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Hydrologic and water quality impacts from perennial crop production on marginal lands

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HYDROLOGIC AND WATER QUALITY IMPACTS FROM PERENNIAL CROP PRODUCTION ON MARGINAL LANDS

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To My Dear Parents, and Zhuzi

献给我的父亲、母亲、竹子

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ABSTRACT

Feng, Qingyu. Ph.D., Purdue University, May 2016. Hydrologic and Water Quality Impacts from Perennial Crops Production on Marginal Lands in the Upper Mississippi River Basin. Major Professor: Indrajeet Chaubey.

Marginal lands are proposed as a viable option for producing biofeedstocks as these lands are not heavily engaged in agricultural production or may not be suitable for intensive row-crop food/feed production. However, meeting biofeedstock production goals will require large amount of marginal lands and the unintended consequences of producing biofeedstocks on marginal lands are not fully clear. The overall goal of this study was to evaluate the productivity of biofeedstocks on marginal lands and the potential impacts on hydrologic and water quality processes from the land use conversion.

This study was conducted in the Upper Mississippi River Basin (UMRB). First, the suitability of marginal lands in this region was evaluated for the growth of three candidate biofeedstock crops, switchgrass, *Miscanthus* and hybrid poplar. The evaluation was conducted using a fuzzy logic based land suitability evaluation method. Then, the simulation of switchgrass and *Miscanthus* growth during their establishment periods in the Soil and Water Assessment Tool (SWAT) model was improved. Finally, the model was used to evaluate the impacts on hydrologic and water quality processes due to production of switchgrass and *Miscanthus* on marginal lands in the UMRB region.

The results indicated that 23% of the UMRB area included marginal lands. Among these lands, 40% of them were poorly suitable for the production of biofeedstock crops. Biofeedstocks produced from these marginal lands could be converted to biofuels that contributed 14 to 25% of the 132 billion liter biofuel goals set by the Energy Independence and Security Act (EISA) 2007. The model simulation results indicated that producing perennial biofeedstock crops on marginal land would reduce annual stream flow by 20% and 29% and sediment load by 26% to 35% at the watershed outlet. The reduction was less during the establishment periods of perennial grasses (first 2 to 3 years of switchgrass and 2 to 4 years of *Miscanthus*) than during the post establishment periods.

The results of this study indicated that marginal land in the UMRB region could be a viable choice of land resources for biofuel development and could be used to produce almost one quarter of biofuel production goals. At the same time, water quality in the watershed could be improved. The information could be used by stakeholders to create regional biofuel development and watershed management plans.

CHAPTER 1. INTRODUCTION

1.1 Statement of the Problem

The proposed development of biofuel has trigged the concerns on land requirement for bioenergy feedstock production and the potential environmental impacts as a consequence of land conversion. One of the concerns in large scale biomass feedstock production is how it will affect availability of land for food or animal feed productions. Use of marginal land is advocated to reduce the competition for land among food, feed, and fuel. Preliminary estimation indicates that large areas of marginal land are available and could make meaningful contribution to biofuel development (Campbell *et al.*, 2008; Tang *et al.*, 2010; Cai *et al.*, 2011). However, marginal land is usually less productive land and could have poor land conditions. Therefore, their suitability for biomass crops is not always guaranteed. Thus, even though the total area of marginal land is promising, it is not clear how much is actually suitable for bioenergy feedstock production. This study is proposed to evaluate marginal land's suitability for three representative bioenergy feedstock crops (switchgrass, *Miscanthus*, and hybrid poplar) that can be potentially grown in such areas. The study is conducted in the Upper Mississippi River Basin. The evaluation is performed using a fuzzy logic based method because the method is able to deal with the uncertain and empirical knowledge on environmental factors that may potentially limit the production of bioenergy crops. After the land suitability is evaluated, the potential environmental impacts are evaluated under projected biofeedstock production scenarios. The evaluation is conducted with the Soil and Water Assessment Tool (SWAT) model. The SWAT model is modified to improve the representativeness of establishment stage of switchgrass and *Miscanthus*. This modification is needed because the current SWAT model does not include capabilities to simulate perennial crop establishment stage, which is a time window for potentially higher soil erosion and nutrient losses and associated negative environmental impacts.

1.2 Introduction

Land availability and potential environment impacts are of great concerns in biofuel development. In the U.S, the biofuel development started in 1940s and was accelerated by the enactment of Renewable Fuel Standard (RFS) within the Energy Independence and Security Act (EISA) (Tyner, 2008). The EISA mandated that 132 billion liter biofuels should be used in the transportation section by 2022, and 60.6 billion liter shall come from cellulosic biofuel. Cellulosic biofuel is produced with biomass feedstock that contains cellulose, such as perennial grasses, trees (e.g. hybrid poplar), crop residue, etc. To produce adequate biomass to meet the goal set by the EISA, a considerably large area of land will be required. The United States Department of Agriculture (USDA) estimated that 11 million ha of cropland will be required to meet this goal (USDA Biofuel Strategic Production Report, 2011). The implication of land requirement triggers concerns on the availability of land. Currently, available arable land is already under great pressure for the production of food, feed, and fiber. The potential increase in population and projected climate change is adding further pressure on land productivity to meet these goals. Thus, proper land choices for biomass production are needed to reduce the competing demands. The large scale biomass feedstock production can also have unintended impacts on environment due land use/land management changes. These potential impacts need to be evaluated carefully to minimize potential negative impacts.

Marginal lands are proposed to be viable solutions for biomass feedstock production (Tilman *et al.*, 2006; Field *et al.*, 2008; Searchinger *et al.*, 2008; Kang *et al.*, 2013a). Marginal lands generally have poor land quality and are not actively engaged in agricultural production (Wiegmann *et al.*, 2008; Kang *et al.*, 2013a). In literature, marginal lands are defined in multiple ways. For example, several studies consider marginal lands as land areas that have Land Capability Class (LCC) 3 to 8 based on soil databases (Hamdar, 1999; Gelfand *et al.*, 2013). Cai *et al.* (2011) define marginal land as land with low productivity according to soil quality, slope, and climate conditions. Similarly, other studies consider marginal land from land use data as idle land, waste land, abandoned land, and buffer areas (Gopalakrishnan *et al.*, 2009; Tang *et al.*, 2010). Irrespective of the definition used, these studies suggest that marginal lands are promising for biofuel feedstock production due to their vast availability (Campbell *et al.*, 2008; Gopalakrishnan *et al.*, 2009; Cai *et al.*, 2011; Niblick *et al.*, 2013).

Previous studies on land availability estimation of marginal land do not include the consideration of marginal lands' heterogeneity in terms of their suitability for bioenergy feedstock production. In reality, not all marginal lands may be suitable to meet specific biofuel crop growth requirements. For example, growth of switchgrass could be affected by soil properties such as salinity, pH and climatic conditions such as growing degree days and precipitation (Monti, 2012). In addition, the marginal lands should be suitable in terms of machinery accessibility and operational safety. Machinery operation safety could be low on high slope marginal lands (Elsheikh *et al.*, 2013). A land suitability analysis of marginal land specific to these possible perennial biomass feedstock crops and operational constraints can improve our assessment of the amount of land available for biomass feedstock production. In addition, land suitability will also facilitate making decisions and policies related to land distribution for biofuel feedstock crop production and reduce uncertainty in environmental impact evaluations.

Land suitability analysis is a procedure for assessing land qualities for given purposes (Joss *et al.*, 2008; Elsheikh *et al.*, 2013). This procedure will help determine the suitability of marginal land for bioenergy feedstock crop growth based on their growth requirement and marginal land properties. Among many available procedures and techniques to conduct land suitability analysis, fuzzy logic based techniques is one of the most popular techniques (Malczewski, 2004) due to its ability to address problems that include imprecise and uncertain data (Joss *et al.*, 2008). The basic concept of fuzzy theory is fuzzy set, which includes a collection of elements with their membership (Zadeh, 1965). Membership describes the degree of belongingness of the element to the fuzzy set and is defined by a membership function (Joss *et al.*, 2008). In traditional set theory, the belongingness of one element to a set only includes two values, belonging to the set or not. In fuzzy set theory, the membership value ranged from 0 to 1. An element with membership value of 0 is considered completely not belonging to the fuzzy set, while an element with membership value of 1 is considered completely belonging to the fuzzy set. An element with membership value between 0 and 1 is considered belonging to the fuzzy set to some degree. This concept of membership value provided a quantitative method to process qualitative variable values, such as tall, short, large, high, low, etc. Fuzzy methods have been applied in land suitability evaluation since the 1990s (Baja *et al.*, 2001; Sicat *et al.*, 2005). Currently, the available knowledge about biofuel feedstock crops such as switchgrass and *Miscanthus* are mainly qualitative and based on expert opinions. Thus, fuzzy logic based technique can be appropriate for land suitability analysis for production of these crops.

Environmental impact is another important concern in biomass feedstock production, especially when they are grown on marginal lands. The unfavorable features of marginal lands generally resulted into fragile environmental conditions, such as thinner soil layers, poor drainage conditions, infertile soils, higher slope condition, etc. With these features, marginal lands tend to cause low crop productivity and have higher soil and nutrient losses. Some marginal land could also be areas that contribute significant nonpoint source (NPS) pollutants to water bodies. Furthermore, these features make the land more sensitive to changes of land use types. When marginal land are converted to biomass feedstock production, the impacts could be either positive or negative depending on the properties of land quality, growth characteristics of biofuel feedstock crops, and the management practices (Engel *et al.*, 2010; Cibin *et al.*, 2012). It is expected that perennial biomass feedstock crops, such as, switchgrass, *Miscanthus*, and hybrid poplar are suitable to grow on marginal land and could bring positive environmental impacts, especially when these lands are high in NPS pollutions. Both field measurement and model simulations studies have found that growing perennial grasses could help reduce sediment and nutrient loss to water bodies. These positive impacts could be further enhanced if perennial grasses are incorporated in best management practices such as vegetated filter strips and grassed waterways (Gopalakrishnan *et al.*, 2009; Cibin *et al.*, 2012). However, negative impacts are also possible with improper biomass production plans. The large areas required to produce biomass indicates watershed scale is appropriate to evaluate impacts on hydrologic and nutrient loss processes and develop proper biomass production allocation plans to enhance positive impacts and reduce potential negative impacts.

Watershed scale impacts from possible biomass production scenarios have been mainly conducted using simulation models. Soil and Water Assessment Tool (SWAT) is identified as a potential tool to assess the potential impacts of biomass production on hydrologic and water quality (Engel *et al.*, 2010). The SWAT model includes a plant growth module in which the growth of perennial grasses such as switchgrass and *Miscanthus* can be simulated. The representation of these perennial grasses is improved by developing growth parameters from field measured data (Trybula *et al.*, 2014). However, the model in its current representation does not include establishment phase of the bioenergy crops. In reality, these perennial biomass feedstock crops take multiple years to reach full growth potential, and these periods are called establishment period. The canopy cover during establishment phase might be smaller and could protect the ground from soil erosion less efficiently than during the post establishment period. Similarly transpiration and nutrient uptake may also be different during establishment phase. Consequently, the establishment stage could be one time period when significant soil erosion and nutrient loss could happen (Seth Dabney, personal communication). Several studies suggest up to 3 years of establishment period for switchgrass (Sharma *et* *al.*, 2003; Heaton *et al.*, 2004; McLaughlin & Adams Kszos, 2005) and 5 to 6 years for *Miscanthus* (Lesur *et al.*, 2013). An improved representation of establishment stage of these perennial crops in the SWAT model is needed to accurately evaluate potential impacts of biofeedstock production during this period.

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CHAPTER 2. MARGINAL LAND SUITABILITY FOR SWITCHGRASS *MISCANTHUS* AND HYBRID POPLAR IN THE UPPER MISSISSIPPI RIVER BASIN

2.1 Abstract

Marginal lands are recommended as a viable land resource for biofeedstocks production, but their suitability for biofeedstock crops growth are poorly understood. This study assessed the suitability of marginal lands in Upper Mississippi River Basin (UMRB) for three promising biofeedstock crops, switchgrass, *Miscanthus* and hybrid poplar. The land suitability was categorized into 5 suitability classes (not-, poorly-, moderately-, good- and highly-suitable) based on a fuzzy logic based land suitability evaluation procedure. The results showed that 60% of marginal lands in UMRB were moderately to highly suitable for growth of the targeted biofeedstock crops. Predicted bioethanol production from marginal land in the UMRB with consideration of suitability level was two thirds of the production predicted without consideration of suitability level. Our results better constrain the potential of marginal land for biofuel production as well as the importance of land suitability evaluation for policy analysis targeting biofuel development on marginal lands.

2.2 Introduction

In response to climate change and energy crisis, biofuel is considered a partial solution to meet future energy requirements. Many countries including the U.S. have developed ambitious biofuel goals which require producing vast quantities of biomass. Achieving these ambitious biomass production goals is challenging due to the potential competition for agricultural resources already being used to produce food, animal feed, and fiber (Harvey & Pilgrim, 2011). Agricultural land is already under pressures from various sources including the demand for food to feed by the current and projected population, land degradation, urbanization, among others (Harvey & Pilgrim, 2011; Kastner *et al.*, 2012). Consequently, marginal land is proposed for biofuel production to alleviate the potential risk of competing for land currently used for agricultural production of conventional food/feed crops (Gelfand *et al.*, 2013; Cobuloglu & Büyüktahtakın, 2015). For biomass production, marginal land is generally considered as a set aside land and unsuitable for row crop production (Kang *et al.*, 2013a). Marginal land availability has been estimated to be ranging from 0.1 to 1 billion ha, globally (Kang *et al.*, 2013b). However, the actual conversion of marginal land for biofeedstock production is not straightforward and efforts are needed to quantify the potential economic and environmental impacts on hydrology and water quality processes (Lewis *et al.*, 2014).

Heterogeneous quality of marginal land is one of the difficulties for practically converting marginal land for biomass production. Land could be considered marginal for many reasons including poor soil structure, soil degradation, site abandonment (Campbell *et al.*, 2008; Milbrandt *et al.*, 2014) or environmental contamination (Gopalakrishnan *et al.*, 2011). Lands located along streams and roads are also considered as marginal

(Gopalakrishnan *et al.*, 2009; Lu *et al.*, 2009). The quality and productivity of these different types of marginal lands vary considerably. Theoretically, all of these lands could well-suited for biofeedstock crop production, which is the assumption made by previous studies estimating the contribution of marginal land to the US biofuel production (Campbell *et al.*, 2008; Cai *et al.*, 2011). This assumption could not be verified in reality since their heterogeneous qualities result into different suitability for biomass crop growth (Shortall, 2013).

Generally, perennial biomass crops such as switchgrass, *Miscanthus*, and hybrid poplar are recommended to be produced on marginal lands (McLaughlin & Adams Kszos, 2005; Heaton *et al.*, 2008; Sannigrahi *et al.*, 2010; Werling *et al.*, 2014). These perennial crops are selected as candidate biofeedstock crops due to their higher biomass yield and relatively low input requirement compared to traditional annual crops (McLaughlin & Adams Kszos, 2005; Heaton *et al.*, 2008). These properties not only are ideal for being candidates of biofeedstock crops, but also could bring positive impacts on environment, ecosystem services and sustainability of marginal land (Kang *et al.*, 2013b). For example, the high biomass production often reduce erosion by providing better surface protection and minimizing runoff (Vaughan *et al.*, 1989; Parrish & Fike, 2005; Feng *et al.*, 2015). These benefits are based on successful establishment and good aboveground growth, which, in turn, depend on quality of land and proper management practices. Even though these perennial crops are considered to be more widely adaptive than annual crops, their production could still be constrained by environmental factors such as climate conditions, slope, soil depth, salinity, and others. Indeed, marginal lands tend to have more of these constraints than does prime farmland. Therefore, evaluating the suitability of marginal land to support proper land use planning for sustaining both biomass production and environment is needed.

