBIO \overset{CO_2\uparrow}{\Rightarrow} \\ \overset{CO_2\uparrow}{\Rightarrow} C_{SOC} \end{array} \right.}_{NCE} \tag{4.1}$$

Modeled N_2O accounts for soil N_2O fluxes from both nitrification and denitrification, as in Eqn. 4.2 (Qin *et al.*, 2013a):

$$\left.\begin{array}{l} NH_4^+ \overset{NO}{\Rightarrow} N_2O_{\mathrm{ntf}} \\ NO_3^- \overset{N_2}{\Rightarrow} N_2O_{\mathrm{dtf}} \end{array}\right| \Rightarrow N2O \tag{4.2}$$

where N_2O_{ntf} is N_2O produced from the nitrification process of the biological oxidation of ammonia (NH_4^+) with oxygen, and N_2O_{dtf} is N_2O produced from soil nitrate (NO_3^-) through denitrification process; N2O is the total N_2O fluxes of N_2O_{ntf} and N_2O_{dtf}. Nitric oxide (NO) and nitrogen (N_2) are also produced from the processes of nitrification and denitrification, respectively, but not quantified in this study.

The original version of AgTEM 1.0 was calibrated and applied at regional scale to assess regional C dynamics (Qin *et al.*, 2011), biomass production (Qin *et al.*, 2012) and water balance (Zhuang *et al.*, 2013). The further developed AgTEM 2.0 incorporated processes such as biomass allocation, N cycling and agricultural management, and was validated (Qin *et al.*, 2013a) and used to assess regional biomass production and C and N dynamics (Qin *et al.*, 2013b). In the AgTEM 2.0 used here, most parameters describing and constraining generic ecosystem processes were either inherited from TEM (e.g., Zhuang *et al.*, 2003; Zhuang *et al.*, 2010) or pre-defined in previous studies (e.g., Qin *et al.*, 2011; Qin *et al.*, 2012). Some vegetation-specific parameters were also calibrated for cellulosic crops selected in this study, namely switchgrass and *Miscanthus* (Qin *et al.*, 2013a, b).

4.2.3 Model Simulations and Regional Analyses

By assuming that switchgrass and *Miscanthus* will be grown on available marginal lands in the conterminous United States (**Figure** 4.1), we applied the AgTEM 2.0 separately for these two crop systems to simulate ecosystem C and N dynamics along with crop growth, using spatially referenced data describing climate, soil, vegetation, atmospheric CO_2 and agricultural management. Model estimates were then used to assess spatial distribution of output variables of interest including NPP, HBIO, NCE and N_2O. Spatial analyses were finally conducted to estimate spatial and national biomass/biofuel production, CO_2 mitigation, N_2O emissions and total GHG emissions.

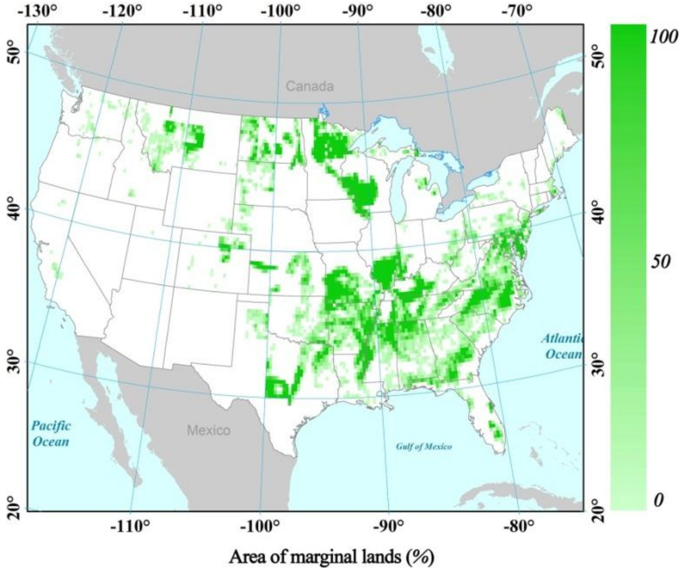

Figure 4.1 Area of marginal lands (%) capable of growing energy crops. Data were derived from Scenario 1 of Cai *et al.* (2011). Marginal lands were identified according to marginal agricultural productivity based on land suitability indicators such as topography, climate conditions and soil productivity; Fuzzy Logic Modeling method was used to determine land productivity (Cai *et al.*, 2011).

For spatial simulations, model was run grid-by-grid to estimate C and N dynamics at a daily time step with available forcing data from 1989 to 2008. First, we ran the AgTEM to equilibrium using the first year data for model initialization. The model was then spun up for 100 years repeatedly using the first 10 years' data to reach equilibrium state. We then ran the transient simulations continuously from 1989 to 2008 using transient forcing data. Spatial forcing data were organized at a 0.25º latitude × 0.25º longitude resolution for the study region. Specifically, climate data describing temperature, precipitation, cloudiness were obtained from the ECMWF (European Centre for Medium-Range Weather Forecasts) Data Server (www.ecmwf.int) and organized at a temporal resolution of one day from 1989 to 2008. Annual atmospheric CO_2 concentrations were collected from the NOAA Mauna Loa CO_2 record (www.esrl.noaa.gov/gmd/ccgg/trends/). The elevation data were derived from the Shuttle Radar Topography Mission (SRTM) (Farr *et al.*, 2007) and soil texture data were based on the Food and Agriculture Organization/Civil Service Reform Committee (FAO/CSRC) digitization of the FAO/UNESCO soil map of the World (1971). Scenario 1 in Cai *et al*. (2011) includes marginal lands from abandoned land and mixed crop and vegetation land, and yet without sacrificing large amounts of cropland and natural lands (forest and grassland) (**Figure** 4.1). The scenario was therefore considered to represent spatial distribution of marginal lands in the United States in this study. Nitrogen fertilization was set at four input rates as 0 (N0), 50 (N1), 100 (N2) and 150 g N ha^{-1} (N3) for both switchgrass and *Miscanthus* systems, according to field experiments (Fike *et al.*, 2006; Heaton *et al.*, 2008; Propheter *et al.*, 2010; Nikièma *et al.*, 2011).

Spatial analyses were conducted for each crop ecosystem based on model simulations, using geographic information system techniques. Regional analyses based on grid outputs were presented as average of the 1990s. NPP and HBIO were computed for both spatial and national levels as primary and harvested biomass production, respectively. Using biomass-to-biofuel conversion efficiencies, biofuel production was further calculated from HBIO results. Under current technologies, the efficiency of converting biomass to biofuel is estimated to be about 282 L ethanol Mg^{-1} DM. The potential efficiency could reach about 399 L ethanol Mg^{-1} DM if advanced technologies available (Lynd *et al.*, 2008). Net CO_2 balances (NCE) and total N_2O emission (N2O) were also computed to estimate spatial and national GHG emissions in terms of global warming potential (GWP). The GWP of N_2O was calculated in units of CO_2 equivalent (CO_2eq) over a 100-year time horizon. Additionally, GWP was related to energy production by computing global warming intensity (GWP_i) in terms of total GWP relative to biofuel production (Qin *et al.*, 2013b).

4.3 Results

4.3.1 Biomass and Biofuel Production on Marginal Lands

With increasing use of N fertilizer, the biomass production at ecosystem scale also increases, in both switchgrass (**Figure** 4.2) and *Miscanthus* ecosystems (**Figure** 4.3). At N0 level, the switchgrass produces NPP (area weighted) of less than 400 g C m^{-2} in most areas (**Figure** 4.2a). With N addition, the NPP production increases dramatically, especially in those areas with intense cropping, e.g., Wisconsin (**Figure** 4.2b-d). When the N rate reaches N2 (**Figure** 4.2c) and N3 (**Figure** 4.2d) levels, most of the southern areas have NPP of 400-800 g C m^{-2}. In terms of biomass harvested (**Table** 4.1), switchgrass produces a national average of 3.5 Mg DM ha^{-1} each year without N application, with additional 1.4 Mg DM ha^{-1} if applied 50 kg N ha^{-1} (N1). The average HBIO could reach 5.7-5.9 Mg DM ha^{-1} when sufficient N fertilizer available. *Miscanthus* generally has higher biomass productivity than corresponding switchgrass at the same N application levels (**Figure** 4.3). Without N application, the NPP reaches over 600 g C m^{-2} in most intense cropping areas (**Figure** 4.3a), with a national average HBIO production of about 10 Mg DM ha^{-1} (**Table** 4.1). With each additional kg of N application, the *Miscanthus* HBIO increases about 50 kg DM ha^{-1} each year on average, with highest increase of 64 kg DM ha^{-1} from N0 to N1 level and lowest increase of 28 at DM ha^{-1}

Table 4.1 Estimated harvestable biomass and biofuel production from energy crops grown on marginal lands under different nitrogen application scenarios.

Energy crops	Nitrogen application	Estimated harvestable biomass production (Mg DM ha^{-1} land) [*]	Estimated biofuel production (kL ethanol ha^{-1} land)	
			Current level[†]	Potential level[‡]
Swithchgrass	N0	3.5 (0.3)	1.0 (0.1)	1.4 (0.1)
	N1	4.9 (0.5)	1.4 (0.1)	1.9 (0.2)
	N2	5.7 (0.6)	1.6 (0.2)	2.3 (0.2)
	N3	5.9 (0.6)	1.7 (0.2)	2.3 (0.2)
Miscanthus	N0	10.2 (1.0)	2.9 (0.3)	4.1 (0.4)
	N1	13.4 (1.3)	3.8 (0.4)	5.3 (0.5)
	N2	15.8 (1.7)	4.5 (0.5)	6.3 (0.7)
	N3	17.2 (2.0)	4.9 (0.6)	6.9 (0.8)

[*] DM, dry matter.

[†] Current and [‡] potential levels of biofuel production are estimated according to current and potential biomass-to-biofuel conversion efficiencies (Lynd *et al.*, 2008).

from N2 to N3 level. When the N rate reaches N3, *Miscanthus* produces the highest HBIO of 17.2 Mg DM ha^{-1}, which almost triples the switchgrass production (**Table** 4.1).

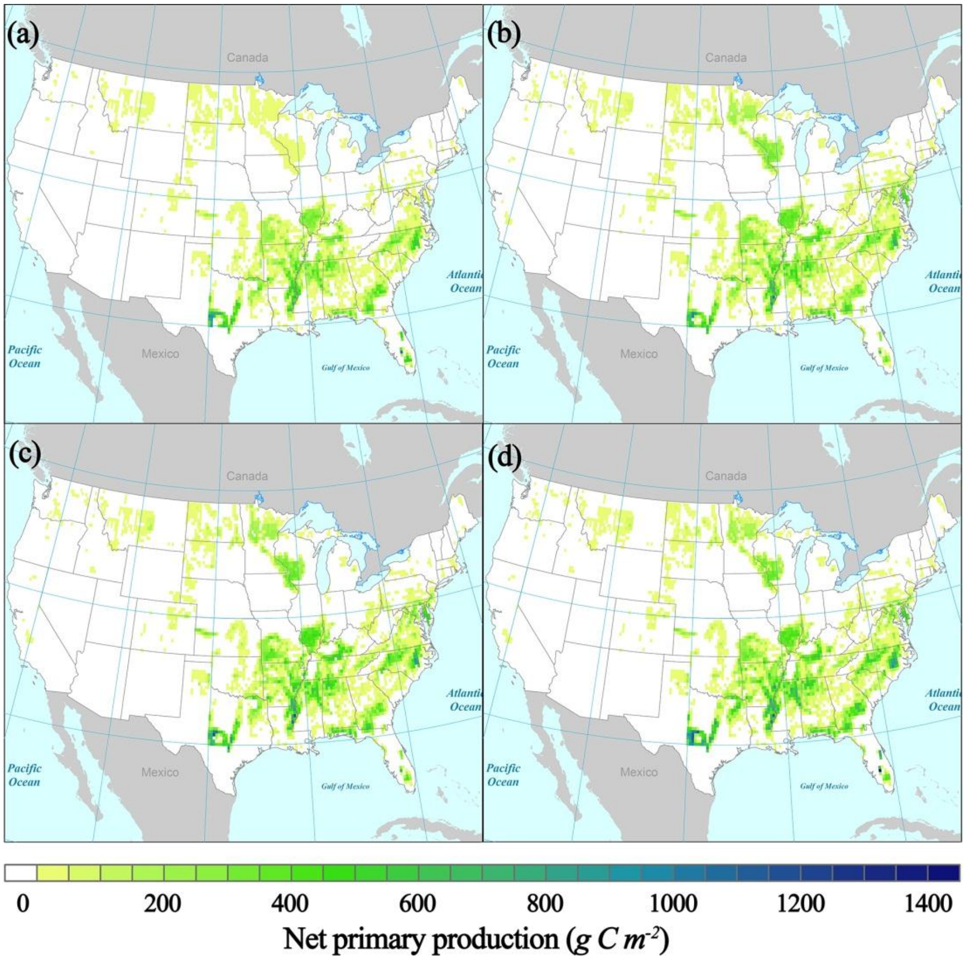

Figure 4.2 Model estimated net primary production of switchgrass from marginal lands. Area weighted estimates were made for switchgrass grown under nitrogen application levels of (a) N0, (b) N1, (c) N2 and (d) N3.

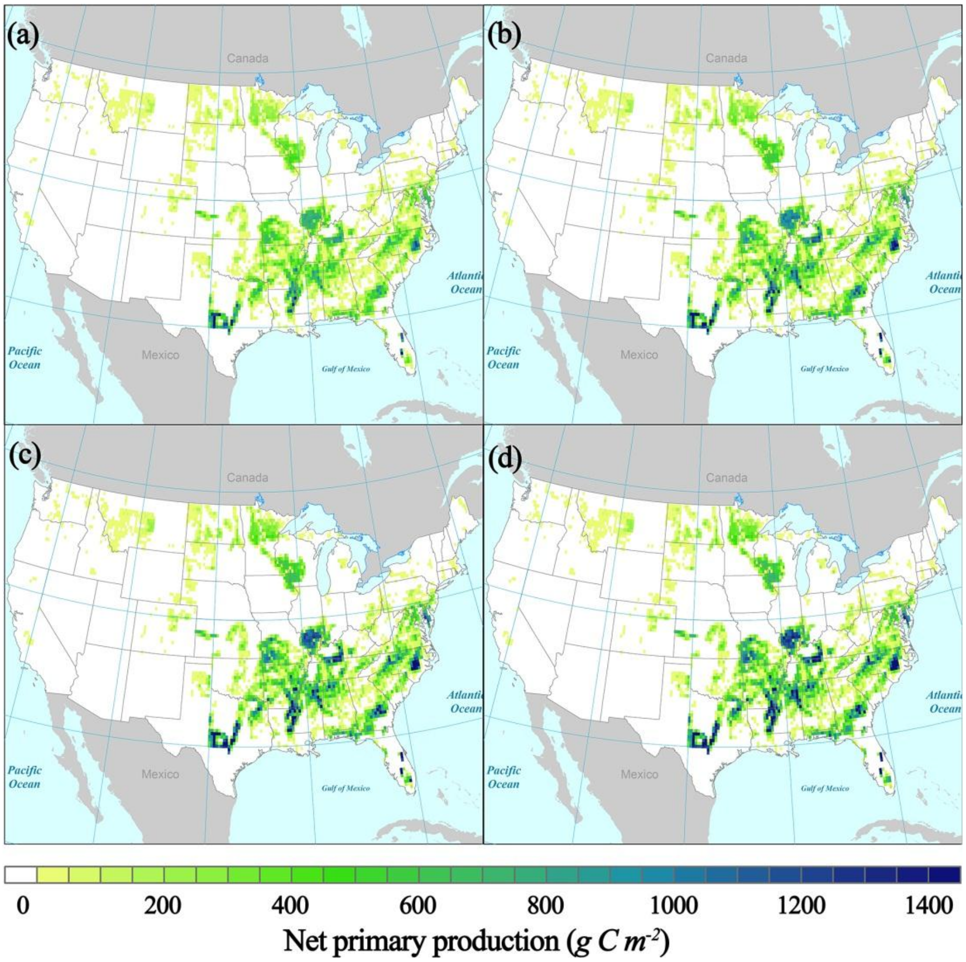

Figure 4.3 Model estimated net primary production of *Miscanthus* from marginal lands. Area weighted estimates were made for *Miscanthus* grown under nitrogen application levels of (a) N0, (b) N1, (c) N2 and (d) N3.

Production of cellulosic ethanol using the harvested biomass is highly dependent on biomass-to-biofuel conversion technologies (**Table** 4.1). Under currently available technology, switchgrass could produce about 1.0-1.7 kL ethanol from each hectare of marginal land, depending on N application and biomass production. *Miscanthus*, however, could produce 2.9-4.9 kL ethanol ha^{-1} land due to its high biomass productivity. With advanced technology available, the biofuel conversion efficiency could increase 41.5%. Switchgrass harvested from marginal lands could therefore produce 1.4-2.3 kL ethanol ha^{-1} land and productive *Miscanthus* could produce 4.1-6.9 kL ethanol ha^{-1} land.

Generally, with advanced technology and application of high-rate N fertilizer, cellulosic crops grown on marginal lands could have considerably higher land use efficiency, in terms of biofuel production at given land, than otherwise with current technology and less use of N. *Miscanthus*, in particular, has higher land use efficiency than switchgrass at each scenario of technology × N application level.

4.3.2 Greenhouse Gas Emissions in Bioenergy Ecosystems

GHG emissions (GWP) are determined by the effects of both ecosystem CO_2 and N_2O emissions (**Figure** 4.4, 4.5). Our model experiments indicate that, most of the cropping areas in the southern US act as net sources of GHG emissions, and estimated *Miscanthus* GWP (**Figure** 4.5) has much higher variation than the corresponding switchgrass GWP (**Figure** 4.4) at any specific location. Specifically, in the switchgrass ecosystems, with increasing use of N fertilizer, the GHG emissions increase significantly, especially in the intense cropping areas in the middle US (**Figure** 4.4). For example, after increasing use of N, net GHG sinks in some areas become GHG sources, e.g., Texas (**Figure** 4.4a,b), and some GHG sources become even larger sources, e.g., South Illinois (**Figure** 4.4b, c). In the *Miscanthus* ecosystems, however, the GHG emissions do not necessarily increase with increasing use of N (**Figure** 4.5). It is evident that, for those areas that are already GHG sources without N fertilization, e.g., Missouri, Kentucky and Tennessee in the middle of the United States (**Figure** 4.5a), the net GWP tends to be larger after use of N fertilizer (**Figure** 4.5b-d); but for the areas that are originally GHG sinks, e.g., Texas and Louisiana in the South US (**Figure** 4.5a), their GWP become even smaller, suggesting these areas become even larger GHG sinks.

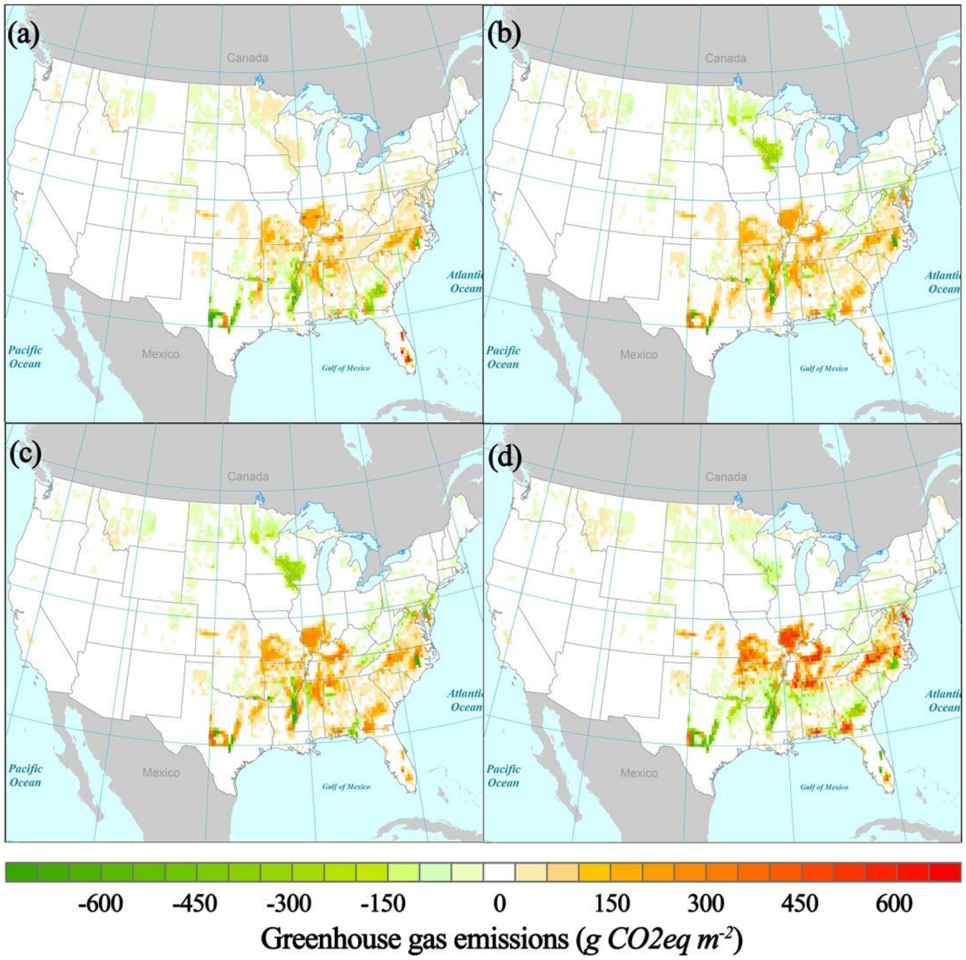

Figure 4.4 Model estimated GHG emissions from switchgrass on marginal lands. Maps show area weighted total emissions of CO_2 and N_2O (GWP) for switchgrass grown under nitrogen application levels of (a) N0, (b) N1, (c) N2 and (d) N3. A positive value indicates a net GHG sink while a negative value indicates a net GHG source.