Land use suitability evaluation is a procedure determining qualities of a given land type for a desired purpose (Elsheikh *et al.*, 2013). There are two broad classes of methods, which are the computer-assisted overlaying based methods and the multi-criteria decision making-based methods (Malczewski, 2004). These methods have been developed and applied within Geographic Information System (GIS) frameworks to evaluate land suitability for various land use types including biomass crop production (Malczewski, 2004). The procedure based on fuzzy logic system is among the most popular methods for its ability to deal with evaluation problems involving imprecise and uncertain data (Malczewski, 2004; Joss *et al.*, 2008). For the land suitability evaluation of biofeedstock crops, the fuzzy logic based land suitability assessment procedure is suitable for two reasons: (1) the understanding of growth constraints on biofuel crops are empirical; and (2) even though multiple plot/field years of study data have been collected on biofeedstock crop growth, these crops have not been widely planted like corn (*Zea Mays*), soybeans (*Glycine Max*) and wheat (*Triticum*). Understanding growth limitations of these biomass crops currently relies on experts' opinion or limited experimental evidence. Moreover, scaling up inferences from plots/fields to larger area brings uncertainty embedded in the data for large area analysis. For example, soil properties are commonly included in land suitability assessment (Joss *et al.*, 2008; Elsheikh *et al.*, 2013). Soil data were available for the entire continental US (e.g., the Soil Survey Geographic Database or SSURGO). In reality, values in soil properties change gradually across the land surface instead of having crispy boundaries such as "mapunit" in the

SSURGO database. In addition, the static databases may not be able to represent the dynamic nature of soil properties in time and space. The fuzzy logic system could help reduce the effects on suitability evaluation conducted with the empirical understanding of crop growth constraints and the precise and time-invariant properties in the available data.

A significant gap in our knowledge exists because we do not know the site-specific suitability of marginal land for biofeedstock crops. The overall goal of this study is to evaluate the suitability of marginal land to growth of switchgrass, *Miscanthus*, and hybrid poplar. Specific objectives include: 1) identify marginal land resources in the Upper Mississippi River Basin (UMRB) area; 2) conduct a comparative analysis of marginal land suitability for growth of switchgrass, *Miscanthus* and hybrid poplar based on fuzzy logic modeling; and 3) predict biofuel production from three biofuel crops in the context of land suitability information.

2.3 Methods

2.3.1 Study area

The UMRB is located in the center of the Corn Belt in the US, with almost half (43%) of its total area (493,000 km^2) covered by row-crop agricultural land (primarily corn and soybean land) (USDA National Agricultural Statistics Service Cropland Data Layer. 2014) and another 16% by pasture land. The great amount of corn production makes this region an important source area not only for food/feed but also for grain based biofuel (Wu *et al.*, 2012) as well as the major contributor of nitrogen losses to the Gulf of Mexico (Srinivasan *et al.*, 2010). The predicted reduction of 20% nitrate nitrogen loss from the Mississippi and Atchafalaya River Basin by producing switchgrass (Costello *et* *al.*, 2009) indicates the potential of environmentally sustainable production for biofeedstock. Especially, the production of perennial biofuel crops on marginal land would probably bring greater environmental benefits. Thus, it is meaningful to evaluate the suitability of marginal land in this region for the production of three promising biofuel crops.

2.3.2 Marginal land in the UMRB region

This study focused on three marginal land types: 1) cropland and grassland with land capability class (LCC) 3 to 8 (Gelfand *et al.*, 2013) and other agricultural land with LCC 5 to 8; 2) land located within 10 meters along streams and roads (Gopalakrishnan *et al.*, 2009, 2011; Tang *et al.*, 2010), where forest and developed land were excluded from the analysis; and 3) idle/barren/fallow land. After mapping these three types of marginal land, those that were identified as protected lands based on the national Protected Areas Database (PAD-US v1.3) were removed from the analysis. Datasets used to identify these marginal land are described in the Supporting Information (SI) Table S1.

2.3.3 Marginal land suitability evaluation system

Figure 1 provided a flowchart of methods used in this study. The ultimate products of this study were land suitability class maps for switchgrass, *Miscanthus*, and hybrid poplar. Suitability class was determined based on Land suitability index (LSI), which represented the degree of land suitability for growth of the three targeted biofeedstock crops. The LSI values ranged from 0 to 1, indicating suitability of marginal land for the crops increased from not suitable at all to completely suitable. First, marginal land is identified within the UMRB. Second, factors (limiting factors in the rest of this paper) that might limit the growth of three biofeedstock crops were identified according to literature and expert's opinion and one raster map for each factor was generated. Third, the marginal land area and maps of limiting factors was used as input layers to a suitability evaluation procedure based on fuzzy logic theory (including fuzzification, fuzzy rule inference, and defuzzification). The evaluation system was first applied to locations where switchgrass yield was reported from literature. The LSI values at these sites were compared to observed switchgrass yields for verification of system accuracy. Finally, the system was applied to all marginal land in the UMRB region to generate the suitability maps for three targeted perennial grass. At last the biomass prediction incorporating suitability information was made with yield and bioethanol conversion rate for the three biofuel crops. Each step is described in detail below. The fuzzy logic system was coded in python (python 2.7) and run in ESRI ArcGIS 10.2.2.

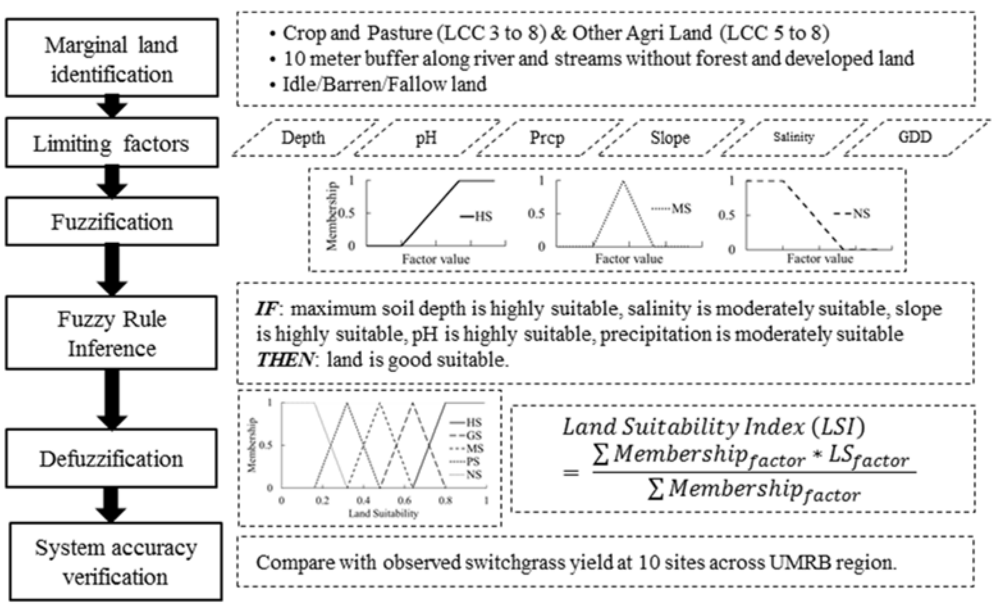

Figure 2.1 Flowchart of evaluation system based on fuzzy logic theory for marginal land suitability to growth of switchgrass, *Miscanthus* and hybrid poplar.

2.3.3.1 Factors limiting growth of switchgrass, *Miscanthus*, and hybrid poplar

Growth of switchgrass, *Miscanthus* and hybrid poplar could potentially be affected or limited by factors either relating to natural growth conditions like climatic conditions and soil properties, or by management practices such as tillage and fertilization. For characterizing land suitability, only factors relating to the natural growing conditions were considered. First, a list of environmental factors affecting growth of these biofeedstock crops, and their suitable ranges between which the three biofeedstock crops were suitable to grow (Table 2.1), was summarized from literature. Then, the identified factors and their suitable ranges were evaluated and finally determined by experts of the three biofeedstock crops. A raster map for each factor was generated and provided in SI Figure S1 and S2 with their corresponding data sources. The parameters and their suitable ranges are described below.

Table 2.1 Factors and their suitable ranges for switchgrass, *Miscanthus* and hybrid poplar

Factors	Switchgrass		*Miscanthus*		Hybrid poplar		Actual Range in UMRB[3]	
	Min	Max	Min	Max	Min	Max	Min	Max
Maximum soil depth (cm)	15	40	15	45	20	40	10	307
Soil Salinity (dS/m)	5.0	14.5	9.8	15.0	2.2	21.4	0	12
Slope (%)	15.3	4.4	15.3	4.4	15.3	4.4	0	70
pH[1]	3.7 (7.6)	6.0 (8.0)	3.7 (7.5)	5.5 (8.0)	3.7 (7.8)	5.5 (8.0)	1.0	8.0
Growing season precipitation[2] (mm)	200	600	--	--	240	375	390	664
Growing degree days (°C)	572	1200	553	1600	1150	1300	2367	4027
Average annual precipitation (mm)	--	--	500	762	--	--	527	1227

[1]: For pH, the highly suitable level had a trapezoidal shape membership function. The 4 values were for the four corners of the trapezoid. The order was (for switchgrass as example): 3.7~bottom left, 6.0~upper left, 7.6~upper right, 8.0~bottom right. Shapes of the function was provided in SI Table S2. Detailed description for how these were defined was provided in 2.3.2.
[2]: Growing season ranged from April 1st to September 30th in this analysis.
[3]: Actual Range of variables in the UMRB is the range of each variable based on measured database in the UMRB area. The maps for the actual range of each variable was provided in SI Figure S1 and S2.
--: The values for this factor were not available for the corresponding plants.

Soil depth

Soil depth could reduce land suitability for two reasons. First, soil depth might limit root system development if soil was shallower than a certain depth. Second, limited soil depth indicates potentially reduced less and nutrient availability. The suitable ranges of soil depth were determined mainly based on the root system distribution of three biofeedstock crops. Approximately 68% to 78% of total switchgrass roots were reported to occur in the top 0.15 m of soil (Ma *et al.*, 2000; Bolinder *et al.*, 2002) and 94% of coarse roots located in the upper 0.4 m of soil (Garten & Wullschleger, 1999). For *Miscanthus*, an increase in root distribution was observed up to 0.45 m even though 90% of their roots concentrated on the upper 0.35 m soil (Neukirchen *et al.*, 1999; Monti & Zatta, 2009). The recommended minimum planting depth was 0.1 m and a minimum value of 0.15 m was determined for *Miscanthus* for the minimum need of root development (Williams & Douglas, 2011). In the case of hybrid poplar, 0.2 m was selected as minimum value because only 17 to 25% of coarse and 11 to 24% of fine root biomass distributed in this depth of soil (Fortier *et al.*, 2013). This was considered inadequate for hybrid poplar growth. While 61 to 73% of coarse and 60 to 78% of fine root biomass distributed within 0.4 m soil and this depth was selected as the maximum value.

Soil salinity

High soil salinity could affect plant growth and limit crop yields by causing low osmotic potential of soil solution and affecting nutritional imbalance (Ashraf & Harris, 2004). Switchgrass is reported to have a low emergence and poor stand establishment at 5 dS/m soil salinity (Kim *et al.*, 2012) and could not survive in soils with salinity exceeding 14.5 dS/m (Dkhili & Anderson, 1990). Similarly *Miscanthus* growth was restricted when salinity was 9.8 dS/m and plant did not survive under 15 dS/m soil salinity (Ye *et al.*, 2005; Agnieszka Płażek, 2014). Growth of hybrid poplar can be limited by soil salinity levels of 4.5 dS/m and greatly reduced by soil salinity greater than 21.4 dS/m (Steppuhn *et al.*, 2008).

Slope

High slope could reduce land suitability by reducing machine operation safety and increasing the risk of soil erosion. Slope values used in existing land suitability evaluation for traditional crops and perennial crops under non-irrigated condition were summarized from literature (SI Table S2). Included studies generally used the 5 suitability classes suggested by the Food Agriculture Organization of the United Nations (FAO) (Hanson & Johnson, 2005). The average values for the thresholds of the highest suitability class (4.4%) and not suitable class (15.3%) were selected as the minimum and maximum values for slope variables used for the three biofuel crops.

pH

Proper pH ranges are important for plant growth. The optimal pH range for switchgrass growth was from 6 to 8 (Hanson & Johnson, 2005) and seedlings of switchgrass could tolerate pH from 3.7 to 7.6 (McLaughlin & Adams Kszos, 2005; Parrish & Fike, 2005). For *Miscanthus*, the optimal pH range for its growth was 5.5 to 7.5 and a pH of 8 was reported to limit *Miscanthus* growth (Williams & Douglas, 2011). Hybrid poplar was recommended to grow on soils with pH ranging from 5.5 to 7.8, and a pH greater than 8.0 was considered to limit poplar growth (Segal R, 2015). The minimum value of pH for *Miscanthus* and hybrid poplar was not available. Thus, a pH of 3.7 available for switchgrass was used for the other two crops as an assumption.

Climatic conditions

Precipitation and temperature are the two major variables that could greatly impact growth and final yield of biofuel crops (Matt A. Sanderson, 1997; Joss *et al.*, 2008; Maughan *et al.*, 2012). Possible precipitation and temperature variables include as average, maximum, and minimum annual and growing season precipitation and temperature. Upland switchgrass yield is limited by growing season (April 1st to September 30th) precipitation and yield, with low biomass production when the growing season precipitation was less than 200 mm. Biomass yield was not limited when growing season precipitation exceeded 600 mm (Davis *et al.*, 2008). Growing degree days (GDD) represented the cumulative heat requirements for plant growth. Upland switchgrass required a minimum GDD of 578 with a base temperature at 10 ºC to complete leaf and stem elongation (Sanderson & Wolf, 1995) and 1200 GDD to reach maturity (Trybula *et al.*, 2014). For *Miscanthus*, 500 mm average annual precipitation (growing season precipitation threshold for *Miscanthus* growth was not available) was considered the minimum amount for its growth, whereas 762 mm (30 inches) was considered ideal precipitation (Jensen *et al.*, 2013). *Miscanthus* required a minimum GDD of 553 for floral initiation (Porzio *et al.*, 2012) and 1600 GDD to reach maturity (Trybula *et al.*, 2014). The suitable ranges of growing season precipitation and GDD values for hybrid poplar were retrieved from Joss *et al.* (2008). By comparing suitable ranges of GDD with the actual GDD ranges in the UMRB, GDD was not a limiting factor and was not used in the following land suitability evaluation procedures.

2.3.3.2 Fuzzification

Fuzzification is the process in which the values of environmental factors were converted to membership values using fuzzy membership functions. The purpose of this method was to map the crispy factor values into common scale for further analysis. As the methods used by Joss *et al.* (2008), 3 suitability levels were created for each environmental factors: highly suitable (HS), moderately suitable (MS) and not suitable (NS). One membership function was defined for each suitability level. The function and shapes of all environmental factors are provided in SI Table S3.

Generally, the membership function for HS level was developed first using the minimum and maximum values summarized in Table 2.1. For maximum soil depth, and growing season precipitation, the increase of values for these two factors increased the potentially suitability of the land for growth of plants. Thus, the membership functions for HS level of the two factors were increasing functions. The membership value started to increase from 0 at the minimum factor value (for example, 15 cm of maximum soil depth for switchgrass) to 1 at the maximum factor value (for example ≥40 cm of maximum soil depth for switchgrass). This indicated that a land did not belong to the group of HS level when values of these two factor was smaller than their minimum value, and completely belonged to that level when larger than their maximum value. For slope and salinity, the membership functions for the HS level were decreasing functions because the larger the values of these two factors, the less one land was suitable for the crop growth. For these two factors, the membership values started to decrease from 1 at the factor's minimum value (for example, 6 of slope for switchgrass) to 0 at the factor's maximum value (for example, 18 of slope for switchgrass). This indicated that a land completely belonged to the group of HS level when values of these two factor were smaller than their minimum values and not belong to the group of HS level when larger than their maximum values. For pH, the membership function for the HS level had a shape of trapezoid. The reason was because both the increase of pH to 14 from around 7 and decrease of pH values to 1 reduced the suitability of land for crop growth. Thus, the membership values started to decrease from 0 at the minimum value (bottom left in Table 1) to 1 at the maximum value (upper left in Table 2.1) when the value was less than 7. The membership value started to decrease from 1 at the maximum value (upper right) to 0 at the minimum value (bottom right).

Based on the membership functions for the HS levels, the membership function for NS levels were the inverse of those for HS levels. The membership functions for MS had a triangle shape. Membership values of a land for the MS level decreased from 1 at the average of maximum and minimum factor value (for example, 27.5 cm of maximum soil depth for switchgrass) to 0 at the maximum or minimum factor values. This indicated that a land completely belonged to the group of MS level at the average value and did not belong to the group when the values were smaller than the minimum or larger than the maximum factor value.