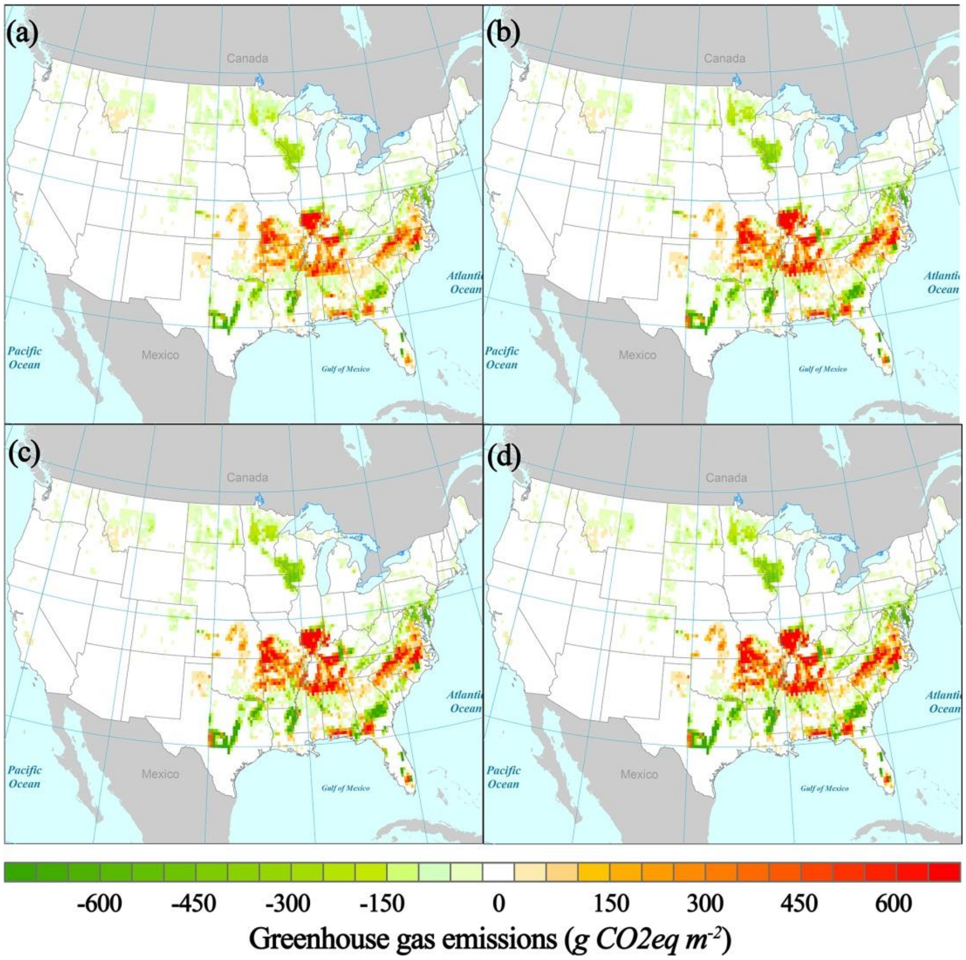

Figure 4.5 Model estimated GHG emissions from *Miscanthus* on marginal lands. Maps show area weighted total emissions of CO_2 and N_2O (GWP) for *Miscanthus* grown under nitrogen application levels of (a) N0, (b) N1, (c) N2 and (d) N3. A positive value indicates a net GHG sink while a negative value indicates a net GHG source.

From the perspective of national average GHG emissions, the changes of net GWP are simply the results of GWP changes in both CO_2 and N_2O (**Table** C 1). Both ecosystems act as GHG sources at national level and at all N application levels (**Figure** 4.6a). Switchgrass and *Miscanthus* have a similar amount of N_2O emissions at each N application rate, and even similar C sinks at lower N rates (N0, N1). But *Miscanthus* has

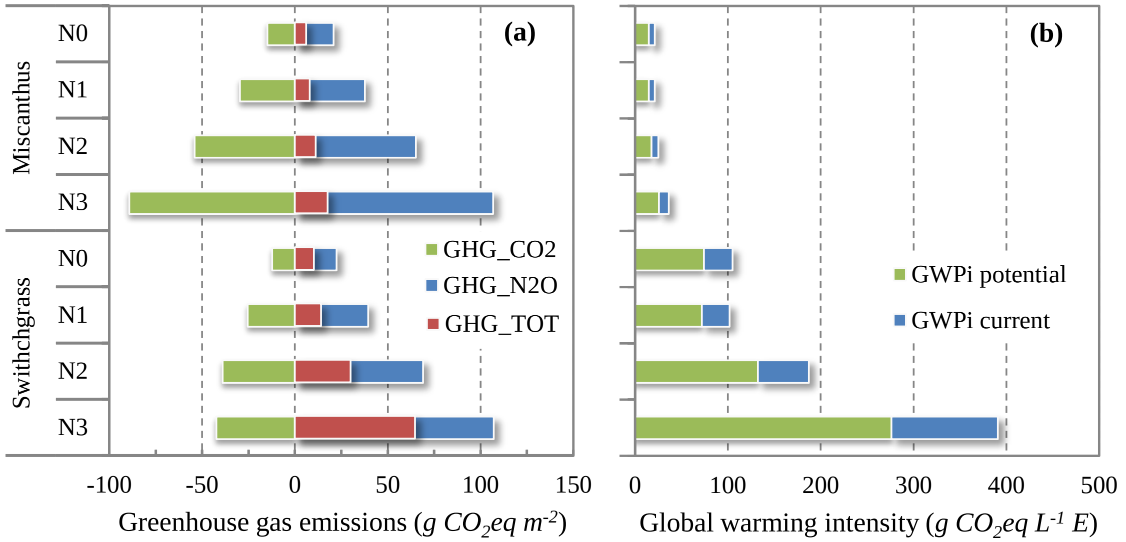

Figure 4.6 National average GHG emissions from switchgrass and *Miscanthus* grown on marginal lands. (a) Contributions of CO_2 (GHG_CO2) and N_2O (GHG_N2O) to total GHG emissions (GHG_TOT) under different nitrogen application levels; a positive value indicates a net GHG sink while a negative value indicates a net GHG source; (b) global warming intensity, in terms of GWP relative to ethanol (E) production under current or potential conversion efficiencies.

a much larger C sink than switchgrass at higher N rates (N2, N3). For instance, in the switchgrass ecosystem, with increasing use of N, both N_2O emissions and CO_2 mitigation increase, but the former has a relatively larger value than the latter, resulting in a net source of GHG emissions. This is especially true when the N rate reaches N2 and N3 levels where the total GHG emissions reach 30 and 65 g CO_2eq m^{-2} respectively, compared with 10 g CO_2eq m^{-2} at N0 level. By contrast, N_2O emissions and CO_2 mitigation do not change much in *Miscanthus* ecosystems, even when the N rate increases. For example, the GWP (N0) of CO_2 and N_2O are -15 and 20 g CO_2eq m^{-2}

respectively, making the net ecosystem GHG of only 6 g CO_2eq m^{-2}. The GWP of CO_2 and N_2O reaches up to -89 and 107 g CO_2eq m^{-2}, respectively, when the N application gets to the N3 level, but the net ecosystem GHG is still only 18 g CO_2eq m^{-2} – about 27% of switchgrass GWP at the same N level.

By relating GHG emissions to biofuel production, our model results show that, *Miscanthus* has much smaller global warming intensities than switchgrass, at all N application levels (**Figure** 4.6b). Under currently available technologies, for each liter of ethanol produced, *Miscanthus* system releases 21-36 g CO_2eq of GHG; with increasing N application, the GWPi also increases. Switchgrass, however, releases much more GHG per unit biofuel than *Miscanthus*, with lowest GWPi of about 100 g CO_2eq L^{-1} at N0 and N1 levels and highest GWPi of 390 g CO_2eq L^{-1} at N3 level. To produce same amount of biofuel, switchgrass on average releases 4-10 times more GHG than *Miscanthus*. With advanced conversion technology, the GWPi can be lowered for both systems by reducing about 40% GHG release relative to current GWPi levels. But still, *Miscanthus* is more environmentally viable than switchgrass in producing biofuel with significantly lower GHG emissions.

4.4 Discussion

4.4.1 Cellulosic Crops as Biomass Feedstocks

Cellulosic crops, such as switchgrass and *Miscanthus*, normally have higher nutrient use efficiency (Lewandowski *et al.*, 2003; Fargione *et al.*, 2010) and possibly higher water use efficiency than food crops (Stewart *et al.*, 2009; Zhuang *et al.*, 2013). They could therefore grow on marginal lands instead of competing with food crops for fertile croplands. However, the results here and elsewhere (Gelfand *et al.*, 2013) also show that, biomass production from marginal lands may be lower than that from croplands. Our previous studies suggested that, an average of about 5-8 Mg DM ha^{-1} of switchgrass or around 20 Mg DM ha^{-1} of *Miscanthus* could be produced from cropland (Qin *et al.*, 2013b), which is higher than those grown on marginal lands even with high N input (**Table** 4.1). This may be partly explained that, besides nutrient (e.g., N), other factors could also affect biomass production on marginal lands, for example, water availability, climate conditions and soil fertility (Cai *et al.*, 2011).

N application affects not only biomass production but also the ecosystem GHG emissions. On the one hand, use of N fertilizer could improve soil nutrient condition and therefore stimulate crop growth. With increasing rate of N application, for each unit of N use, biomass production increment decreases gradually (**Figure** C 1a, c), i.e., marginal HBIO production decreases with N addition (**Figure** C 1b, d). On the other hand, increasing use of N leads to more N loses through gaseous emissions, leaching and runoff. With increasing N application, the GHG release also gets stronger (**Figure** C 1a, c), the marginal GHG emissions increase with N addition (**Figure** C 1b, d). It is therefore very important to analyze how N use affects the benefits (e.g., biomass or biofuel production) and costs (e.g., GHG emissions) in marginal lands in our future studies.

4.4.2 Land Use and GHG Emissions Regarding 2022 Biofuel Target

Totally 136 billion liters of renewable fuels, including 79 billion liters of cellulosic ethanol, are expected to be produced annually by 2022 in the United States (US Congress, 2007). In order to reach the ambitious cellulosic ethanol target, a total of about 280 million ton of cellulosic biomass will be required under current biofuel conversion technology. If switchgrass were grown on the marginal lands for biofuel feedstocks, a total of 48-81 Mha of land would be required (**Figure** C 2). According to estimates made by (Cai *et al.*, 2011), large area of cropland or natural ecosystems might have to be sacrificed for this purpose. Additionally, 8-31 Tg CO_2eq of GHG would be produced due to cropping, depending on N input levels (**Figure** C 2). However, if *Miscanthus* were grown, large quantity of land could be saved compared with growing switchgrass, only 16-28 Mha of available marginal lands could be sufficient to produce required biofuel feedstocks. More importantly, using *Miscanthus* could reduce a considerable amount of GHG emissions; only a total of 1.7-2.9 Tg CO_2eq of GHG would be released to meet the 2022 target (**Figure** C 2).

If biofuel conversion efficiency could be improved, i.e., from 282 to 399 L ethanol Mg DM (Lynd *et al.*, 2008), the biomass demand would be dramatically reduced to 200 million ton of dry matter. The land demand and GHG emissions could also be reduced to 71% of those under current technology, for both switchgrass and *Miscanthus* systems. Considering biofuel productivity alone, *Miscanthus* grown under N3 level has the highest land use efficiency. Under this scenario, only 11.6 Mha of marginal lands will serve the purpose of producing 79 million liters ethanol (**Figure** C 2). However, if environment is the only concern, then *Miscanthus* grown under the N0 level release the smallest amount of GHG of just 1.2 Tg CO_2eq, but yet requires 19.6 Mha of land (**Figure** C 2).

By comparing with previous estimates for biomass produced from cropland (Qin *et al.*, 2013b), we find that, cellulosic crops have lower productivity grown on marginal lands, and therefore require relatively more land to reach 2022 target, than they were otherwise grown on fertile cropland. However, compared with maize grown on cropland, marginal land – based *Miscanthus* requires comparable or even less land resources and releases remarkably less amount of GHG, irrespective of N application and technology. While this study focuses on land demand and GHG emissions, other aspects including societal, economic, and environmental impacts should also be factored into the cost-benefit analysis of large-scale biomass bioenergy development in future studies.

4.4.3 Limitations and Future Needs

Modeling study is often limited by data availability and model deficiency. In this study, data of climate, soil and vegetation were used to initialize model and make regional estimates. Most of these data (e.g., temperature, precipitation) are derived and reanalyzed from site/field observations, which inevitably introduce uncertainties into the spatially referenced model simulations due to observation errors, spatial heterogeneity and possible interpretation biases (Smith *et al.*, 1997; Huang *et al.*, 2009; Melillo *et al.*, 2009). In particular, due to lack of data, the fertilization rate was assumed to be constant throughout the whole US. Even with several different N rates (N0-N3), the fertilization scenario may not necessarily reflect the real management practice, simply because that soil fertility is spatially heterogeneous and fertilization rate can be adjusted accordingly. In addition, due to incomplete mechanism understanding and data unavailability for certain cellulosic crop systems, AgTEM used in this study only incorporates one major management component (i.e., fertilization) and leaves others (e.g., water availability, rotation) not specifically modeled (Qin *et al.*, 2013b). As observational and spatial data become available and our understanding regarding bioenergy ecosystems advances, we shall incorporate them into AgTEM analysis with higher accuracy.

As for cost-benefit analysis of energetic, environmental and economic aspects regarding large-scale bioenergy development (e.g., Hill *et al.*, 2006), life cycle assessment (LCA) will be needed to account for energy system processes along with cellulosic ethanol's life "from-cradle-to-grave" (e.g., Davis *et al.*, 2009; Scown *et al.*, 2012). Ecosystem analysis made in this study consists of only one link of the whole LCA chain, which estimates only those processes that occurred inside specific ecosystems. Other system processes, such as transportation, manufacturing and biofuel use, should also be factored into the LCA. It worth noting that, in future analysis, we may also consider the data and modeling uncertainties (Qin *et al.*, 2013b), technology advances (Lynd *et al.*, 2008), climate change impacts (Tulbure *et al.*, 2012) and time scale (Kendall *et al.*, 2009), by using LCA together with various uncertainty analysis techniques (e.g., Monte Carlo uncertainty analysis) (Wang *et al*., 2012). The total GHG emission estimates shall be revised if we conduct LCA.

4.5 Conclusion

Growing biomass from marginal lands is becoming an increasingly attractive choice for producing biofuel as an alternative energy source to fossil fuels. In this study, by using a biogeochemical model, we estimated bioenergy potential and possible greenhouse gas (GHG) emissions from bioenergy crops grown on marginal lands in the United States. Modeling experiments show that, cellulosic crops, especially *Miscanthus*, could produce a considerable amount of biomass and thus ethanol. *Miscanthus* has much lower global warming intensity, in terms of GHG emissions per unit ethanol produced, than switchgrass. To reach the mandated cellulosic ethanol target in the United States, growing *Miscanthus* could save large amounts of land and reduce remarkable GHG emissions than growing switchgrass. High-accuracy data assimilation, model improvement and life cycle assessment, still await future study.

4.6 Acknowledgement

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CHAPTER 5. SUMMARY AND FUTURE OUTLOOK

5.1 Dissertation Summary

Generally, my dissertation research is to assess land use change caused environmental impacts in the context of climate change and bioenergy development, by using model-data fusion approaches. Increasing concerns about energy security and environmental sustainability have prompted development of bioenergy, which is most likely to cause direct land use change due to biomass production. Cropland and marginal lands could be potentially converted to lands that support development of biofuel crops. Then, what are the major energetic consequences, environmental impacts and agricultural implications of the cropland- or marginal-land-supported biofuel cropping?

In this dissertation and our previous studies (Qin *et al*., 2011; 2012; Zhuang *et al*., 2013), we looked into diverse aspects of food security, bioenergy production, sustainability and environment. Below, we only summarize the results, findings and discussion in the dissertation:

1. An agroecosystem model (AgTEM) was developed based on the Terrestrial Ecosystem Model. The model was incorporated with biogeochemical and ecophysiological processes including crop phenology, biomass allocation, nitrification and denitrification as well as agronomic management of irrigation and fertilization. Once parameterized and validated, AgTEM is capable of

simulating C and N dynamics of certain ecosystems. In the study, AgTEM was specifically validated for three major crops: maize, switchgrass and *Miscanthus*. The model reproduced the annual net primary production and nitrous oxide emissions of most sites, with over 85% of total variations explained by the model. Local sensitivity analysis was conducted to test the response of the model to different sources of variance in input data. The study indicated that the model sensitivity varies among different ecosystems.

2. Cropland-supported biofuel production and potential GHG emissions were estimated using AgTEM. By assuming maize, switchgrass and *Miscanthus* grown on the current maize-producing areas in the conterminous United States, the modeling experiments indicated that, the maize ecosystem acts as a mild net carbon source while cellulosic ecosystems (i.e., switchgrass and *Miscanthus*) act as mild sinks. Among all three bioenergy crops, *Miscanthus* is the most biofuel productive and the least GHG intensive at a given cropland. Substituting *Miscanthus* for maize to produce biofuel on cropland could potentially save land and reduce GHG emissions.
3. Biomass/biofuel productivity and capability of climate change mitigation were assessed for marginal lands that could potentially be used for biofuel development. Two cellulosic crops, switchgrass and *Miscanthus*, were assumed to be grown on the abandoned land and mixed crop-vegetation land with marginal productivity. AgTEM was used for spatial simulation and regional estimation. The analyses showed that, cellulosic crops, especially *Miscanthus*, could produce a considerable amount of biomass and thus biofuel. *Miscanthus* has much lower

global warming intensity than switchgrass. To reach the mandated cellulosic ethanol target of the US, growing *Miscanthus* could save a large amount of land and substantially reduce GHG emissions compared with growing switchgrass.

5.2 Future Outlook

5.2.1 Modeling Uncertainties and Improvement

Generally, three major sources of uncertainties contributed to the modeling variance and uncertainty: observation, model and data (**Table** 5.1). Observation error, aka, experimental error, comes from experimental variability due to biased method, design and measurement. It directly affects model algorithms and model validation. Model itself is another key factor determining simulations, introducing uncertainties into modeling results through uncertain model structure, algorithm, parameter and variable. Data includes observational data used for model development and simulations, and forcing data used for regional estimation. Their variability contributes significantly to the modeling uncertainties (Kennedy & O'hagan, 2001). Interpretation errors mainly refer to the post-process of model results and using the results to inform policy-making.

Constraining uncertainties of any of these categories could help improve model performance (**Table** 5.1). More observational data will help to parameterize and validate AgTEM at locations under different environmental conditions. Better understanding of model-data fusion can be achieved via dedication to cross-site experimental research that are long-term with appropriate time intervals during sufficient time courses, covering various climate and management. Regional estimates are still limited in terms of modeling accuracy and precision due to incomplete understanding of ecosystem

Table 5.1 Major sources of uncertainties contributed to AgTEM modeling and simulations.

Sources	Possible causes	Examples	Possible improvements
Observation	Experiment design, methodology, measurements	Site-level yield and N_2O measurements, NPP calculation, lack of consistent evidence, lack of record for detailed management practices.	cross-site experimental research that are of consistent methodology and appropriate representation
Model	Structure	AgTEM is based on natural ecosystem model, without considering such agricultural management as tillage, rotation.	Future study should consider improving the management module in AgTEM. The further uncertainty and
	Algorithms	Numerical errors and approximations in equations used to describe ecosystem processes, e.g., in empirical functions.	sensitivity analysis at large scales should also improve modeling capability. Improved observation will help build, calibrate and validate models.

Table 5.1 Continued.

	Parameters	Some parameters are not constant across space or species, e.g., HI. Some are calibrated upon site observation which may not be accurate.	
	Variables	Imprecise representation of certain environmental conditions.	
Data	Validation data, model forcing data	Cross-site data of NPP and N_2O may not be accurate. Regional forcing data could represent large-scale but may not fine-scale climate.	Enhancing experiment and modeling cooperation, and improving model-data fusion methods.
Interpretation	Model output	NPP and N_2O at regional scale cannot represent local simulations and therefore may not match site-level observations.	Understanding modeling mechanisms, uncertainties and limitations of certain estimation.

mechanisms, data unavailability, model uncertainties and study boundary limitations. Some suggested that, by applying “code of best practices” to the model-data fusion framework, estimations could be improved by constraining uncertainties from both data and model (e.g., Keenan *et al*., 2011).

5.2.2 Limitations and Future Needs

The intrinsic characteristics of ecosystem modeling limited the way we interpret the large-scale simulation results. First of all, ecosystem system models, including AgTEM, represent certain biophysical and biogeochemical processes at a relatively large spatial scale compared with crop models. The model simulations may reproduce or reflect regional or global observations but may not necessarily inform the site-level or field practices such as agricultural management. In this study, the ability of AgTEM to simulate the G×E×M (gene/species × environment × management) interactions is limited to a certain degree. Future model improvement and model-data integration may potentially link ecosystem models with specific crop models (see also discussion in Section 2.4.2).