2.3.3.3 Fuzzy rule inference

This step intended to determine the membership value of one land to 5 integrated suitability levels based on all environmental factors instead of just one factor. The 5 suitability levels include: integrated highly suitable (iHS), integrated good suitable (iGS), integrated moderately suitable (iMS), integrated poorly suitable (iPS) and integrated not suitable (iNS). The membership values indicated the degree of a land's belongingness to each of the 5 integrated suitability levels. The determination of membership value based on all environmental factors was completed by using empirical IF-THEN rules. One example of the IF-THEN rule was "IF the maximum soil depth is HS, salinity is MS, slope is HS, pH is HS, precipitation is MS, and GDD is HS, THEN, the land is iGS". The suitability levels used in the IF part was the 3 suitability levels from the fuzzification step, and those used in the THEN part was 5 integrated suitability levels. The following rules were used in generating a single IF-THEN rules:

- When there is at least one not suitable, the combinations will be considered as integrated not suitable (iNS).
- When there are all highly suitable variables, the combination will be considered as integrated highly suitable (iHS)

- When there is one marginally suitable variables, the combination will be considered as integrated good suitability (iGS)
- When there are 2 and 3 marginally suitable variables, the combination will be considered as integrated marginal suitability (iMS).
- When there are 4 marginally suitable, the combination will be considered as integrated poor suitable (iPS).

The minimum membership value of all components in the IF part was assigned as the membership value for integrated suitability level of the land in the THEN part. For each suitability level, one or several rules might be included from different combination of IF part. The maximum value from different rules with same integrated suitability level in the THEN part was assigned as final membership values of the land for that suitability level. This IF-THEN rule was actually calculating the logical intersections (AND) and unions (OR) of fuzzy sets for suitability levels defined in the fuzzification step. By using a combination of both intersections and unions (known as ANDOR), the fuzzy rule inference system tried to get a balance between the two extremes achieved by using only one operator, either AND or OR.

2.3.3.4 Defuzzification

Defuzzification converted the membership values of land for each of 5 integrated suitability levels from fuzzy rule inference step into one representative value, which was called the Land Suitability Index (LSI) in this study. LSI represented the overall suitability of each land pixel for growth of targeted biofeedstock crops. LSI was calculated using the Center of Maximum (COM) defuzzification method. First, membership functions were developed (SI Figure S3) to represent the membership values of LSI for each suitability level. Mean of the maximum LSI values for each suitability level were then determined. At last, a final weighted average LSI was achieved by using the membership values determined for each suitability level in the fuzzy rule inference as weights (Figure 2.1)

2.3.3.5 LSI accuracy verification

In existing literatures, accuracy of land suitability from fuzzy logic based procedure (Bolinder *et al.*, 2002; McLaughlin & Adams Kszos, 2005) were checked with experts' opinion or empirical opinions. The accuracy of LSI values calculated in this study were checked by comparing the measured yield values of switchgrass and LSI values. This method was considered more practical and reliable. LSI was a concept that could not be measured objectively. However, yield of crops could be considered as an objective indicator that could reflect the degree of land suitability. Switchgrass was tested in multiple sites across a wide geographic range across the study area in the last two decades. Yield data from different sites with their geographic location (Latitude, Longitude) were summarized from literature (SI Table S4). Totally, data from 9 sites were included in the validation. Land in these location included both marginal and non-marginal land. It was reported that the switchgrass yield from both marginal and non-marginal land did not show significant difference (Wullschleger *et al.*, 2010). The relationship between the yields and LSI values at all sites were analyzed using the regression module in SAS9.4.

After the verification, LSI values for switchgrass, *Miscanthus*, and hybrid poplar were generated using the same data sources, parameters and procedures as used in the verification step. The LSI maps was reclassified into 5 suitable classes, similar as used by Reshmidevi et al (2009). The classes included: not suitable (0 ~ 0.3), poorly suitable (0.3 ~ 0.45), moderately suitable (0.45 to 0.6), good suitable (0.6 ~ 0.8), highly suitable (0.8 ~ 1).

2.3.4 Biofuel production prediction

Biofuel production was calculated in two ways to explore the impacts by incorporating marginal land suitability on the prediction of potential contribution from marginal land to biofuel production in the UMRB. The first way used an average yield of switchgrass, *Miscanthus* and hybrid poplar from field experiments for all marginal lands. The yield values used are provided in SI Table S4-6. The average yield used for switchgrass was 9 Mg/ha, for *Miscanthus* 31 Mg/ha, and for hybrid poplar 8 Mg/ha. In the second method, yield of biofeedstock crop was scaled down by the LSI values. This method assumed that the average yield could be achieved on marginal land when its LSI value was 1. For example, if LSI values for one land was 0.6, the yield of switchgrass would be 5.4 Mg/ha, of *Miscanthus* would be 18.6 Mg/ha and of hybrid would be 4.8 Mg/ha. A bioethanol yield of 80 gal/dry Mg biomass, which was close to the average published bioethanol yield that could be achieved practically from lignocellulose biofeedstock (Lovett *et al.*, 2009; Gao *et al.*, 2014; Liu *et al.*, 2015), was used for all three biofuel crops to calculate the total bioethanol that could be produced from marginal land in the UMRB region.

2.4 Results

2.4.1 Marginal land availability

Table 2.2 presents the availability of marginal land in the UMRB area. Marginal land with LCC 3 to 4 and 5 to 8 are separated because LCC 1 to 4 are suitable for cultivation of traditional crops and land with LCC 5 to 8 are not suitable. In this study, the targeted crops are all perennial plants and might be suitable for growing on land with LCC ranging from 5 to 8. As shown in Table 2.2, all types of marginal lands comprise 23% of the entire UMRB area. The largest areas of marginal land come from cropland with LCC 3 to 4, followed by grassland with LCC 3 to 4 and grassland with LCC 5 to 8. Land area under cropland with LCC 5 to 8 is relatively small, as well as other crops with LCC 5 to 8. Combined areas of marginal lands from buffer area and idle/barren/fallow lands are much smaller than those from Type 1 marginal land. Overall, 29% of cropland in the UMRB area are marginal land and nearly two thirds (62.3%) of grasslands are identified as marginal land.

Table 2.2 Marginal land (ML) availability in Upper Mississippi River Basin (UMRB)

Types of marginal land		Area (km^2)	% over total ML area	% over total UMRB[1] area	% over corresponding original land class area
Type 1	Cropland with lcc 3 to 4	56,426	51	11	27
	Cropland with lcc 5 to 8	3,965	4	1	2
	Grassland with lcc 3 to 4	36,423	33	7	47
	Grassland with lcc 5 to 8	11,139	10	2	14
	Other crops with lcc 5 to 8	172	0.15	0.03	5
Type 2	10 m strips along stream	2,894	3	1	
	10 m strips along road	41	0.04	0.01	
Type 3	Idle/fallow/Barren	625	1	0.13	
Summary	Total area of ML in UMRB	111,660	100	23	

2.4.2 LSI accuracy validation

Figure 2.2 presents the results for validation of LSI values calculated with the fuzzy logic based land suitability framework. The trend for the changes in switchgrass yield and changes in LSI values indicated that the calculated LSI value effectively ($p<0.05$) explained the yield of switchgrass from these lands. The yield value, corresponding LSI value and reference for each site is provided in SI Table S4.

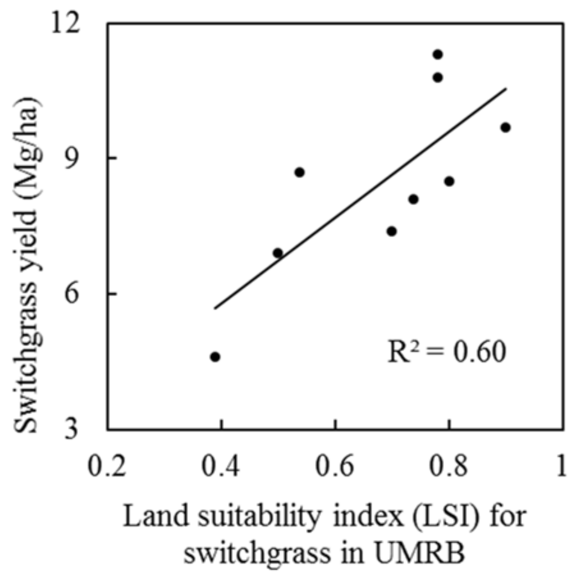

Figure 2.2 Influence of Land Suitability Index (LSI) on where switchgrass yield from previously published studies (SI Table S4).

2.4.3 Marginal land suitability

Figure 2.3 and Figure 2.4 presented the area and spatial distribution of 5 suitability classes based on LSI of switchgrass, *Miscanthus*, and hybrid poplar. The total area of land with classes of not suitable, poor suitable, and moderate suitable were 38% for switchgrass, 41% for *Miscanthus*, and 34% for hybrid poplar. Area of land with class of not suitable were similar for both three crops. For land with classes of poorly and moderately suitable, the area was largest for *Miscanthus*, followed by switchgrass and then hybrid poplar. The area of land with good suitable class was much higher for switchgrass than for *Miscanthus* and hybrid poplar, while the reverse pattern happened for land with highly suitable classes.

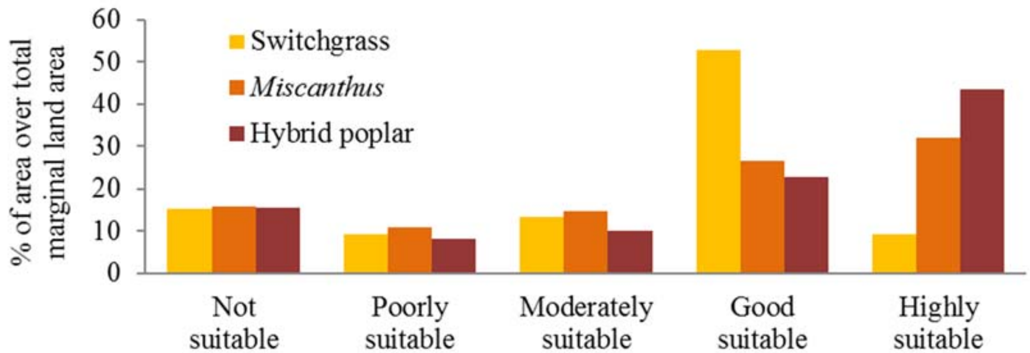

Figure 2.3 Histogram of areas for each suitability class

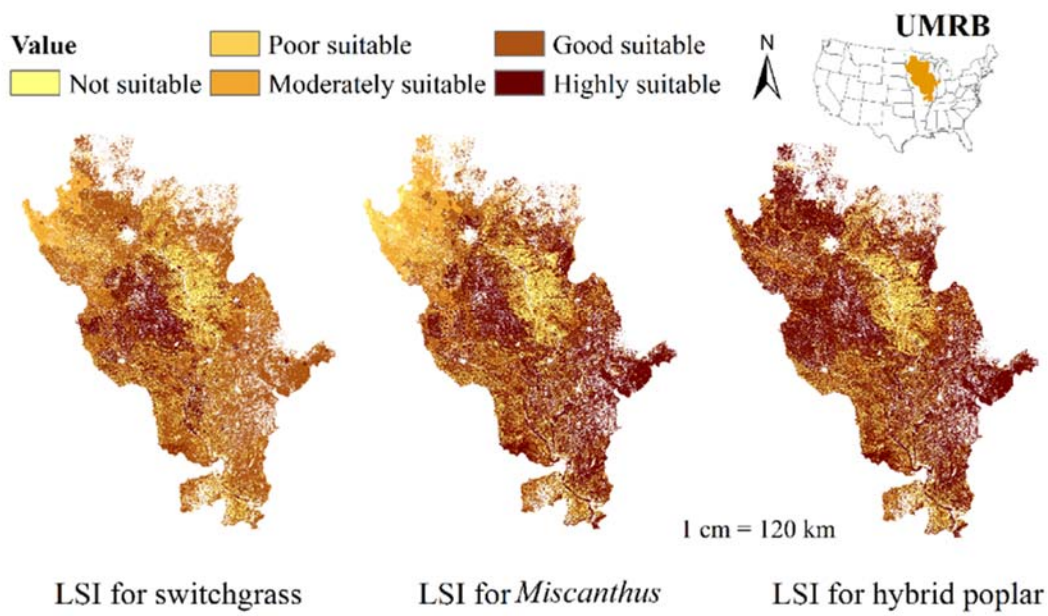

Figure 2.4 Land Suitability maps (LSI) for switchgrass, *Miscanthus*, and hybrid poplar in the Upper Mississippi River Basin (UMRB)

2.4.4 Biofuel production in UMRB

Due to the higher average measured yield of *Miscanthus*, the total biomass and predicted bioethanol from this perennial biofeedstock crop on marginal land in the UMRB region is about 3 times that from switchgrass or hybrid poplar (Table 2.3). When land suitability information was incorporated into biomass production prediction, the predicted biomass and bioethanol from these three crops were about two thirds of the prediction made with average yield of these biofuel crops. The final prediction of bioethanol production was close to that of switchgrass.

Table 2.3 Biomass and bioethanol yield prediction with average biomass yield and marginal land yield based on LSI for switchgrass, *Miscanthus*, and hybrid poplar from marginal land in the UMRB region. Bioethanol was calculated with a bioethanol yield of 80 gal/dry Mg biomass.

	With average yield		With marginal land yield based on LSI	
	Biomass (Million Mg)	Bioethanol (Billion Gallons)	Biomass (Million Mg)	Bioethanol (Billion Gallons)
Switchgrass	101	8	59	5
Miscanthus	302	24	206	16
Hybrid Poplar	89	7	58	5

2.5 Discussion

2.5.1 Marginal land identification

In literature, marginal lands have been defined in terms of 5 aspects. These include economic, biophysical, location, current condition or environmental aspects (Peterson & Galbraith, 1932; Gopalakrishnan *et al.*, 2009; Cai *et al.*, 2011; Kang *et al.*, 2013a). In this study, the types of marginal land defined in terms of their biophysical, location and current location aspects are considered. Marginal land defined by LCC includes crop and pasture land with marginal LCC. This is defined because the Renewable Fuel Standard 2007 specifies that land for biomass production could only come from current crop and pasture land (Schnepf & Yacobucci, 2010). In addition, LCC is an established database that indicates the suitability of land for cultivating current annual agricultural crops. The inclusion of marginal idle/barren/fallow land is triggered by the potential environmental benefits by growing perennial grasses on buffers along streams and roads (Gopalakrishnan *et al.*, 2009). As for type 3 marginal land, they are currently not engaged in agricultural production and could avoid impacting current agricultural production. These three marginal land types meet the expectation of candidate land resources for biofuel development. The total area of marginal land identified is close to the land area identified in Gelfand *et al* (2013) using similar criteria. The framework developed in this study could serve as a starting point for comprehensive suitability evaluation of other marginal land types. Similarly, additional factors that affect the growth of biofuel crops may also need to be evaluated. For example, individual brownfields may have unique characteristics that are detrimental for growth of specific biofuel crops, but not others.

For the marginal land types included in this study, a competition of land between food/feed and fuel production may not be completely avoided. With the exception of marginal idle/barren/fellow land, marginal land defined by LCC and from buffer area all contain land currently used for crop production. They are major sources of marginal land. If they were converted to biofeedstock crop production, agricultural production will be reduced in UMRB area. From the productivity point of view, these lands are suffering certain degrees of limitation for agricultural production. Their poor performance of traditional crops might be a good reason for conversion to biofeedstock crops, which generally have lower input requirements than traditional crops.

2.5.2 Suitability evaluation

This study used a well-established land suitability evaluation procedure based on fuzzy logic theories. This method has been developed and applied in a large number of studies (Malczewski, 2004; Sicat *et al.*, 2005; Reshmidevi *et al.*, 2009; Elsheikh *et al.*, 2013) and even for biofeedstock crops (Joss *et al.*, 2008; Lewis *et al.*, 2014). Even though this study focused only on marginal land area, the framework including the limiting factor values will also be applicable on other land types (such as prime farm land) to evaluate their suitability for growth of these three biofeedstock crops. The LCC class for identifying marginal land provide some insights into the suitability for crop growth, but the targets of LCC classes are for traditional annual crops. LCC classes do not indicate the suitability of land for perennial biofeedstock crops. The evaluation procedure in this study provide more cogent information on land suitability for growth of switchgrass, *Miscanthus*, and hybrid poplar.