In addition, the AgTEM describes the agroecosystem dynamics within its modeling boundary, any processes beyond certain studied ecosystems are not specifically considered in the model and therefore should be further accounted for if system boundary changes. For instance, to study life cycle of biofuels in the energy system, besides ecosystem biomass feedstock production processes, other system processes such as fertilizer production, biomass transportation, biofuel refinery, transportation and end use should also be included and examined (Davis *et al*., 2009; Wang *et al*., 2012) (see also discussion in Section 5.2.3).

Also, energy cropping scenarios applied in the study do not suggest actual practice of certain large-scale land use/cover changes (also in Section 3.4.4). Other environmental issues such as soil fertility, soil erosion and water availability, and societal and economic issues such as farmers' choice (e.g., cost-benefit decisions and farming habits) and commercial efficiency (e.g., intensive cropping area selection, harvest equipment availability and harvest efficiency) could also affect land availability. Future studies of land selection considering these issues may further constrain land use data and suggest possible cropping regions in practice. Biofuel yield is limited by available biomass-to-biofuel conversion technology, and our biofuel production predictions were limited by the conversion efficiency data. Biofuel prediction should be improved when technology advancing and conversion efficiency data become available.

5.2.3 Energy, Environment and Economy Nexus

Energy security is and will still be a major problem in the foreseeable future for economic development. Meanwhile, environmental sustainability is a key factor determining energy development. In contrast to conventional fossil fuels, renewable bioenergy seems to be a promising option considering the balance among energy, economy and environment. This dissertation focuses on evaluating biofuel production and its consequences of GHG emissions. The analysis is at ecosystem scales, but not the upstream and downstream of biofuel production and use, such as resource input, transportation and fuel use. We estimated the GHG emissions in biofuel ecosystems, but did not assess other environmental impacts, such as water balance, air quality. Additionally, our study did not look into the economic impacts. In order to comprehensively evaluate the impacts of bioenergy cropping, energetic, economic and environmental aspects of biofuel development should be further investigated (**Figure** 5.1).

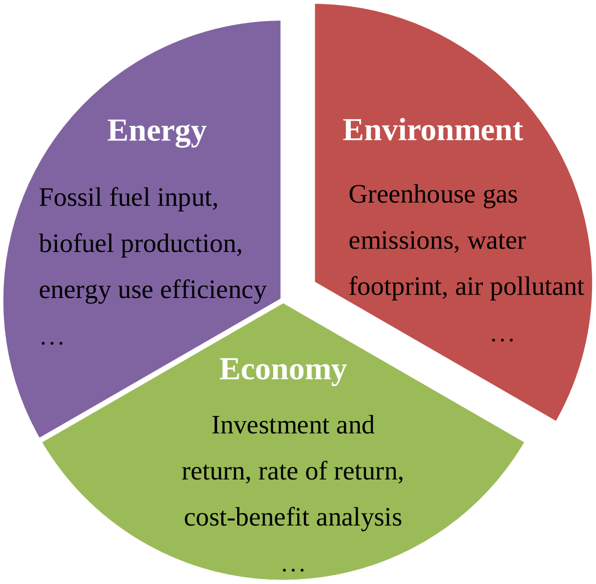

Figure 5.1 Energy, environment and economy nexus in bioenergy development.

Life cycle assessment (LCA) is a useful computational tool that can be used to account for ecosystem processes as well as upstream and downstream industry process along the biofuel's life “from-cradle-to-grave” (Hill *et al*., 2006; Davis *et al*., 2009). By applying LCA to the life cycle of biofuel from manufacture/transport of resources for cropping, to biofuel use (**Figure** 5.2), we shall be able to investigate the following aspects that have not been included in this dissertation:

1. Energy: energy into and out of the system, net energy balance and fuel energy ratio, biofuel energy efficiency.

2. Environment: GHG emissions, potential climate change mitigation (compared with fossil fuels), water footprint, and other air pollutants.
3. Economy: costs in industrial manufacturing, cropping and transportation, benefits from biofuel, co-products and even environmental “credits”, cost-benefit analysis.

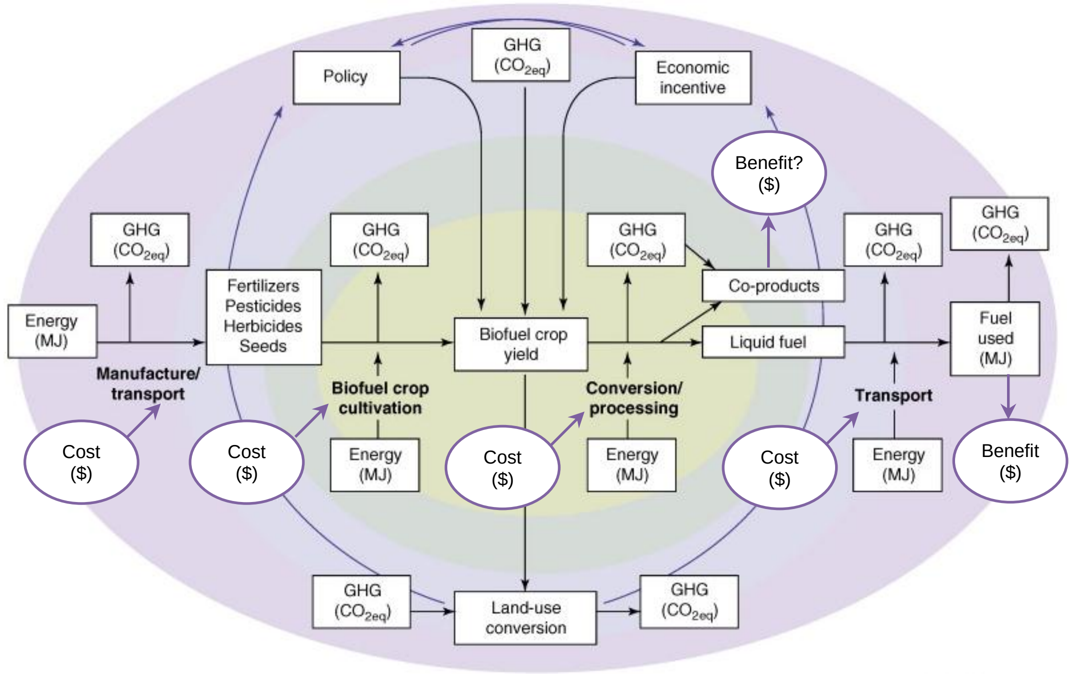

Figure 5.2 A chain of production for biofuels with energy, cost and benefit, GHG requirements (inputs) and emissions (outputs) defined at each step in the production process. The smallest possible system boundary in this case would include only the center box, ‘biofuel crop yield’, where inputs of GHG would include the CO$_2$ required for photosynthesis and outputs of GHG would include CO$_2$ from respiration and decomposition, as well as NO$_x$ and CH$_4$ fluxes from the soil. The background colors represent different system boundaries that become increasingly complicated with size. Adapted from Davis *et al*. (2009).

4. Policy making: above information regarding energetic, environmental and economic costs and benefits of biofuels from different feedstocks and land types should assist policy making on large-scale bioenergy expansion.

Ecosystem estimations here and elsewhere (e.g., Hill et al., 2006; Heaton *et al*., 2008) can be used as input into LCA. Ecosystem models can be coupled into LCA and life cycle modeling framework (e.g., GREET, Wang *et al*., 2012) to link ecosystem-based process of biomass feedstock production with other production, refinery, conversion and transportation processes in the energy system (Davis *et al*., 2009; Kwon *et al*., 2013).

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APPENDICES

Appendix A Technical Notes of Nitrification and Denitrification in AgTEM

In AgTEM (**Figure** A 1), the three major nitrogen oxide (NO_X) fluxes (namely, N_2O, NO and N_2) are modeled in the processes of nitrification and denitrification (**Figure** 2.1 in the main text, **Table** A 1). NO_X (NOX) in the model accounts for the total NO (NO_{ntf}) and N_2O ($N2O_{ntf}$) emissions from nitrification and N_2 ($N2_{dtf}$) and N_2O ($N2O_{dtf}$) emissions from denitrification (Eqn. A1). Total N_2O flux ($N2O$) includes both $N2O_{ntf}$ and $N2O_{dtf}$ fluxes.

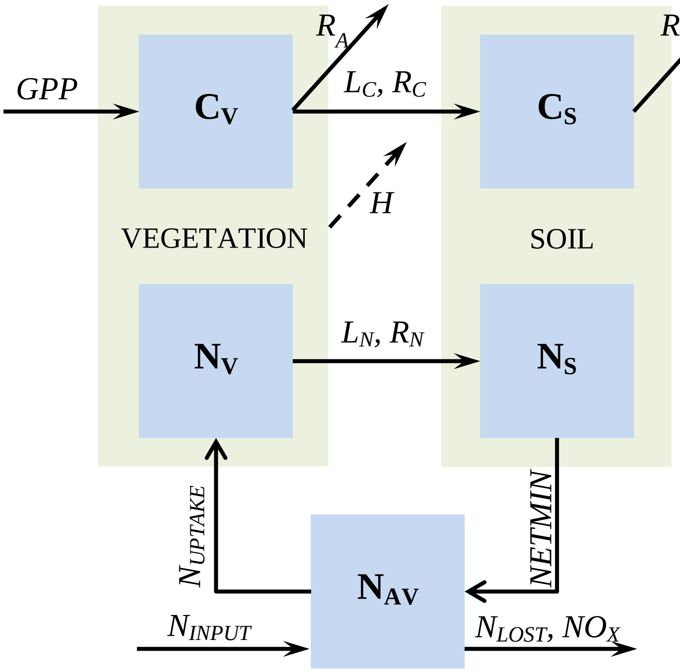

Figure A 1 A schematic flow of carbon and nitrogen in AgTEM. Square blocks show state variable of C and N in vegetation and soils. Arrows indicate C and N fluxes; the dashed arrow shows C and N fluxes due to possible harvest (*H*). See text for more description and acronyms in **Table** 2.2.

$$NOX = N2O_{ntf} + NO_{ntf} + N2O_{dtf} + N2_{dtf} \tag{A1}$$

Nitrification describes the process of the biological oxidation of ammonia with oxygen into nitrite and nitrate (**Figure** 2.1); it is a very important step in the nitrogen cycle in soil. The nitrification rate (N_{ntf}), measuring the nitrification reaction in soil, is highly dependent on a number of environmental factors. These factors include the N concentration, temperature, soil hydrologic properties and soil pH. In AgTEM, the nitrification rate is modeled as:

$$N_{ntf} = N_{NH4}\left[1 - \exp(-k_{ntf}\, f\left(W_{ntf}\right) f\left(T\right) f(pH))\right]\left[1 - \frac{N_{NH4}}{N_{cst} + N_{FET} + N_{NH4}}\right] \tag{A2}$$

where N_{NH4} is the NH_4^+-N concentration in soil layer, N_{FET} is NH_4^+-N concentration in added urea and NH_4^+-based fertilizer, and N_{CST} is a constant value adjusting the maximum nitrification rate and can be calibrated using data showing the maximum flux rate of N_2O as an indication of the maximum rate of nitrification at high NH_4^+-N levels (Parton *et al.*, 1996). k_{ntf} is a parameter used to simulate the environmental impacts on nitrification, set as constant (Bradbury *et al.*, 1993) (**Table** A 2). $f(T)$, $f(W_{ntf})$ and $f(pH)$ are constraints which depend on temperature, soil water content and soil pH, respectively. With increasing NH_4^+-N concentration, the nitrification rate increases asymptotically with an extremely high speed at relatively lower N content, and eventually approximates to an upper threshold level at higher soil N levels (**Figure** A 2a).