The results of validating LSI value from this procedure provide evidence for the effectiveness of the suitability map for indicating the potential growth of targeted biofeedstock crops. Nonetheless, several sources of uncertainties should be noted. The first source of uncertainty comes from determining the variables and their suitable ranges. Even though the variables included in our analysis cover most of the variables considered in the past analysis of suitability for the biofuel crops (Joss *et al.*, 2008; Lovett *et al.*, 2009), there are other variables that are not included in this analysis, such as dryness index (Lewis *et al.*, 2014). It is considered that the effect of water is reflected partially by the precipitation factor. These factors are determined based on empirical knowledge and expert's opinions. It has been pointed out that this way of selecting variables and their impacts is subjective (Elsheikh *et al.*, 2013). In addition, variables and their suitable ranges may vary with cultivation. For example, differences exist between upland and lowland ecotypes of switchgrass for important agronomic traits, like yield, winter hardiness, etc. This is also true for hybrid poplar, which also has many different genotypes. These differences in relationships between cultivars and environmental variables can also introduce uncertainties in the shapes of membership functions. A piece-wise linear function is selected due to its simplicity and its capability of representing the general roles played by each variable on crop growth. Besides the uncertainties from the distance between this linear function and the true relationships between environmental variable and crop growth, the different responses from cultivars of the same crop will result into differences of model output sensitivity to shapes of membership functions. However, a lack of training data to determine the relation between land property and suitability for crop growth is the main reason for not developing more predicting membership functions between variables and suitability of land for growth of targeted crops.

The last source of uncertainty comes from the data used in assessment of the suitability map accuracy. As shown in SI Table S4, the average yield from experimental fields for switchgrass contains different degrees of variance, ranging from less than 1Mg/ha to more than 3 Mg/ha. These variations could be caused by an array of factors including differences in environmental conditions, management practices, and cultivars. In this study, only environmental conditions are used. Even though the relationship between yield and the LSI achieved based on environmental conditions are significant, it is not clear how much contributions to the yield difference are made by other factors. In addition, some management practices might have changed the land properties, thus the input values used in this study. For example, pH values could be managed by liming application. While, the COM defuzzification method could account for impacts from this point because small changes of input values will not change the best compromise value for LSI value. The LSI values were not validated for *Miscanthus* and hybrid poplar due to limited biomass production data. These major sources of uncertainties should be considered and processed in future research to increase the confidence of the marginal land suitability for biofeedstock crop production.

2.5.3 Biofuel production

The bioethanol yield predicted with average yield in this study are comparable to those predicted in other studies. For example, Srinivasan *et al.* (2010) predicted that 42% of all agricultural land in UMRB region planted with switchgrass could produce 345 Million Mg biomass with the simulation by the Soil and Water Assessment Tool (SWAT) model. In this study, the total area of marginal land is 23% of the UMRB region area, which covers 29% (close to one thirds) of corn/soybean land. The biomass production is calculated using yield from experimental sites, instead of farmers' land which generally produce smaller yield than experimental sites. The estimation with yield from farmer's land is not feasible currently because large area production of these perennial crops are not available. While, the current breeding efforts made on these perennial crops could help improve the yield of these crops to the average yields used here. The estimation of biomass and biofuel production here are considered efficient with current knowledge on yield performance of these biofeedstock crops. The predicted of biomass production was 101 Million Mg, about one thirds of the total biomass expected by Srinivasan *et al.* (2010). When marginal land suitability was considered, the biomass and bioethanol prediction was reduced by one-third for all three biofuel crops, but they could still make substantial contribution to the biofuel development goals in the Energy Independence and Security Act of 2007, which mandated that 21 billion gallon cellulose biofuel be produced annually by 2022.

2.6 Conclusion

In summary, this study presents the application of a well-established land suitability evaluation framework based on the fuzzy logic theory. The results of this study characterizes great spatial variance of land suitability for three promising biofeedstock crops, switchgrass, *Miscanthus* and hybrid poplar. Specifically, 23% of the UMRB area are identified as marginal land, and 60% of the marginal land area are moderately to highly suitable for growth of switchgrass, *Miscanthus* and hybrid poplar. The major factor that limited the growth for these biofuel crops were steep slopes, high salinity, or lower soil pH. When suitability of marginal land is considered, the predicted bioethanol production is two thirds of predictions made by considering that the land were all suitable for biofuel crop growth. The information underscores the importance of marginal land's potential contribution for biofuel development. It also underscores the importance of considering marginal land suitability, which is critical for proper biofeedstock placement on the landscape and accurate assessment of biofuel production potential in the UMRB. If less suitable marginal land were going to be used for biofuel crop production, management practices to improve their suitability may need to be developed and implemented.

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CHAPTER 3. SIMULATING ESTABLISHMENT PERIOD OF PERENNIAL BIOENERGY GRASSES IN THE SWAT MODEL

3.1 Abstract

Perennial bioenergy grasses like switchgrass and *Miscanthus* are known to have an establishment period, during which time their biomass increases annually until their maximum potential biomass is reached. This study evaluated the trends of biomass (yield), Leaf Area Index, and biomass partitioning ratio during the establishment period of switchgrass and *Miscanthus*. These trends were incorporated into the Soil and Water Assessment Tool (SWAT) model. Based analysis of measured data, we recommend using expected yields of established grasses as reference yields (i.e., 8.7 Mg/ha for upland switchgrass, 13.5 Mg/ha for lowland switchgrass, 16.4 Mg/ha for *Miscanthus* in Europe, and 23 Mg/ha for *Miscanthus* in the U.S.) to determine the length of establishment period. These reference yields resulted in 2 to 3 years for switchgrass, 2 to 4 years for *Miscanthus* in the U.S. and 3 to 6 years for *Miscanthus* in Europe as the length of establishment period. The modified SWAT model provided reasonable simulated yields during establishment periods for switchgrass and *Miscanthus*. Simulated evapotranspiration (ET) with the modified model was higher, thus more surface runoff and water yield during the establishment period compared with simulation by the unmodified model. Simulated soil erosion and nutrient losses (mineral and organic nitrogen and phosphorus) were also higher by the modified model.The result of this study

study improved the representation of growth processes of perennial grasses and simulation of hydrologic and water quality processes in the SWAT model.

3.2 Introduction

Perennial grasses like switchgrass and *Miscanthus* has been considered as major candidate sources of cellulosic biomass for bioenergy development (McLaughlin & Adams Kszos, 2005; Heaton *et al.*, 2008). These perennial grasses are characterized by higher sustainable yield, relatively lower nutrient and management requirements, and broader adaptability (McLaughlin *et al.*, 2004; Zub & Brancourt-Hulmel, 2012) than annual biomass crops like corn (*Zea mays*). In addition, these grasses are reported to be able to grow reasonably well on marginal lands, a feature that is important for biofeedstock production because bioenergy development might cause competition of land for food production and using marginal land can help avoid this competition (Nonhebel, 2005; Feng *et al.*, 2015). On the other hand, these grasses are also reputed for their difficult or slow establishment to reach their maximum potential biomass production (Parrish & Fike, 2005). The duration from the first year (the year when perennial grasses are planted) to the year when they are able to produce their maximum potential yield is considered as the establishment period. During their establishment periods, relatively lower biomass production has both environmental and economic implications. Lower biomass production causes lower nutrient uptake and poorer protection to land surface, thus increasing the risk of higher nutrient and sediment losses (Thomas *et al.*, 2014). Sarkar & Miller (2014) reported that nitrogen loss from switchgrass field was higher when switchgrass was young than when it was established. Curley *et al.*, (2009, 2010) analyzes the nitrogen and phosphorus loss under establishing *Miscanthus* and reports that losses of these two nutrients could be as high as losses from crop land. From the economic aspect, the lower yield during the establishment period could reduce the contribution to the bioenergy development from these two perennial grasses.

A considerable variability in establishment period for switchgrass and *Miscanthus* has been reported in many studies (Madakadze *et al.*, 1998; Heaton *et al.*, 2004; Miguez *et al.*, 2008, 2012; Hastings *et al.*, 2009; Maughan *et al.*, 2012; Lesur *et al.*, 2013). Generally, it is considered that switchgrass and *Miscanthus* could reach their maximum potential biomass production at least 3 years after planting (Clifton-Brown *et al.*, 2001; McLaughlin & Adams Kszos, 2005; Schmer *et al.*, 2009; Maughan *et al.*, 2012). *Miscanthus* may even take up to 5 years to reach its maximum potential biomass production (Christian *et al.*, 2008; Maughan *et al.*, 2012). There have been few studies analyzing the establishment period of switchgrass. For *Miscanthus*, several studies have been conducted to explore its yield variability using long term observed biomass production data. Lesur *et al.* (2013) reported that establishment period of *Miscanthus* ranged from 3.3 to 7.3 years, with an average of 4.7 years. As pointed by *Arundale et al.* (2014), the observed yield by Christian *et al.* (2008) showed a trend of increasing yield in the first 6 years and staying stable in the next 8 years. The establishment period varies due to many factors, including the specific species of the perennial crop, management practices (such as planting method, density, harvest time and frequency) (Casler & Boe, 2003; Miguez *et al.*, 2008; Pyter *et al.*, 2010), and growth environment conditions (such as temperature, precipitation, and soil properties) (Fike *et al.*, 2006). The annual yield variability caused by these factors contributes to the variability in the length of establishment period for the two perennial grasses.

Due to the economic and environmental implications of establishment period for switchgrass and *Miscanthus*, some efforts have been made to incorporate this period in plant growth models. Miguez *et al.* (2012) represented the establishment period of *Miscanthus* in the BIOCRO model by assuming a 3-year establishment period and using overwintering rhizome size as input for the calculation of the second and third year biomass production. Sarkar and Miller (2014) evaluated the differences in nutrient loss during the establishment and post-establishment period of switchgrass and *Miscanthus* by using two different sets of plant growth parameters in the Soil and Water Assessment Tool (SWAT) model. Thomas *et al.* (2014) assumed 80% in year 2, 90% in year 3, and 100% yield in year 4 to year 8 of expected maximum yields in the Groundwater Loading Effects of Agricultural Management Systems-National Agricultural Pesticide Risk Analysis (GLEAM-NAPRA) model to account for the growth of switchgrass in its establishment period. Simulation with these methods provide some insights to the hydrologic and water quality processes under the two perennial grasses in their establishment and post-establishment period, however, other biophysical models, such as MISCANMOD/MISCANFOR model (Clifton-brown *et al.*, 2004; Hastings *et al.*, 2009) and the empirical model developed by Wullschleger *et al* (2010) ignore the simulation of establishment period.

The SWAT model is developed to evaluate the impacts on hydrologic and water quality processes under various land use, land management and climate change scenarios (Arnold *et al.*, 1998). Algorithms for plant growth module in the SWAT model is adapted from the Environmental Policy Integrated Climate (EPIC) model (Neitsch *et al.*, 2011). In the SWAT model, the Hydrologic Response Unit (HRU) is the smallest simulation unit and is a land area with a unique combination of soil, land cover type and topography (slope). On each HRU, plant growth, hydrology, sediment and nutrient losses processes are simulated with input data including weather, topography, soil, and management practices. A detailed description of the SWAT model is provided in Neitsch *et al.* (2009). This model has been improved for simulating annual growth of switchgrass (Shawnee) and *Miscanthus* (*Miscanthus x. Giganteus*) by Trybula *et al.* (2014) in terms of harvest, plant respiration and nutrient uptake algorithms as well as plant growth parameters based on field observed data. In the current versions of the SWAT model, perennial grasses are allowed to reach their maximum potential biomass productivity from the planting year and their establishment periods are not represented. As SWAT is one of the most widely used models for hydrologic and water quality processes evaluation (Ng *et al.*, 2010; Love & Nejadhashemi, 2011; Wu *et al.*, 2012; Wu & Liu, 2012; Sarkar & Miller, 2014; Trybula *et al.*, 2014), it is important to incorporate the establishment period of switchgrass and *Miscanthus* in the model to accurately predict the environmental impacts under various bioenergy development scenarios, especially during the establishment period of these grasses.

The primary objective of this study was to understand the growth processes of switchgrass and *Miscanthus* during their establishment period and represent these processes in the SWAT model. The specific goals included: 1) Exploring the duration of establishment periods for switchgrass and *Miscanthus*; 2) Understanding the developing trends of yield, Leaf area index (LAI), and biomass partitioning to aboveground and belowground biomass for the two perennial grasses during the establishment period; 3) Modifying the SWAT model to represent those trends during the establishment periods; and 4) Evaluating hydrologic and water quality processes during establishment periods of the two grasses.

3.3 Materials and Methods

3.3.1 Perennial crop growth simulation in the SWAT model

Plant growth module in the SWAT model is used to evaluate the biomass/yield production and the flow of water and nutrient in the soil plant atmosphere continuum (Neitsch *et al.*, 2011). As shown in Figure 3.1, plant growth is controlled primarily by fraction of Potential Heat Unit (fr_{PHU}), which is the total heat units required from the beginning of growing season (emergence) to plant maturity. The growth starts from potential LAI, which develops following a predefined growth curve by fr_{PHU} and six LAI related parameters. LAI converts intercepted Photosynthetically Active Radiation (PAR) into potential total biomass at a rate of Radiation Use Efficiency (RUE) which is a fixed value for each specific plant type. Total biomass is then partitioned into aboveground and belowground biomass with different ratios at different fr_{PHU}. The ratio reduces from 0.4 at the plant emergence (RFR1C) to 0.2 at maturity (RFR2C) by default. These two values are specified for switchgrass and *Miscanthus* by Trybula *et al.* (2014). LAI development also controls the development of crop height. Root depth develops linearly from the beginning of the growing season to fr_{PHU} at 0.4 as a portion of maximum depth. When fr_{PHU} is larger than 0.4, root depth equals to maximum root depth. Root depth might also be restricted by soil depth if the soil is shallower than the maximum potential rooting depth. The potential growth of LAI and biomass will then be reduced according to the degree of stresses from water, temperature, nitrogen and phosphorus, to calculate the actual growth under specific environmental conditions. Crop yield is then calculated from the actual amount of total biomass with harvest related parameters. For the purpose of assessing impacts of plant growth on water and nutrient cycles, plant water and nutrient (nitrogen and phosphorus) uptakes are also calculated and they are determined with evapotranspiration for water uptake and plant nutrient fraction at different growth stages for nutrient uptake. A detailed description of how plant growth processes are simulated could be found in Neitsch *et al.* (2011).

For perennial crops, the SWAT model allows them to maintain their root system throughout their life span as long as a kill operation is not conducted. They go dormant in winters and start growing if the average air temperature in a day goes above the base temperature. Trybula *et al.* (2014) improved the model for representation of the nutrient translocation/remobilization to belowground rhizome organs as a storage of nutrients for regrowth in the following year by modifying nutrient fraction parameters (PLTNFR and PLTPFR for nitrogen and phosphorus, respectively). Based on the information of how the perennial crop growth simulation in SWAT model, the incorporation of establishment period representation requires understanding of lengths of establishment period and developing trends of maximum LAI values, RUE and partitioning ratio for aboveground and belowground biomass during this period.