Table A 1 Variables and parameters used in AgTEM to simulate soil nitrogen dynamics and nitrogen oxide emissions

Variable/Parameter	Definition	Unit
Nitrogen state variables		
N_{FET}	NH_4^+-N concentration in added urea and NH_4^+-based fertilizer	$g\ N\ m^{-2}$
N_{NH4}	NH_4^+-N concentration in soil layer	$g\ N\ m^{-2}$
N_{NO3}	NO_3^--N concentration in soil layer	$g\ N\ m^{-2}$
Nitrogen fluxes		
$N2O_{ntf}$	Flux of nitrous oxide (N_2O) from nitrification	$g\ N\ m^{-2}\ day^{-1}$
$N2O_{dtf}$	Flux of nitrous oxide (N_2O) from denitrification	$g\ N\ m^{-2}\ day^{-1}$
$N2O_{tot}$	Total flux of nitrous oxide (N_2O)	$g\ N\ m^{-2}\ day^{-1}$
$N2_{dtf}$	Flux of nitrogen (N_2) from denitrification	$g\ N\ m^{-2}\ day^{-1}$
NO_{ntf}	Flux of nitric oxide (NO) from nitrification	$g\ N\ m^{-2}\ day^{-1}$
NOX	Flux of total nitrogen oxides (N_2O, NO and also N_2 included)	$g\ N\ m^{-2}\ day^{-1}$
Nitrification variables and parameters		
EET	Actual evapotranspiration	mm
N_{CST}	Parameter adjusting the maximum nitrification rate	$g\ N\ m^{-2}\ day^{-1}$
N_{ntf}	Nitrification rate	$g\ N\ m^{-2}\ day^{-1}$
IR	Daily irrigation	mm
pH	Soil pH	--

Table A 1 Continued.

PR	Daily precipitation	mm
SOC	Soil carbon density	g C m^{-2}
T_{air}	Daily air temperature	°C
n_{N2O}	Parameter determining N_2O from fully nitrified N	--
n_{NOX}	Parameter determining NO_X from fully nitrified N	--
n_{ntf}	Parameter determining N_2O from partially nitrified N at field capacity	--
ω_d	Soil moisture deficit at the permanent wilting point (at -100 kPa)	mm
ω_f	Available water capacity, the difference between field capacity and the permanent wilting point	mm
ω_i	Soil water held in a particular soil layer above the permanent wilting point	mm
ω_s	Difference between saturation and the permanent wilting point	mm
Denitrification variables and parameters		
C_{CO2}	CO_2 produced during mineralization	g C m^{-2} day^{-1}
clay	percentage content of soil clay	%
$N_{0.5}$	soil NO_3^--N concentration at which the reaction rate is half of the potential denitrification rate	g N m^{-2} day^{-1}
N_{dtf}	actual denitrification rate	g N m^{-2} day^{-1}

Table A 1 Continued.

N_{dtfmax}	potential denitrification rate	g N m^{-2} day^{-1}
sand	percentage content of soil sand	%
ρ_{N2}	Parameter determining N_2 lost from denitrified N at field capacity	--
ρ_{NO3}	soil NO_3^--N content at which N is released in equal amount of N_2 and N_2O in the denitrification process	g N m^{-2} day^{-1}

$f(W_{ntf})$ is modeled as a function of soil water held in a particular soil layer above the permanent wilting point (ω_i), available water capacity (ω_f), the difference between saturation and the permanent wilting point (ω_s), and soil moisture deficit at -100 kPa (ω_d) (Bradbury *et al.*, 1993; Smith *et al.*, 2010a; Bell *et al.*, 2012). It is assumed that, when water retention is approximately between -33 kPa and -100 kPa (field capacity), $f(W_{ntf})$ equals 1, and $f(W_{ntf})$ declines when soil water leaves this range:

$$f(W) = \begin{cases} 0, & (\omega_i \le 0) \\ 1 - \dfrac{(1-\omega_0)(\omega_f - \omega_d - \omega_i)}{\omega_f - \omega_d}, & (0 < \omega_i < (\omega_f - \omega_d)) \\ 1.0, & ((\omega_f - \omega_d) < \omega_i < \omega_f) \\ 1 - \dfrac{(1-\omega_0)(\omega_i - \omega_f)}{\omega_s - \omega_f}, & (\omega_f < \omega_i < \omega_s) \\ 0, & (\omega_i > \omega_s) \end{cases} \tag{A3}$$

where ω_0 is a parameter set as constant to adjust the soil water rate for decomposition at the permanent wilting point and at saturation (Smith *et al.*, 2010a). For unknown soil

Table A 2 Values of parameters used to calibrate nitrogen oxide emissions in AgTEM

Parameter	Value	Sources of calibration
N_{CST}	50	Smith *et al.*, 2010a; Smith *et al.*, 2010b
$N_{0.5}$	16.5	Bell *et al.*, 2012
k_{ntf}	0.6	Bradbury *et al.*, 1993
ω_0	0.2	Smith *et al.*, 2010a; Bell *et al.*, 2012
n_{ntf}	0.02	Bell *et al.*, 2012
n_{NOX}	0.02	Bell *et al.*, 2012
n_{N2O}	0.6	Bell *et al.*, 2012
ρ_{N2}	0.5	Bell *et al.*, 2012, Smith *et al.*, 2010a
ρ_{NO3}	200	Bell *et al.*, 2012

water variables, soil water content ω_i is calculated as soil moisture deficit according to Bradbury *et al.* (1993):

$$\frac{d\omega_{i,t}}{dt} = PR_t + IR_t - EET_t \tag{A4}$$

where ω_i at time step *t* is closely related to water input into soil; PR, IR and EET are the daily water budget in terms of precipitation, irrigation and evapotranspiration, respectively. Available water capacity ω_f is defined as the difference between field capacity and the permanent wilting point; ω_f is modeled as a function of percentage content of soil sand (*sand*) and clay (*clay*). ω_s follows the pedotransfer function using soil texture and soil carbon density (*SOC*) (Smith *et al.*, 2010a, b):

$$\omega_s = 0.002SOC + 0.25clay\ (mm) \tag{A5}$$

The temperature impact $f(T)$ on nitrification is modeled according to Bradbury *et al*. (1993), using air temperature (T_{air}):

$$f(T) = \frac{47.9}{1 + \exp\left(\frac{106}{(T_{air} + 18.3)}\right)} \tag{A6}$$

Soil pH modifies nitrification as in Eqn. (A7) (Parton *et al.*, 1996):

$$f(pH) = 0.56 + \frac{tan^{-1}\left[0.45\pi\left(pH - 5\right)\right]}{\pi} \tag{A7}$$

where π is the mathematical constant *Pi*, and *pH* is soil pH. **Figure** A 2 shows the impacts of soil NH_4^+-N concentration (**Figure** A 2a), soil moisture or water content (**Figure** A 2b), temperature (**Figure** A 2c) and soil pH (**Figure** A 2d) on the relative nitrification rate.

The nitrification rate is further used to model N_2O and NO gases emitted during soil nitrification. It is assumed that a certain percentage (n_{NOX}) of the fully nitrified N will be lost as gas, some part of which will be lost (n_{N2O}) as N_2O and the rest (1- n_{N2O}) as NO (Bell *et al.*, 2012). Of the partially nitrified N, a certain proportion (n_{ntf}) is lost as N_2O at field capacity with a linear declining rate as soil water decreases. For the soil at particular soil moisture content, the NO_2 and NO emissions are modeled in Eqn. (A8) and Eqn. (A9), respectively:

$$N2O_{ntf} = \left(\frac{n_{ntf}\omega_i}{\omega_f} + n_{NOX}n_{N2O}\right)N_{ntf} \tag{A8}$$

$$NO_{ntf} = n_{NOX}\left(1 - n_{N2O}\right)N_{ntf} \tag{A9}$$

where $N2O_{ntf}$ and NO_{ntf} are N_2O and NO emissions from nitrification, respectively. n_{ntf}, n_{NOX} and n_{N2O} are parameters used to define the proportion of N_2O from partially nitrified N at field capacity, NO_X from fully nitrified N and N_2O from fully nitrified N, respectively.

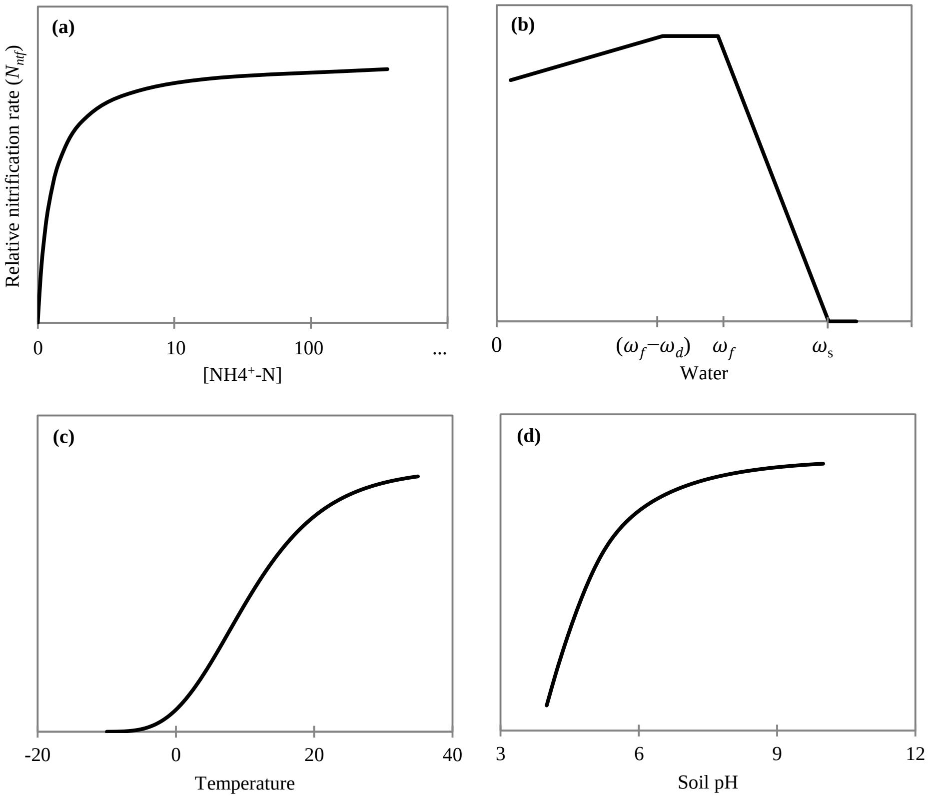

Figure A 2 Simulation of nitrification responding to substrate concentration, climate and soil environment. Nitrification rate depends on (a) soil ammonium concentration [NH_4^+-N], (b) soil water, (c) temperature, and (d) soil pH. The sizes of the axes do not necessarily reflect the actual extent of the variables.