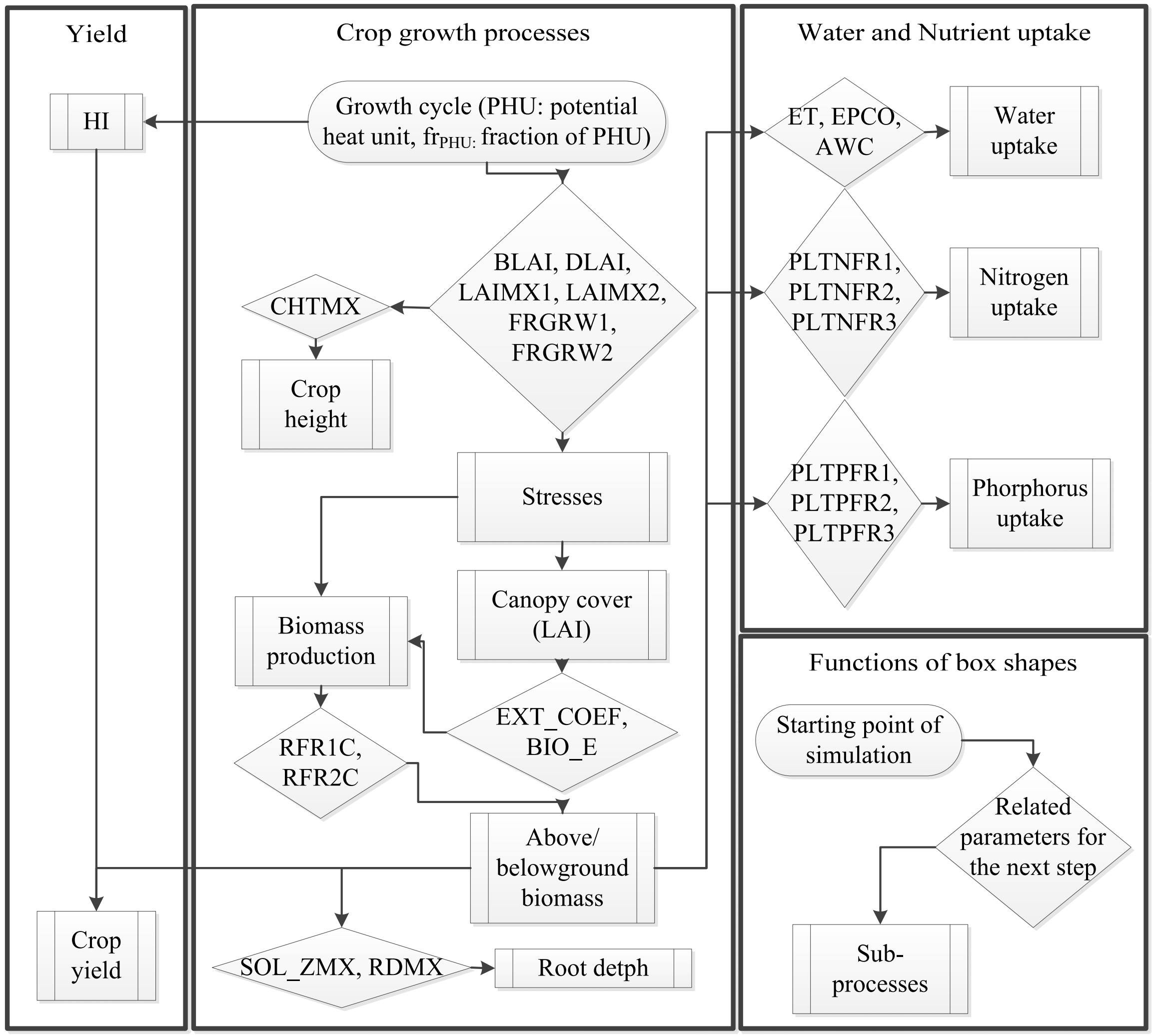

Figure 3.1 Conceptualized flowchart of plant growth module in the SWAT model for annual plant growth. Definition of parameters shown in this chart is provided in Supporting Information (SI) Table S1.

3.3.2 Dataset description

Observed annual growth parameter values was collected from both literature and local experiment sites for switchgrass and *Miscanthus*. These parameters included annual yield, maximum LAI, and biomass partitioning ratio at maturity. When data were shown in figures in literature, they were extracted using the GetData Graph Digitizer (trial version 2.26.0.20). Annual yield data was collected in order to identify the lengths of establishment period. Yield data that were longer than 2 years since the first year were included in the database, which were provided in Supporting Information (SI) Table S2 for switchgrass and SI Table S3 for *Miscanthus*. These yield data were obtained from a wide range of geographic location, where the management practices and growth conditions varied a lot. The main management variables are harvest time/frequency and nitrogen fertilizer application. Monti *et al.* (2008) concluded that one cut system was both adequate to get higher biomass and economically feasible for switchgrass cultivation as a bioenergy crop. Thus, yield from only one cut system was included if there were multiple harvest times reported in one study. There was currently not a definite conclusion on how switchgrass and *Miscanthus* growth responded to different fertilization rates, therefore yields under different nitrogen fertilization rates were all included. The data was organized based on availability for different species, attempting to understand the yield accumulating patterns during their establishment and post establishment periods. Switchgrass yield was grouped for upland (Shawnee and other upland varieties) and lowland (Alamo and Kanlow) ecotypes. *Miscanthus* was for *Miscanthus x giganteus*, but was categorized into the US and the Europe groups. These data were used to recommend a reference yield for determining the turning point from establishment to post establishment period. Due to the limited data for LAI and biomass partitioning ratio (at maturity), data points for all species under different growth conditions were grouped together for upland switchgrass and *Miscanthus*. Studies included in databases for LAI and biomass partitioning ratio are provided in SI Table S4 and S5.

3.3.3 Modification of the SWAT model

In the current SWAT model (revision 635), annual LAI for perennial crops are allowed to reach their maximum values (BLAI) since the first year. While, reported annual LAI observations for switchgrass and *Miscanthus* indicated an increasing trend of BLAI during the establishment period of these two perennial grasses. A non-linear logistic growth equation was fitted for the third quartile of the reported BLAI observations and was added to the grow.f code (SI Table S6) to simulate the annual BLAI of perennial crops as suggested by Miguez *et al.* (2008) for delineating the trends of maximum biomass production of *Miscanthus*:

$$f(x) = \frac{\emptyset_1}{1 + exp((\emptyset_2 - x)/\emptyset_3)} \qquad Equation\ 3.1$$

where $f(x)$ was the annual maximum LAI value. x is the age (in year) of the perennial crop starting at 1 from the planting year. $\emptyset_1$, $\emptyset_2$, and $\emptyset_3$ are parameters specific for each plant. $\emptyset_1$ represented the BLAI that the perennial crops are expected to reach at their post-establishment periods. $\emptyset_2$ represented the approximate time (in year) taken by the plant to reach half of the maximum potential value. $\emptyset_3$ represented the approximate time (in year) taken by plant to reach from half to approximately three quarters of maximum potential value. In the modification, two existing parameters (BIO_LEAF and BMX_TREES) in the current swat parameter database (plant.dat) were used to represent the two new parameters in the proposed equation. These two parameters were originally only used for simulation of trees and not used for other types of plants. BIO_LEAF was used in the simulation for perennial grasses as $\emptyset_2$ and BMX_TREES was used as $\emptyset_3$.

Miguez *et al.* (2008) collected observed yield data mainly from the Europe, where *Miscanthus* was extensively studied and long term yields data were available, and analyzed the changing patterns of long term yields for *Miscanthus*. The authors estimated the model parameters by fitting the equation to each site of their datasets. In our study, the equation was applied to the changes of annual BLAI and RUE values. The suggested BLAI of switchgrass and *Miscanthus* by Trybula *et al.* (2014) was used as $\emptyset_1$. Due to limited data on BLAI observation, $\emptyset_2$ and $\emptyset_3$ were estimated based on the trend of annual yield observations and was validated by comparing the predicted annual BLAI values with the 3rd quartile of observed LAI values. The maximum value for observed LAI of switchgrass was high, but might not be representative for all geographic locations. Table 3.1 provids the suggested ranges of $\emptyset_1$, $\emptyset_2$ and $\emptyset_3$. Observed data for RUE was unavailable for switchgrass and *Miscanthus*. Here, it was assumed that RUE of perennial grasses changes following similar patterns of BLAI and yields of perennial crop yields, which increased during the establishment period and stayed stable during the post-establishment period. The modification of above and below ground biomass portioning simulation was not included.

Table 3.1 Recommended values of $\emptyset_1$, $\emptyset_2$ and $\emptyset_3$ for Shawnee switchgrass and *Miscanthus x Giganteus*

Parameter	Shawnee Switchgrass (*Panicum Virgatum*)		*Miscanthus x giganteus*		Parameter in SWAT plant database
	Suggested	Ranges	Suggested	Ranges	
$\emptyset_1$	8	-	11	10-13	BLAI
$\emptyset_2$	0.75	0.5-1.5	1.5	1-3	BIO_LEAF
$\emptyset_3$	0.32	0.25-0.75	0.75	0.5-1.5	BMX_TREES

3.3.4 Validation of model modification and exploring impacts on hydrologic and water quality

Modification of the SWAT model for simulating establishment periods was validated at 5 sites for switchgrass and 5 sites for *Miscanthus* (Table 3.2), where annual yield data during the establishment periods of switchgrass (Shawnee) and *Miscanthus* (*Miscanthus x giganteus*) were available. At each location, a one-HRU SWAT model was setup. The growth parameters of these two ecotypes from Trybula *et al* (2014) were used in setting up the model at all locations with site-specific information for topography, soil, climate, and management practices, as provided in SI Table S7 and S8. In each location, a 1 to 3 years warmup period was included depending on the availability of climate data. The one-HRU model for the WQFS site was also used to explore the differences of hydrology and water quality related processes between the establishment period and post-establishment period. These processes included the differences in evapotranspiration, surface runoff, water yield, soil erosion, and losses of nitrogen and phosphorus.

Table 3.2 Locations where the SWAT model was setup to test the modification

Location	State	Latitude	Longitude
Water Quality Field Station	Indiana	40.50	-86.99
Throckmorton Purdue Agriculture Center	Indiana	40.30	-86.91
Brookings	South Dakota	44.31	-96.80
Arlington	Wisconsin	43.34	-89.38
Lafayette	Indiana	40.48	-86.82
Schochoh	Kentucky	36.76	-86.77

3.4 Results

3.4.1 Length of establishment periods and development of LAI and Biomass partitioning

Reported yield from field observations (Figure 3.2) indicated that yield of both switchgrass and *Miscanthus* increased during the establishment period and became relatively steady during the post establishment period. Upland and lowland switchgrass entered their post establishment period at the second or third year. *Miscanthus* grown in the U.S. entered its post establishment period at the second to the 4th year and in the Europe at the third to 6th year.

During the post establishment period, upland switchgrass produced 8.7 Mg/ha yield and lowland switchgrass produced 13.5 Mg/ha yield averaged over the second to the eighth year after planting. *Miscanthus* produced 23 Mg/ha yield averaged over the third to the 10th year after planting in the U.S., and 16.4 Mg/ha yield averaged over the 4th to the 14th year after planting in Europe. Observed annual maximum LAI values also showed a clear increasing trend during the establishment periods of upland switchgrass and *Miscanthus* (Figure 3.3). The 3rd quartile of observed annual maximum LAI and projected annual maximum LAI values by the equation from Miguez *et al.* (2008) matched reasonably well, except for the first year (Figure 3.3). The projection of annual maximum LAI for switchgrass at the first year could not be validated due to a lack of measured data. For *Miscanthus*, the projected maximum LAI for the first year was less than half of the observed value. Percentage of belowground biomass also (Figure 3.4) showed a slightly increasing trend, especially for *Miscanthus*. However, this trend was not as clear as that for yield and LAI.

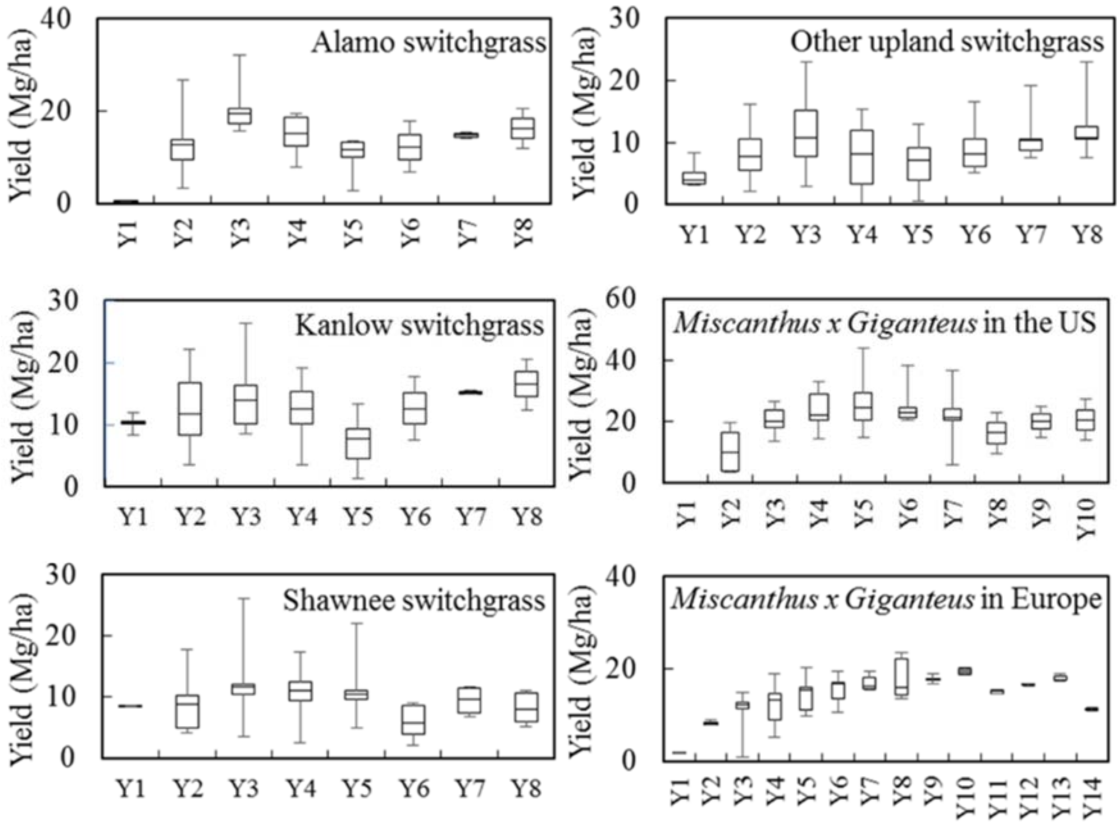

Figure 3.2 Distribution of yields for switchgrass (Lowland species Alamo and Kanlow, Upland species Shawnee and other, all from the U.S.) and *Miscanthus x Giganteus* (from the U.S. and Europe) including observed data for the establishment period from literature and field measurement. Y represented for year and Y1 is the planting year.

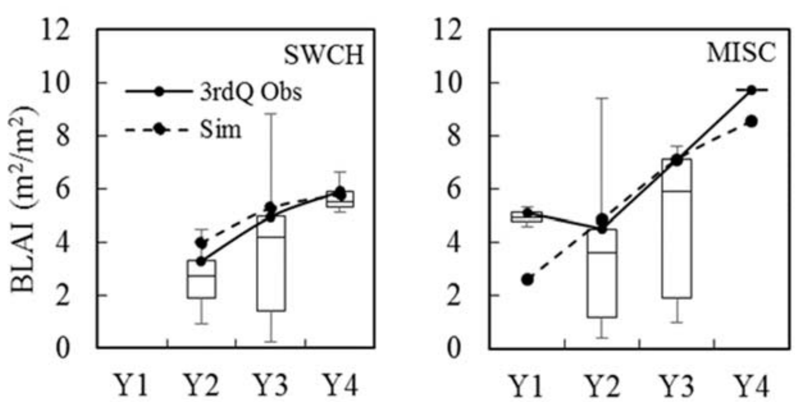

Figure 3.3 Distribution of BLAI values for Upland switchgrass, Shawnee switchgrass and *Miscanthus x Giganteus* during the establishment period from literature. Y represented for year and Y1 was the planting year. The black line with dots were simulated maximum LAI values with the Equation 3.1.

3.4.2 SWAT model improvement for establishment period simulation

Since data for LAI during the establishment periods were not available at all test sites, simulated monthly LAI of switchgrass and *Miscanthus* by the modified SWAT model was compared with the simulation by the unmodified model at all sites (SI Figure S1). The results for WQFS and TPAC are presented in Figure 3.5 as an example. The simulation by the unmodified model reached maximum LAI values (BLAI in SWAT) starting from the first year. While, simulated annual maximum LAI values by the modified model increased during the establishment period and stayed stable after that. The trends of annual maximum LAI for both perennial grasses followed the pattern found in the observed values (Figure 3.3).

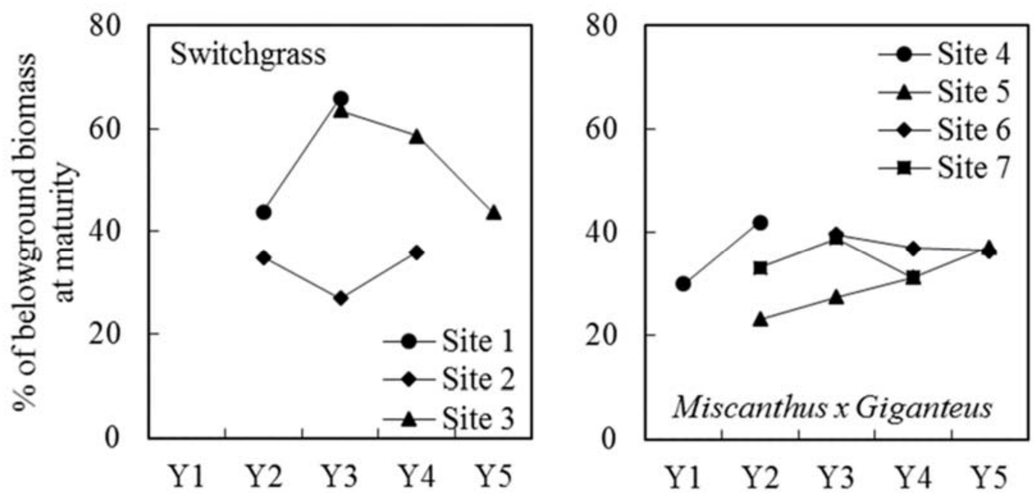

Figure 3.4 Percentage of belowground biomass at maturity for switchgrass and *Miscanthus* (*Miscanthus x Giganteus*). Y represented for year. Site 1: Frederiction Research Centre of Agricultural and Agri-Food Canada (Bolinder *et al.*, 2002); Site 2: Mandan, North Dakota, US (Frank *et al.*, 2004); Site 3 and Site 7: West Lafayette, Indiana, US (Burks, 2013); Site 4: Essek, UK (Beale & Long, 1995); Site 5: Hertfordshire, UK (Riche & Christian, 2001); Site 6: southeast England (Christian *et al.*, 2006)

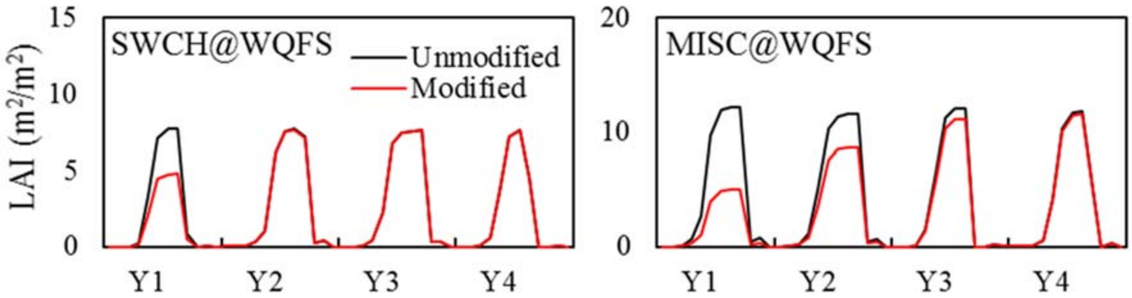

Figure 3.5 Simulated monthly Leaf area index (LAI) with the unmodified (version 635, default) and modified (for establishment period in this study) SWAT models for switchgrass (SWCH) and *Miscanthus* (MISC) at Water Quality Field Station (WQFS). Y represented for year and Y1 was the first year when the grass was planted. At this site, Y1 for SWCH is 2007 and for MISC is 2008.

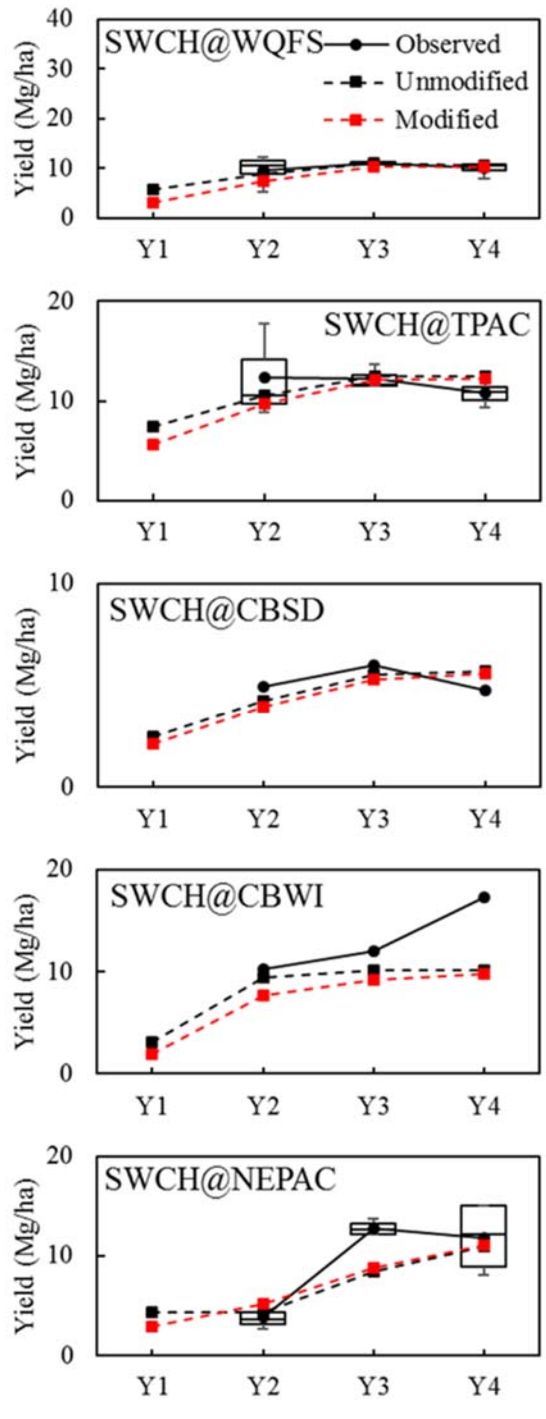

Figure 3.6 Observed and simulated yields for switchgrass (SWCH, Shawnee) with the unmodified (version 635, default) and modified (for establishment period in this study). WQFS: Water quality field station, IN; TPAC: Throckmorton Purdue Agriculture Center, IN; CBSD: Brooking, SD; CBWI: Arlington, WI; NEPAC: Northeast Purdue Agricultural Center, IN.

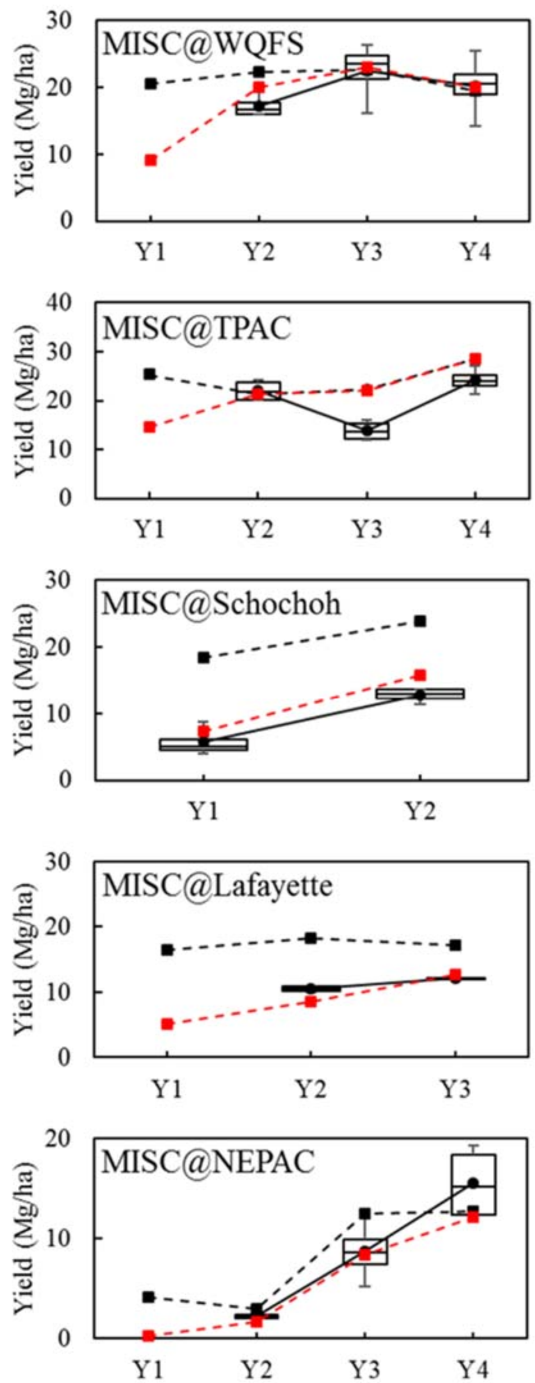

Figure 3.7 Observed and simulated yields *Miscanthus* (MISC, *Miscanthus x giganteus*) with the unmodified (version 635, default) and modified (for establishment period in this study). WQFS: Water quality field station, IN; TPAC: Throckmorton Purdue Agriculture Center, IN; Schochoh: Schochoh, KY; Lafayette: Lafayette, IN WI; NEPAC: Northeast Purdue Agricultural Center, IN.

3.4.3 Hydrologic and water quality responses to model modification

The simulated Evapotranspiration (ET) by the modified SWAT model was lower during the establishment period than the simulated ET by the unmodified SWAT model (Figure 3.8). Less ET resulted into more surface runoff and water yield during this period under both grasses during the establishment periods. Higher surface runoff resulted in increased soil erosion. During the establishment period, mineral nitrogen was most affected compared to organic nitrogen and mineral/organic phosphorus for both perennial grasses (Figure 3.9). Simulated mineral nitrogen losses by the modified model was about half of that by the unmodified model during the establishment period. The differences for the other three nutrient loss variables (organic nitrogen, mineral and organic phosphorus) were very small.

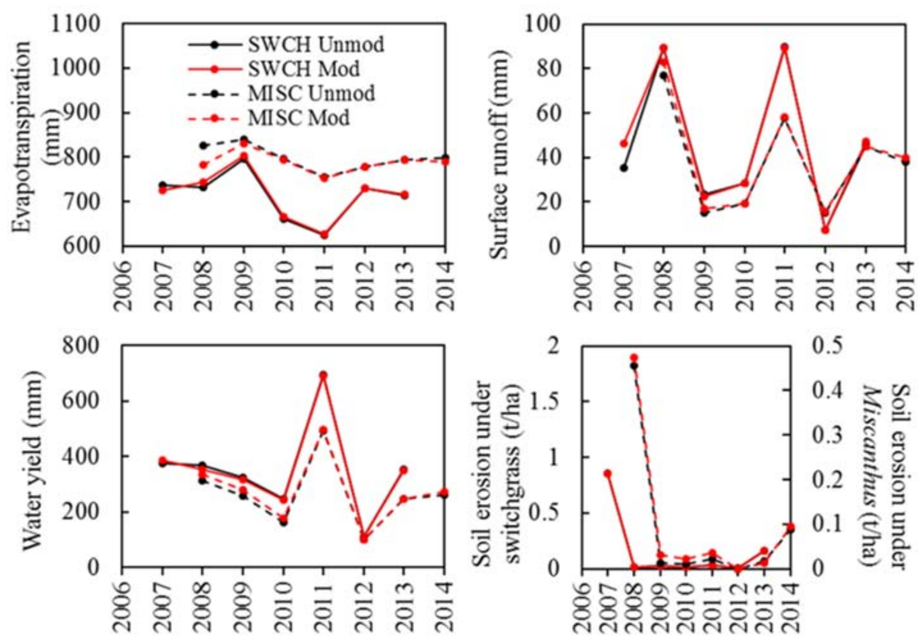

Figure 3.8 Comparison of hydrologic processes and soil erosion under switchgrass (SWCH, Shawnee) and *Miscanthus* (MISC, *Miscanthus x giganteus*) using the unmodified (version 635, default) and modified (for establishment period in this study) SWAT model at Water Quality field Station (WQFS), IN with a two HRU model (one for Shawnee switchgrass and one for *Miscanthus x Gigantues*)

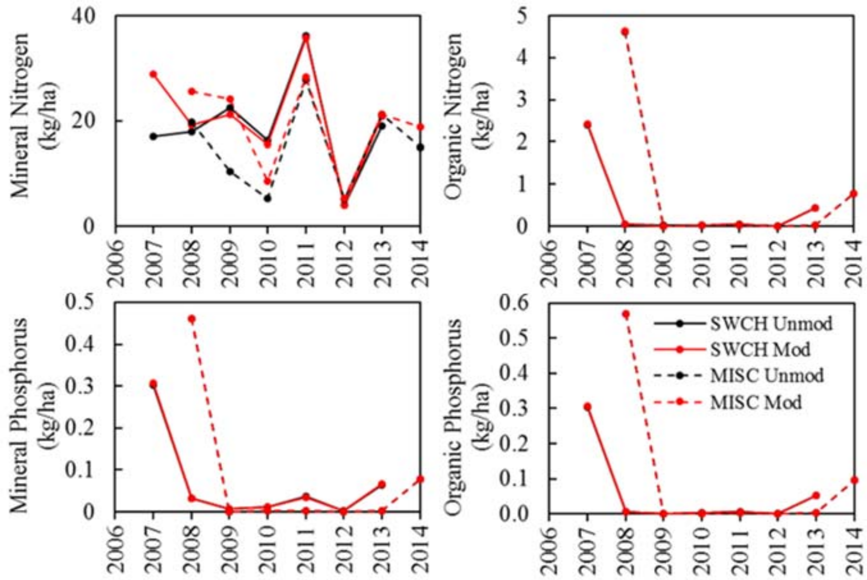

Figure 3.9 Comparison of nutrient loss processes and soil erosion under switchgrass (SWCH, Shawnee) and *Miscanthus* (MISC, *Miscanthus x giganteus*) using the unmodified (version 635, default) and modified (for establishment period in this study) SWAT model at Water Quality field Station (WQFS), IN with a two HRU model (one for Shawnee switchgrass and one for *Miscanthus x Gigantues*).

3.5 Discussion

3.5.1 Duration of establishment periods for switchgrass and *Miscanthus*

Yield is currently the most frequently collected data for perennial bioenergy grasses like switchgrass and *Miscanthus*. Analysis of the published data indicated that switchgrass (both upland and lowland) has a length of establishment period ranging from 2 to 3 years. The establishment period of *Miscanthus* ranges from 2 to 4 years in the U.S. and 3 to 6 years in the Europe. These lengths of establishment period are close to reported 3 to 5 years establishment periods of switchgrass and *Miscanthus* in literature (Jung *et al.*, 1990; Bullard *et al.*, 1995; Lewandowski *et al.*, 2000, 2003; Heaton *et al.*, 2004; Schmer *et al.*, 2009; Maughan *et al.*, 2012). The determination of the establishment period in this study was based on the average yield during their post establishment periods. Thus, this study also recommended that the expected yield reported in the results part can be used as a reference yield to determine whether the grass is in the establishment or post establishment period.

Ceiling, peak or maximum potential yield of perennial grasses has been considered as the indicator for the turning point from establishment to post-establishment period (Bullard *et al.*, 1995; Parrish & Fike, 2005). However, yield is a function of biophysical stress including soil characteristics, environmental (precipitation and temperature), and pest stresses. Therefore, it is possible that yields could be higher during establishment period. Therefore, these ceiling yields should be considered carefully for determination of establishment period (Lesur *et al.*, 2013). Lesur *et al.* (2013) assumed 85% of maximum potential yield as a threshold to identify duration of establishment period and their modeled results indicate that establishment periods of *Miscanthus* in Europe ranged from 3.3 to 7.3 years, with an average of 4.7 years. These values may only be applicable to the Europe since all the data for *Miscanthus* were obtained from that region. The establishment period for *Miscanthus* in Europe determined in this study (3 to 6 years) is close to their value, and is longer than the length in the US. Existing literatures on establishment period lengths of switchgrass and *Miscanthus* are mostly based on expert's opinion, especially for switchgrass (Bullard *et al.*, 1995; McLaughlin & Adams Kszos, 2005; Schmer *et al.*, 2009; Maughan *et al.*, 2012). This study determined the values based on observed data and can serve as a general guidance for determination of establishment period in areas where no historical data were available for these perennial grasses.