Nitrogen oxide emissions also come from the soil NO_3^--N through denitrification. In AgTEM, the denitrification rate is modeled following Henault *et al.* (2000, 2005), depending on the soil nitrate concentration, soil water content and soil biological activity:

$$N_{dtf} = N_{dtfmax} f\left(NO3\right) f\left(W_{dtf}\right) f\left(BIO\right) \quad \text{(A10)}$$

where *f(NO3)*, $f(W_{dtf})$ and *f(BIO)* are the impacts of soil NO_3^--N concentration (**Figure** A 3a), soil water content (**Figure** A 3b) and soil biological activity (**Figure** A 3c) on

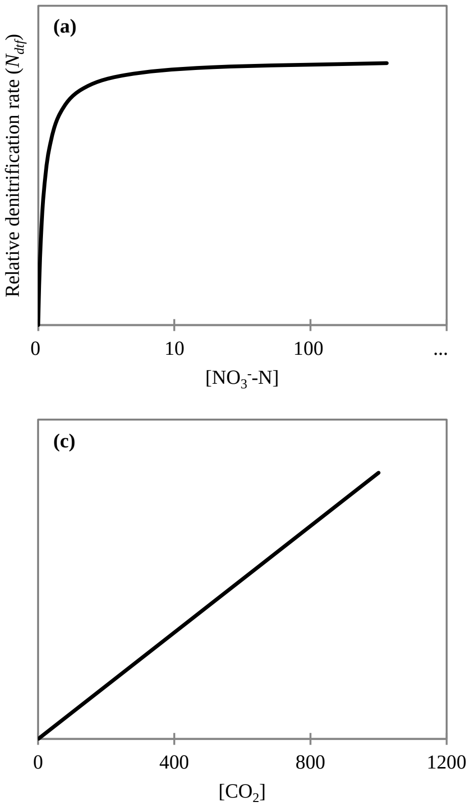

Figure A 3 Simulation of denitrification responding to substrate concentration and soil environment. Denitrification rate relates to (e) soil nitrate concentration [NO_3^--N], (f) soil water and (g) CO_2 change in soil. The sizes of the axes do not necessarily reflect the actual extent of the variables.

potential (N_{dtfmax}) and therefore actual denitrification rate (N_{dtf}), respectively. N_{dtfmax} is a site-specific parameter, and can be calibrated by scaling it to output peaks at times of optimal denitrification conditions (Henault *et al.*, 2000).

Soil nitrate affects the nitrification rate through *Michaelis-Menten* kinetics (Henault *et al.*, 2000):

$$f\left(NO3\right) = \frac{N_{NO3}}{N_{0.5} + N_{NO3}} \tag{A11}$$

where N_{NO3} is the real time soil NO_3^--N concentration, and the *Michaelis* constant $N_{0.5}$ is the NO_3^--N concentration at which the reaction rate is half of the N_{dtfmax}.

The soil water factor $f(W_{dtf})$ is modeled according to (Grundmann *et al.*, 1987), and the soil biological activity factor *f(BIO)* is calculated as a function of CO_2 produced during mineralization, following Bradbury *et al.* (1993):

$$f\left(W_{dtf}\right) = \left[\frac{\left(\omega_i / \omega_f\right) - 0.62}{0.38}\right]^{1.74} \tag{A12}$$

$$f\left(BIO\right) = 0.05C_{CO2} \tag{A13}$$

The N lost via denitrification is then released as N_2 ($N2_{dtf}$) and N_2O ($N2O_{dtf}$). The proportion of N_2 gas lost is modeled as a function of soil water and soil nitrate content, as discussed in Parton *et al*. (1996) and Bell *et al*. (2012):

$$N2_{dtf} = N_{dtf}h\left(W_{dtf}\right)h\left(NO3\right) \tag{A14}$$

where soil water content $h(W_{dtf})$ and soil nitrate content $h(NO3)$ constraints on the denitrification rate are modeled in Eqn. (A15) and Eqn. (A16), respectively (Bell *et al.*, 2012):

$$h\left(W_{dtf}\right) = \rho_{N2}\left(\frac{\omega_i}{\omega_f}\right) \tag{A15}$$

$$h\left(NO3\right) = 1 - \left(\frac{N_{NO3}}{\rho_{NO3} + N_{NO3}}\right) \tag{A16}$$

where ρ_{N2} is the proportion of N_2 lost from denitrified N at field capacity, and ρ_{NO3} is a parameter indicating the soil NO_3^--N content at which N is released in equal amount of N_2 and N_2O in the denitrification process. The proportion of N_2O lost by denitrification is then calculated as:

$$N2O_{dtf} = N_{dtf}\left[1 - h\left(W_{dtf}\right)h\left(NO3\right)\right] \tag{A17}$$

Total N_2O ($N2O_{tot}$) emitted from soil can then be calculated as:

$$N2O_{\mathrm{tot}} = N2O_{ntf} + N2O_{dtf} \tag{A18}$$

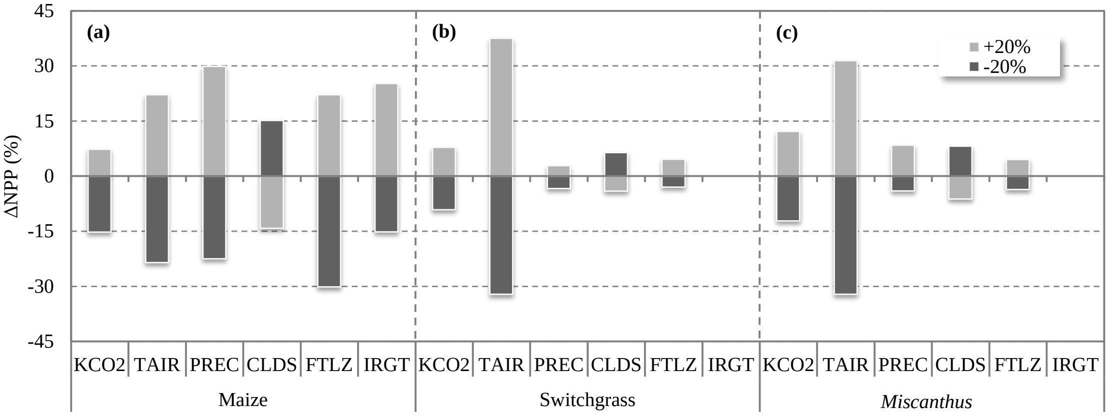

Figure A 4 Sensitivity of NPP responding to model input (±20% change) in different ecosystems. Estimates were made for (a) maize at site Fort Collins, CO, (b) switchgrass at site Chatham, MI and (c) *Miscanthus* at site Urbana, IL. Abbreviations are same as in **Figure** 2.3.

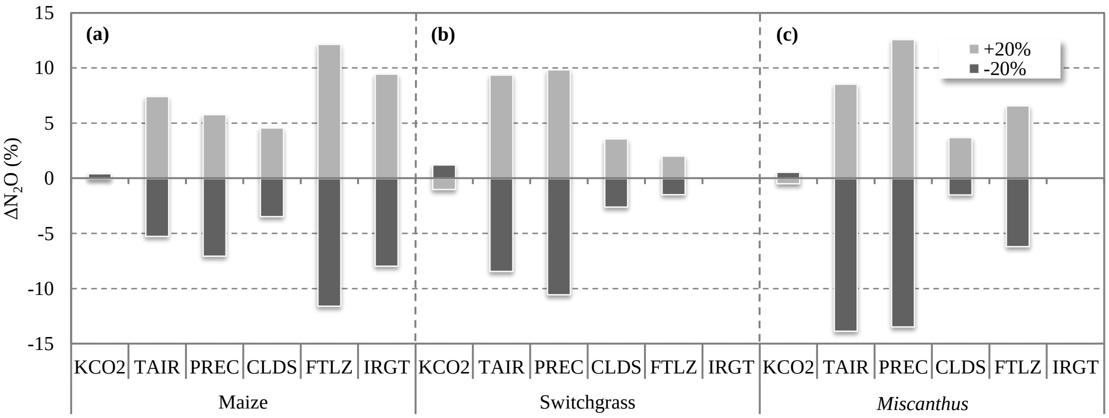

Figure A 5 Sensitivity of N_2O responding to model input (±20% change) in different ecosystems. Estimates were made for (a) maize at site Fort Collins, CO, (b) switchgrass at site Chatham, MI and (c) *Miscanthus* at site Urbana, IL. Abbreviations are same as in **Figure** 2.3.

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Appendix B Biomass, Land and GHG in Cropland

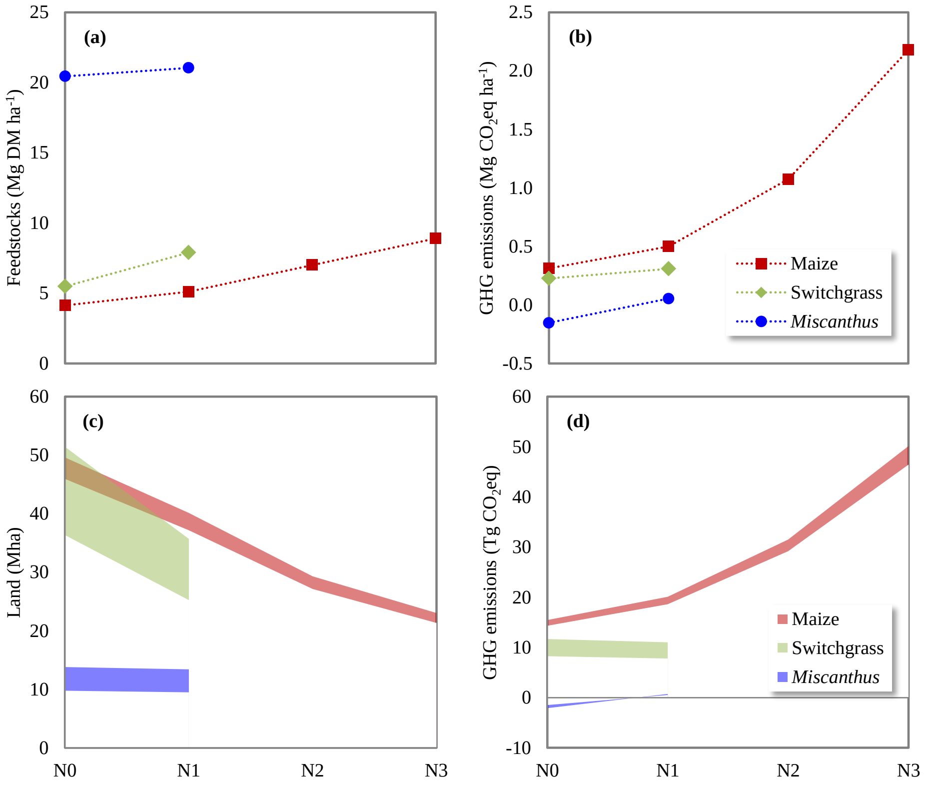

Figure B 1 Biomass feedstocks production and GHG emissions of maize, switchgrass and *Miscanthus*. (a) Biomass production and (b) corresponding GHG emissions at given land under different N input levels. (c) Total land required and GHG emitted to reach the 2022 biofuel target of 79 billion liters of cellulosic ethanol. The upper and lower bounds in (c) and (d) indicate corresponding levels under current and potential biofuel conversion technologies.