3.5.2 Physiological processes during the establishment period for switchgrass and *Miscanthus*

Establishment period is required for belowground rhizome organs to be fully developed in perennial grasses (Miguez *et al.*, 2012). Data analyzed in this study indicated that belowground biomass of switchgrass and *Miscanthus* shows a slightly increasing trends during the first 3 to 4 years. The rate of increases varies due to the species differences and specific growing conditions. Planting methods and density are also reported to affect the time required by *Miscanthus* to get established (Miguez *et al.*, 2008; Lesur *et al.*, 2013). Higher planting densities tend to increase the rate of belowground biomass development and shorten establishment period. However, a lack of data availability limits our ability to quantify the role of planting density on establishment period. There is also a scarcity of data related to nutrient dynamics and RUE of switchgrass and *Miscanthus* during the establishment period. Burks (2013) analyzed changes of nitrogen and phosphorus concentration and mass in above- and below- ground biomass for 3 years after the planting year of Shawnee switchgrass and *Miscanthus x Giganteus* at the WQFS. The result indicated that the concentration of nitrogen and phosphorus in biomass did not vary among years. But the mass of the two nutrients in the plant increased with the biomass accumulation. Additional measured data from multiple locations are needed to generalize such trends.

3.5.3 Modification of SWAT model to incorporate establishment period simulation

Development of LAI is the driving factor of biomass development simulation in the SWAT model. In this study, the modification of SWAT model was mainly on the simulation of BLAI values, which was further modified to update annually instead of a static value as the default model. The updating was conducted using a logistic equation developed by Miguez *et al.* (2008). In their study, the parameters were estimated as a function of growing condition at different country and season. In our study, the parameters were estimated from the observed yield data as the observed data for LAI was unavailable. Parameter estimation using yield data was possible as the growing conditions and management practices can be represented by the SWAT model. The incorporation of this function combined with growth parameters for Shawnee switchgrass and *Miscanthus x Giganteus* by Trybula *et al.* (2014) improves the simulation of yields, especially for *Miscanthus*.

The modification on LAI simulation improved the representation of perennial grass yield development during their establishment period by the SWAT model though the improvement was less obvious for switchgrass than for *Miscanthus*. For switchgrass, the improvement is not obvious if total yield values are considered. Due to the short establishment period (2 year) for switchgrass in these sites, the simulated yields by the unmodified and modified SWAT model are both low and similar during the establishment period. The lower simulated yield of switchgrass by the unmodified model during the first year tends to lead to a false impression that the unmodified model is representing the establishment periods. What actually happens is that switchgrass needs to develop rhizomes and roots in the first year of growth. This is represented by partitioning 49% of whole biomass to belowground biomass (RFR2C in the SWAT model) in the SWAT model. In addition, the belowground biomass can be maintained from one year to another by the perennial grass. This caused the lower yield of switchgrass in the first year. In addition, LAI was over-estimated by the unmodified model compared to the measured values (Figure 3.3). The modified SWAT model improved biomass partitioning and LAI values during the establishment period. For *Miscanthus*, the model improvement is more obvious than switchgrass. Simulated *Miscanthus* yields by the unmodified model are high in the first year at study sites except at NEPAC. Similar to switchgrass, *Miscanthus* also partitions its total biomass into above- and belowground biomass, but the proportion to be partitioned to belowground biomass is much lower than for switchgrass.. The suggested value of RFR2C for *Miscanthus* is 18% (Trybula *et al.*, 2014). Here, it might be recalled that observed LAI in the first year is high as shown in Figure 3.3. The yield of *Miscanthus* during the first year might be expected to be true in reality due to higher observed LAI. While, observed yield in the Europe (Figure 3.2) and in Schochoh, KY (Figure 3.6) both indicate that *Miscanthus* yield in the first year is lower than later years. It could be possible that the higher observed LAI in the first year as shown in Figure 3.3 is not as representative as later years due to limited data points.

The simulated yield for switchgrass and *Miscanthus* during their establishment period was acceptable compared with observed yield. The modified SWAT model satisfactorily simulated the trends and magnitudes of observed yields at 2 out of the 5 sites (i.e. WQFS and TPAC;) for switchgrass and 4 out of 5 sites for *Miscanthus* (WQFS, Schochoh, Lafayette, and NEPAC). In CBSD, the observed yield was relatively low and did not meet the recommended reference yield in this study. In CBWI, the yield in the year 4 was much higher than the expected yield for Shawnee switchgrass during the post establishment period. As pointed out by Casler and Boe (2003), Shawnee switchgrass shows broader adaptability than other upland switchgrass cultivars (such as Cave in Rock and Dacotah) and produces generally higher yields. However, the average observed yield at these two locations (CBSD and CBWI) are quite different during both the establishment and post establishment period. There could be two reasons for this differences in observed yield. One reason is the growing conditions at CBWI is more favorable for crop growth (personal communication with Dr. Jeffrey Volenec). The lower observed yield in CBSD might be caused by some soil properties that limited the growth of switchgrass. The simulation result by the unmodified model indicated that switchgrass in CBSD experienced on average 70 days' water stress and 202 days' temperature stress. While in CBWI, there was no water stress and the average temperature stress was 208 days. The other is the higher weight per tiller in the CBWI site than in the CBSD site (Casler and Boe, 2003). This property of crop growth was not represented in the SWAT model for crop growth. These could be possible reasons that caused the poor performance of the model at the CBSD and CBWI sites. At NEPAC and TPAC, the growth of switchgrass and *Miscanthus* was affected by a severe drought that occurred in 2012 (Y2 for NEPAC and Y3 for TPAC data), which also affected the duration of establishment period and yield trends. The differences between simulated and observed yields of switchgrass and *Miscanthus* indicate that there are still efforts required to further understand the reasons for yield variability and the capability of model to capture the variability.

Another point that is worthy of discussion is the simulation of yield decline for *Miscanthus* in the long run. In this study, the equation proposed was based on the assumption that yield under optimal growth condition will be stable during the post establishment period. Lesur *et al.* (2013) presented an equation that represents both increasing of yield in the establishment period and declining of yield in the long term. In the data from the U.S., yield decline is also reported for *Miscanthus* (Arundale *et al.*, 2014). Reasons for yield decline include depletion of soil nutrient, soil compaction, and pest and disease pressure (Cadoux *et al.*, 2012; Lesur *et al.*, 2013; Arundale *et al.*, 2014). In this study, yield decline is not considered. There is a need to collect long-term yield data and utilize the data to develop model algorithms that could simulated expected long term decrease in *Miscanthus* yields. As a comprehensive model, the SWAT model might be able to account for some reasons, like the depletion of soil nutrients. However, impacts of disease and pests are not simulated in the SWAT model.

3.5.4 Differences in hydrologic and water quality processes between establishment and post establishment periods

The simulation with the unmodified and modified SWAT model verifies the hypothesis that hydrologic and water quality processes in the establishment period are different from those in the post-establishment period. Even though these simulations are not calibrated at WQFS due to unavailability of observed data, the simulated results are comparable to observations reported in literature. Reported ET for switchgrass is 676 mm in literature (Yimam *et al.*, 2014). Mineral nitrogen leaching from *Miscanthus* ranged from 10 to 20 kg/ha with 60 kgN/ha fertilization (close to 56kgN/ha used in the simulation). The changes of hydrologic and water quality variables, such as lower evapotranspiration and higher sediment/nutrient loss during the establishment period, were same as reported in literature (Sarker & Miller, 2014; Curley *et al.*, 2009; Curley *et al.*, 2010). Even though the differences in the simulation under switchgrass is small at the test sites with the modified and unmodified SWAT model, it may be not the case at areas where switchgrass establishment is longer than 2 years. In addition, a small change of sediment and nutrient losses at the field scale (HRU in this study) might accumulate and cause larger loss at the watershed outlet. The life span for maintaining ceiling yield of switchgrass is expected to be 10 to 20 years (Hopkins *et al.*, 1995; Fike *et al.*, 2006), and of *Miscanthus* between 15 to 20 years (Lewandowski *et al.*, 2000). Even though establishment period is short compared to the life span of these two perennial grasses, the environmental impacts could be substantial during this period. The model improvement made in our study will enable quantification of hydrologic/water quality impacts during establishment periods of bioenergy crops and could provide insights on best management practices needed to minimize the unintended negative impacts.

3.6 Conclusions

Switchgrass and *Miscanthus* both have establishment periods. However, the understanding of the establishment periods of the two perennial grasses is limited. This study summarizes data for various physiological processes of the two perennial grasses and explores their evolution during the establishment period. The extracted knowledge on these processes is incorporated into the SWAT model to improve the model's simulation of these two perennial grasses during their establishment periods. The modified model is then used to quantify the differences in hydrologic and water quality processes during the establishment and post-establishment periods. This study recommends using yield values that established switchgrass and *Miscanthus* are expected to produce as threshold yields to determine their establishment periods. Upland switchgrass generally produces 10 Mg/ha yield and lowland switchgrass generally produce 15 Mg/ha yield once they are fully established. Based on these threshold yields, both ecotypes of switchgrass have a 2 to 3 year establishment period. Established yield of *Miscanthus* is expected to be 15 Mg/ha in Europe and 20 Mg/ha in the U.S. The establishment periods for *Miscanthus* is 3 to 6 years in Europe and 2 to 4 years in the U.S., respectively. During the establishment period, maximum LAI of the two perennial grasses increases but varies considerably among the two crops. The ratio of above- to below- ground biomass for the two perennial grasses increase during the establishment period but the rate of increasing varies significantly at different sites.

The measured crop growth data availability during the establishment period is quite limited. Even though yield data was collected for these two candidate bioenergy crops, the biomass partitioning, LAI and yield values during the establishment period are largely missing. For example, out of all the sites tested in this study, only one site had yield data for *Miscanthus* in the first year. The improvement of the model in this study was partially based on the assumptions of RUE changes, and should be validated with the availability of measured data.

3.7 Acknowledgements

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CHAPTER 4. BIOMASS PRODUCTION AND HYDROLOGIC/WATER QUALITY IMPACTS FROM SWITCHGRASS AND *MISCANTHUS* GROWTH ON MARGINAL LAND IN THE UPPER MISSISSIPPI RIVER BASIN (UMRB)

4.1 Abstract

Availability of considerably large areas of marginal land in the Upper Mississippi River Basin (UMRB) provides valuable land resources for growth of perennial biofuel crops and brings environmental benefits. This study predicted the biomass production from switchgrass and *Miscanthus* on marginal lands and the potential impacts on flow and sediment load in the UMRB region using the Soil and Water Assessment Tool model. The results indicated that 22% to 37% of the biofuel development goal (132 billion liters) set by the Energy Independence and Secure Act (EISA) 2007 could be achieved by growing switchgrass and *Miscanthus* on marginal lands in the UMRB region, respectively. The production of the two perennial grasses on marginal lands caused 8% and 12% reduction of flow and 8% to 13% reduction of sediment load at the watershed outlet by growing switchgrass and *Miscanthus*, respectively. In addition, the reduction of flow and soil erosion was smaller during the establishment period than during the post establishment periods of these perennial biofeedstock crops. The results from this study can be utilized in developing watershed management plans, especially targeting at both biofuel development and solving environmental problems in the UMRB region.

4.2 Introduction

As an important agricultural region, the Upper Mississippi River Basin (UMRB) produces 49% of corn (*Zea mays*) and 41% of soybeans (*Glycine max*) for the US (*USDA National agricultural statistics service: Quick Stats*, 2014). However, the UMRB region is also well-known for considerable nutrient losses from agricultural land and contributes about 50% of nutrient loads from the Mississippi River Basin to the Gulf of Mexico (Srinivasan *et al.*, 2010). Approximately 34% of the existing agricultural lands in this region are marginal lands (Feng *et al.*, unpublished). These lands are considered at the margin of cultivation because they could not be remuneratively cultivated for traditional crops due to various limitations such as poor physical properties on the production practices (Lubowski *et al.*, 2006). These lands are also environmentally sensitive and more vulnerable to erosion than prime farmland. These lands may potentially serve as hotspots and contribute more sediment and nutrient losses than prime agricultural lands in this region. Conservation practices targeted on these lands for water quality improvement might be more effective than focusing in other areas within the basin that may contribute relatively smaller losses of nonpoint source pollutants.

Perennial grasses, such as switchgrass (*Panicum virgatum*) and *Miscanthus* (*Miscanthus x giganteus*), installed as buffer strips or hedges are recommended to reduce sediment and nutrient losses from fields (Dabney *et al.*, 1995, 2004, 2009; Meyer *et al.*, 1995; Curley *et al.*, 2009, 2010). These perennial grasses protect the land surface year around and avoid disturbance from tillage required by producing traditional annual crops. They also have lower requirement for agricultural chemical application. There grasses are reported to reduce sediment loss by 63% to 99%, nitrogen loss by 46 to 81% and phosphorus by 34 to 78% when switchgrass is grown as buffer strips (Blanco-Canqui *et al.*, 2006; Curley *et al.*, 2009; Dabney *et al.*, 2009; Lee *et al.*, 2012). Concurrently, these grasses could also be utilized as biofeedstock crops because of their high biomass production potential. The average annual biomass production of switchgrass is 10 to 15 Mg/ha, and of *Miscanthus* is 15 to 20 Mg/ha (Heaton *et al.*, 2008; Wullschleger *et al.*, 2010). In addition, these grasses are reported to be able to grow well on marginal lands (Woodson, 2011; Feng *et al.*, 2015). Availability of large areas of marginal lands in the UMRB region makes it ideal for utilizing these perennial grasses as biofeedstocks and for conservation purposes to reduce non-point source pollution from this region.

Biomass production and their environmental impacts in the UMRB region have been evaluated in several studies (Jha *et al.*, 2006; Srinivasan *et al.*, 2010; Demissie *et al.*, 2012; Wu & Liu, 2012). These studies focus mainly on environmental impacts from increased corn production for biofuel development by either assuming expansion of current cropland or more fertilizer application. The use of marginal lands to produce biofeedstocks has been recommended but not evaluated extensively. One of the challenges is the inadequate representation of candidate perennial grasses in the currently available biophysical models. Ng *et al.* (2010) simulated the growth of *Miscanthus* using the SWAT model with the crop growth parameters from another model or values derived from literature. Srinivasan *et al.* (2010) simulated the growth of switchgrass on all agricultural lands. Love & Nejadhashemi (2011) considered both growth of perennial crops and marginal land. In their study, marginal land included lands that were not used for agricultural production, such as fallow cropland, pasture, or wetland. Feng *et al.* (2015) simulated the growth of switchgrass and *Miscanthus* on marginal lands using the

Agricultural Policy Environmental Extender (APEX) model. Other studies did not include the consideration of perennial grasses as biomass feedstock crops. Recent advances in understanding of marginal land quality and spatial distribution combined with the recent improvements in the SWAT model to simulate perennial grasses enable evaluation of biomass production on marginal lands and associated environmental benefits. Systematic evaluation methods for marginal land identification for biomass production are proposed in recent years in several studies (Gopalakrishnan *et al.*, 2011; Kang *et al.*, 2013; Feng *et al.*, 2015). Similarly, Trybula *et al.* (2014) modified the SWAT model algorithms to improve simulation of upland varieties of switchgrass and *Miscanthus* using evidence-based parameter values. In addition, Feng *et al.* (unpublished) incorporate the simulation of establishment periods of switchgrass and *Miscanthus* in the SWAT model. These improvements enabled the SWAT model in better representing the growth of switchgrass and *Miscanthus* and evaluation of associated hydrologic and water quality impacts.

The objective of this study is to evaluate the growth of switchgrass and *Miscanthus* on marginal land in the UMRB region. Specifically, the following goals are achieved: 1) setting up SWAT model that includes marginal land in the UMRB region; 2) estimating the biomass production of switchgrass and *Miscanthus* by simulating their growth on marginal lands; and 3) quantifying the impacts on hydrology and water quality when these perennial grasses are produced on marginal lands in the region.

4.3 Methods

4.3.1 General description

This study set up a SWAT model (Arnold *et al.*, 1998) specifically for the simulation of land use change scenarios for growing perennial crops on marginal lands for switchgrass and *Miscanthus* production in the UMRB region. Detailed description of the SWAT model is provided by Neitsch *et al.* (2011). This section describes former works that this study utilized, land use scenarios, and the steps for setting up SWAT model to incorporate marginal lands in a large area for the UMRB.