Appendix C Carbon and Nitrogen Dynamics in Marginal Lands

Table C 1 Estimated net carbon exchange (NCE) and N_2O fluxes at different nitrogen input levels in the conterminous United States

N input	NCE (g C m^{-2} yr^{-1})		N_2O (g n m^{-2} yr^{-1})	
	Switchgrass	*Miscanthus*	Switchgrass	*Miscanthus*
N0	-3.3 (0.3)	-4.0 (0.4)	0.05 (0.00)	0.05 (0.01)
N1	-6.9 (0.6)	-8.1 (0.7)	0.08 (0.01)	0.08 (0.01)
N2	-10.6 (1.0)	-14.8 (1.6)	0.15 (0.02)	0.14 (0.01)
N3	-11.6 (0.2)	-24.3 (2.2)	0.23 (0.03)	0.23 (0.02)

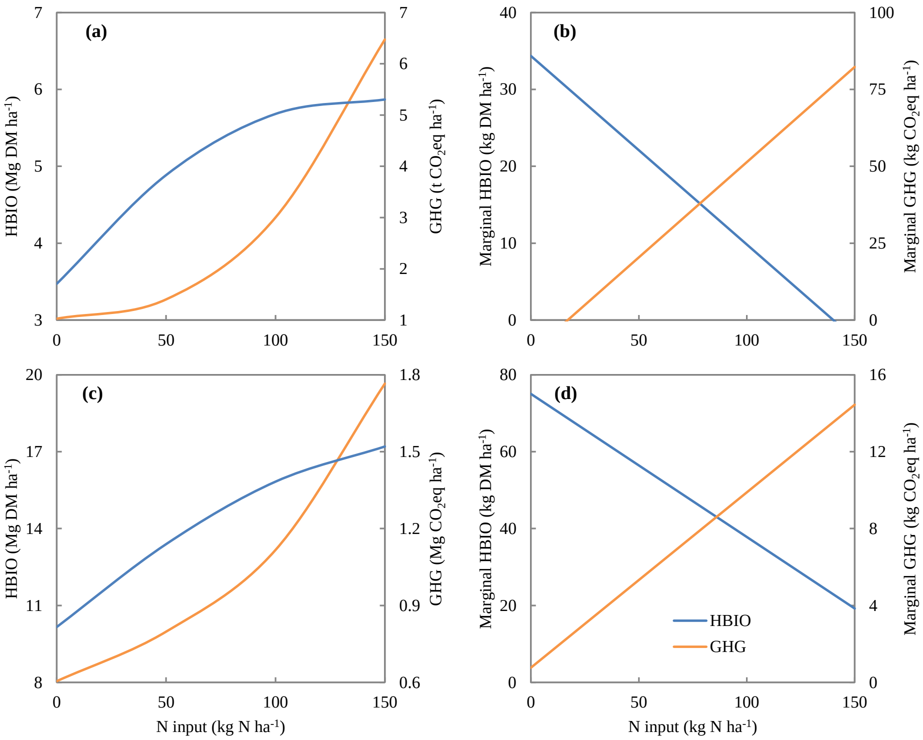

Figure C 1 Estimated HBIO and GHG from marginal lands with increasing use of N. Estimates for HBIO and GHG of (a) switchgrass and (b) *Miscanthus* were based on national average results (**Table** 4.1); marginal HBIO and marginal GHG of (c) switchgrass and (d) *Miscanthus* were based on polynomial (order 2) relationships between HBIO or GHG and N input.

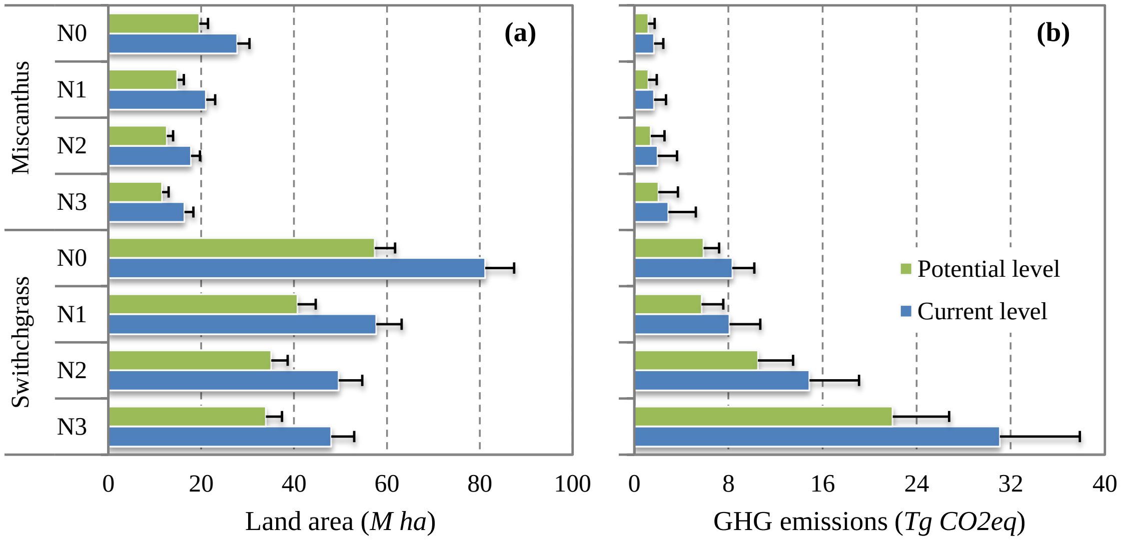

Figure C 2 Estimated demand of marginal lands and GHG emissions to achieve the 2022 biofuel mandate of 79 billion liters of cellulosic ethanol. Model estimates of (a) land demand and (b) GHG emissions were made for switchgrass and *Miscanthus* under current and potential biofuel conversion efficiencies.

VITA

VITA

ZHANGCAI QIN

web.ics.purdue.edu/~qin9
Graduate school, Purdue University

EDUCATION

PURDUE UNIVERSITY
Doctorate of Philosophy
Earth, Atmospheric & Planetary Sciences
Research: *ecosystem modeling, global biogeochemical cycling, ecohydrology, bioenergy and environment*

December 2013
West Lafayette, IN, US

CHINESE ACADEMY OF SCIENCES
Master of Science
Atmospheric Physics & Environment
Research: *modeling, soil carbon, carbon sequestration potential*

July 2010
Beijing, China

CHINA AGRICULTURAL UNIVERSITY
Bachelors of Agronomy and Business Administration
Resources & Environmental Sciences, Business
Research: *land use change, soil carbon/nitrogen dynamics, fertilizer marketing*

July 2007
Beijing, China

RESEARCH INTERESTS & SKILLS

Interactions, feedbacks and biogeochemical cycling among atmosphere, terrestrial ecosystems and human dimensions under climate change, with special foci on: 1) ecosystem modeling and remote sensing; 2) land use change, climate change and greenhouse gas emissions; 3) hydrology and ecosystem water balance; (4) bioenergy, environment and economy.

Field & lab experiment; statistics; empirical & mechanistic modeling; remote sensing & GIS analysis; life cycle assessment and cost-benefit analysis.

SCIENTIFIC EXPERIENCE

RESEARCH ASSISTANT 2010-2013
Purdue University West Lafayette, IN, US
Department of Earth, Atmospheric & Planetary Sciences
Participated in projects funded by NSF, NASA and DOE; assisted PI with project management; conducted researches.

RESEARCH ASSISTANT 2007-2010
Chinese Academy of Sciences Beijing, China
Institute of Atmospheric Physics
Participated in several national and international research projects; conducted researches.

RESEARCH ASSISTANT 2006-2007
China Agricultural University Beijing, China
Undergraduate Research Program
Assisted PI with experiment design and lab analysis; conducted researches.

PUBLICATIONS

See PUBLICATIONS Section.

SELECTED PRESENTATIONS

Qin Z. Bioenergy vs. Environment: estimating biofuel, land, water and greenhouse gas emissions using a data-model fusion approach. *Argonne National Laboratory*. Chicago, US. Aug. 22, 2013.

Qin Z. Bioenergy, land, water and greenhouse gases: what can we expect from the croplands? *EAPS department seminar 2013 spring, Purdue University*. Indiana, US. Feb. 14, 2013.

Qin Z. Energy vs. Environment: modeling the biofuel production and GHG emissions from bioenergy ecosystems using biogeochemical model. *Modeling ecosystems and biogeochemical cycles, Purdue University*. Indiana, US. Oct. 10, 2012.

Qin Z., Zhuang Q., Chen M., He Y. Thermal acclimation impacts on global carbon dynamics. *2012 ESA Annual Meeting*. Portland, US. Aug. 5-10, 2012.

Zhuang Q., **Qin Z**., Chen M. Potential land use change effects on water balance due to bioenergy development in the conterminous United States. *AGU Chapman conference on remote sensing of the terrestrial water cycle*. Hawaii, US. Feb. 19-22, 2012.

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PROFESSIONAL SERVICES

Member of
  American Geophysical Union
Reviewer/Referee for
  African Journal of Agricultural Research; Applied Geography; Ecological Modelling; Environmental Science & Technology; Global Change Biology Bioenergy; GTAP Technical Paper Series; PLOS ONE; Renewable & Sustainable Energy Reviews

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PUBLICATIONS

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Qin Z, Zhuang Q, Zhu, X (2013) Carbon and nitrogen dynamics in bioenergy ecosystems: 2. Potential greenhouse gas emissions and global warming intensity in the conterminous United States. *Global Change Biology Bioenergy*, doi: 10.1111/gcbb.12106.

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