4.3.2 Study area

The UMRB basin covers 7 states (Figure 4.1) and has a total drainage area of 492,000 km^2. This basin is located in the "corn belt" region of the US and has 43% of its area devoted to corn, soybean, and wheat (*Triticum aestivum*) production (USDA National Agricultural Statistics Service Cropland Data Layer, 2014). Other major land cover types include 22% of forests, 16% of pasture and hay, 10% of water and wetlands, 8% of developed area, and 1% of other agricultural crops. Fertile soil, adequate water supply and mild climate in this region make it an important food provision area, especially for corn and soybean (Wu *et al.*, 2012). The large amount of agricultural production in this region also makes it ideal for providing biofeedstock for producing more than 50% of the US biofuel production (Wu *et al.*, 2012). Almost all current biorefineries are using corn as feedstock with only one cellulosic biorefinery (DuPont, in Nevada, Iowa) with ethanol production capacity of 30 million gallon per year. Growth of switchgrass and *Miscanthus* as a candidate biofeedstock has been tested across this region at several location (Supporting Information, SI Table S1).

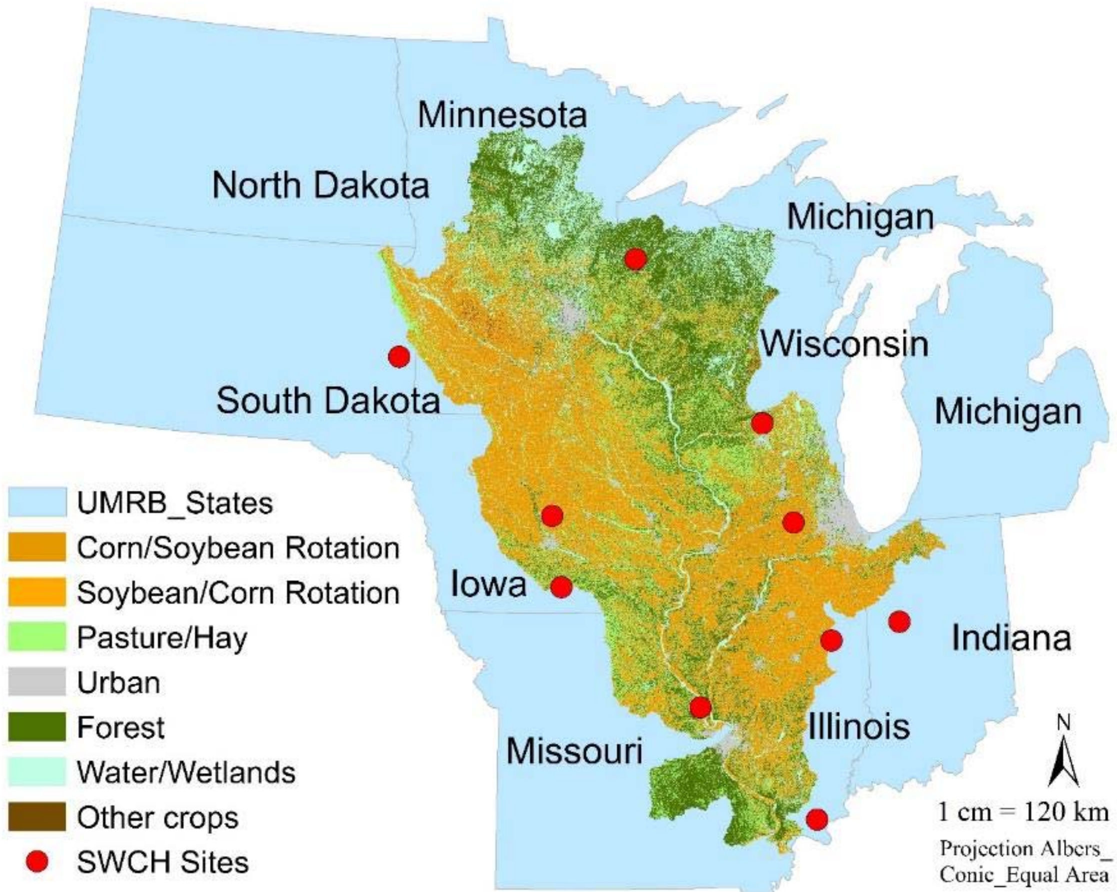


Figure 4.1 Location, major land use types and fields for switchgrass (SWCH) sites of the Upper Mississippi River Basin

4.3.3 Marginal land and their suitability for perennial grass growth in the UMRB region

Feng *et al.* (unpublished, Chapter 2) found that 23% of the UMRB areas were marginal land based on the land cover type information from National Agricultural Statistics Service (NASS) and soil properties information from Soil Survey Geographic (SSURGO) database. These marginal lands were mainly from land for other agricultural crops, corn and soybean, and pasture, with the majority from land for corn, soybean and pasture with Land Capability Class (LCC) 3 and 8. The suitability of these marginal lands were also evaluated for growth of switchgrass and *Miscanthus* based on Land suitability index (LSI), ranging from 0 (not suitable) to 1 (completely suitable). Among these marginal lands, 60% of them had LSI values larger than 60. This indicated that these marginal lands were moderately to highly suitable for the growth of these perennial grasses.

4.3.4 Land cover change scenarios

Six scenarios for producing perennial grasses were evaluated (Table 4.1). Marginal land was classified into three groups in this study in order to limit the total number of Hydrologic Response Units (HRUs) in the SWAT model. The three groups included: Not suitable (LSI 0 to 0.3), Moderately suitable (LSI 0.3 to 0.6) and Highly suitable (LSI 0.6 to 1.0). The purpose of designing these scenarios was to test the growth of switchgrass and *Miscanthus* on marginal lands with different suitability levels, and impacts on hydrologic and sediment loads at the edge of field and watershed scales. The specific grass species evaluated were Shawnee switchgrass (*Panicum virgatum L.*) and *Miscanthus* (*Miscanthus x giganteus*) for which the SWAT model has been parameterized by Trybula *et al.* (2015) for this region.

Table 4.1 Land cover change scenarios included in this study

Scenario	Land cover	Plant
Baseline	Land cover types based on NASS2013	Original
Not Suitable	Mostly not suitable marginal land	switchgrass *Miscanthus*
Moderately Suitable	Moderately suitable marginal land for switchgrass	switchgrass *Miscanthus*
Highly Suitable	Highly suitable marginal land for switchgrass	Switchgrass *Miscanthus*

4.3.5 SWAT model setup

The land cover change scenarios required the SWAT model to include simulation of marginal land areas in the UMRB region. This was achieved by manipulating the soil and land use layers for setting the SWAT model up. The SSURGO raster layer for marginal land area and the STATSGO raster layer (obtained from the SWAT_US_Soils.mdb and resampled from 250 meter original resolution to 30 m resolution) in non-marginal land area were combined. The soil properties for soils in the STATSGO raster layer was also extracted from the SWAT_US_Soils.mdb files and imported into the SWAT_US_SSURGO.mdb file. In order to include marginal land and its suitability information into the model, the marginal land suitability map was first classified into 12 categories, representing marginal land from four major land cover types (corn, soybean, pasture, and other agriculture land) and three suitability levels (not suitable, moderately suitable and highly suitable) for each of the four major land cover types. Then the map with 12 categories was incorporated into the NASS 2013 layer. In this way, the baseline scenario could be represented (with original land cover types on these marginal lands) as well as projected biomass production scenario (with converting marginal land of different suitability level to switchgrass and *Miscanthus*) in the model setup. These steps were needed to preserve the location of marginal lands and to meet the file and memory size limitations of the SWAT model. For example, if these two data sets were used and no thresholds were applied on soil, land use or slope in the HRU definition step in ArcSWAT, there would be too many HRUs present in the model to perform simulations in a timely manner or would exceed the memory size limitation for ArcSWAT (i.e. 2 GB). If any thresholds were applied (even 1% for soil or l% for land use and 1% for slope), marginal land area would be lost due to the fact that most of these lands were scattered and had small land area within each sub-basin.

After these two layers and the database for ArcSWAT were prepared (adding new land cover types to the crop table in the project.mdb), a 30-m DEM data layer was used, with the predefined HUC12 watershed boundary and streamline for the study area to delineate the watershed. The soil and land cover layers were then added to the soil/landuse/slope definition step, with two classes of slope (0 to 5%, >5%). A threshold of 20% on an area basis of soil and land use types was applied in the HRU definition step. This threshold value was set based on the distribution of STATSGO soil types for the non-marginal land area and the number of HRUs that were allowed by ArcSWAT database (see explanation later in this paragraph). Then, data for point source, management practices of corn/soybean, and tile drainage were incorporated in the model database. Management practices for corn, soybean, pasture, switchgrass and *Miscanthus* was the same as those used by Cibin *et al.* (2015). For switchgrass and *Miscanthus*, a 2- and 3-year establishment periods were assumed, respectively. Tile drainage was installed on soil of somewhat poor, poor and very poor drainage conditions (extracted from SSURGO database) on corn and soybean lands with slopes less than 2%. There were 9,375 HRUs with tile drainage with the total area of tiled drained HRUs consisting of 18.2% of the UMRB area. Weather data were downloaded for 732 weather stations located within the UMRB region from National Climate Data Center (NCDC, https://gis.ncdc.noaa.gov/). Stations with more than 20% missing data for precipitation were removed from the SWAT modeling with a total number of 440 stations used in the analysis. If any short-term data were missing for any of these 440 weather stations, missing data were filled by data from the closest stations located within 50 km of the target station using the Inverse Distance Weighting method. The SWAT model inputs were then written in ArcSWAT. This was done by writing one type of input table (for example, hru files) at a time. After writing each type of input file, the ArcSWAT project was saved, closed and reopened. Before reopening, the projectname.mdb file was compressed either using Access Database (Open .mdb, click “File”, click “Compact & Repair Database”) or using ArcCatalog (Right click on the .mdb file, select “Administration” and then “Compact Database”). The largest number of HRUs for one ArcSWAT project that could be stored was approximately 150,000, based on several trials. Finally, the model was setup with 5,732 USGS HUC12 subbasins, and 136,079 HRUs.

The model was then calibrated against observed data from 6 USGS gauge stations (Table 4.2) within the basin for flow and 2 for sediment load at monthly scale for 1995 to 2000 and validated for 2001 to 2005. The parameters for calibration of flow and sediment load are provided in SI Table S2. The calibration and validation was evaluated using the coefficient of determination (R^2) and the Nash-Sutcliffe efficiency (NS) (Equation 1) as the objective functions, where O and P represent for observed and simulated values, respectively, and i represents months in this study. The calibrated model was used to simulate the scenarios listed in Table 4.2 for the period of 1995 to 2005. The yield of corn, soybean, switchgrass and *Miscanthus* were summarized for HRUs with different marginal land suitable classes. Total biomass was calculated by summing up the products of yield and area at each HRU. Total bioethanol production was calculated as the products of total biomass and bioethanol yield of 302 Liter/Mg dry biomass (80 gallon/Mg dry biomass) (Feng *et al.*, 2015). The results for flow and sediment load were summarized at the watershed outlet. In addition, evapotranspiration, soil moisture change, soil erosion and biomass production potential were evaluated at the HRU level.

$$NS = 1 - \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n}(O_i - \bar{O})^2} \qquad (1)$$

4.4 Results and Discussion

4.4.1 Model calibration and validation results

The model was first evaluated to simulate major crops (corn and soybean) in the study area. Simulated corn grain yield ranged from 0.1 to 11.7 Mg/ha with an average yield at 8.3 Mg/ha. Simulated soybean grain yield ranged from 0.1 to 4.0 Mg/ha, with an average of 3.3 Mg/ha. These ranges and average values of yields were close to those reported by NASS for the simulation period (ranged from 2.3 to 11.3 Mg/ha, averaged at 8.6 Mg/ha).

The model was calibrated and validated for flow simulations at 6 stations and for total sediment load at 2 stations (Table 4.2). Time series comparison between observed and simulated flow and total sediment load at the watershed outlet (Mississippi River below Grafton, IL, 05389500) are provided in Figure 4.2. The monthly statistics for both flow and total sediment load at all sites were mostly over 0.5, indicating a good model performance (Santhi *et al.*, 2001; Engel *et al.*, 2007) (Santhi *et al.*, 2001; Engel *et al.*, 2007)

Table 4.2 Monthly calibration/validation statistics for flow and total sediment load at various stations in the Upper Mississippi River Basin

Station	USGS Gauge No.	Calibration (Monthly)		Validation (Monthly)	
		R^2	NS	R^2	NS
Flow					
Minnesota River near Jordan, MN	05330000	0.84	0.79	0.92	0.91
Chippewa River at Durand, WI	05369500	0.65	0.43	0.79	0.63
Mississippi River at McGregor, IA	05389500	0.72	0.58	0.83	0.53
Skunk River at Augusta, IA	05474000	0.88	0.87	0.87	0.84
Mississippi River below Grafton, IL	05587455	0.89	0.87	0.86	0.78
Illinois River at Valley City, IL	05586100	0.79	0.73	0.81	0.73
Total sediment load					
Mississippi River below Grafton, IL	05587455	0.76	0.72	0.76	0.31
Illinois River at Valley City, IL	05586100	0.67	0.56	0.71	0.37

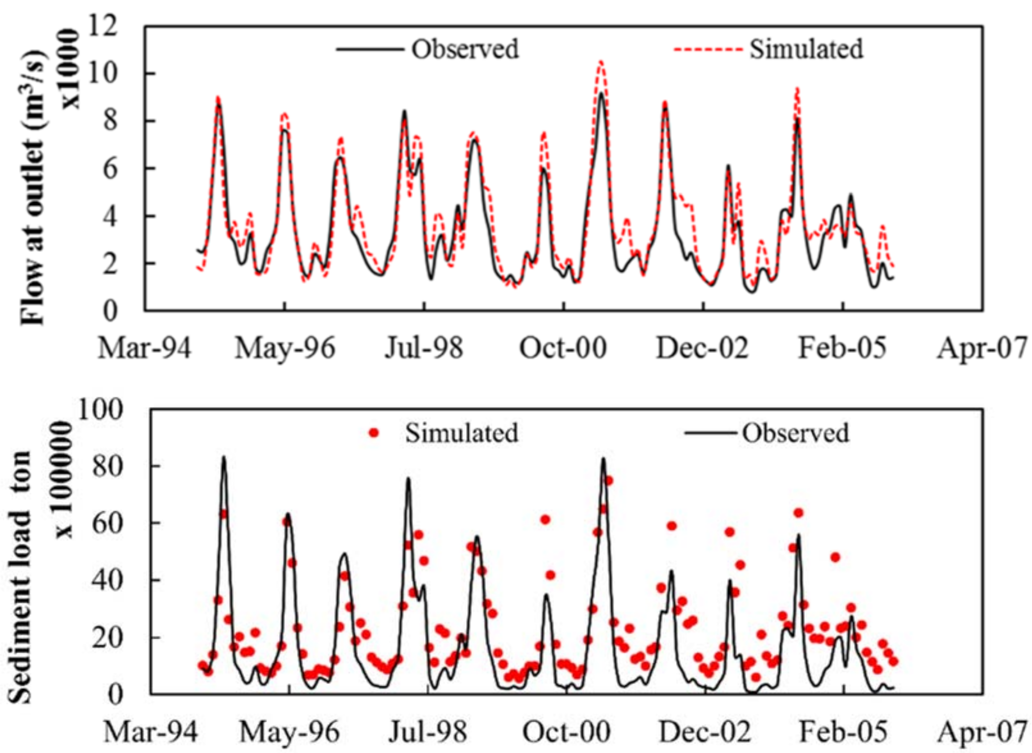


Figure 4.2 Comparison between monthly time series of observed and simulated flow and total sediment load at the outlet of the Upper Mississippi River Basin for the calibration (1995 to 2000) and validation (2001 to 2005) periods.

4.4.2 Biomass production

The average simulated yields of switchgrass and *Miscanthus* across all marginal lands (three suitable classes) increased during their establishment periods (Table 4.3, Figure 4.3). Switchgrass yield monotonically increased during its establishment period (year 1 and year 2) and the beginning of the post establishment period (3^{rd} till the 11^{th} year in this study). *Miscanthus* yield also increased during its establishment period (1^{st} to 3^{rd} year), but yield during the post establishment period (4^{th} till 11^{th} year in this study) was lower than the establishment periods. The yield distributions of the two grasses were similar among marginal lands with different suitability levels (Figure 4.3), indicated by the Land suitability index (LSI) (Feng *et al.* unpublished). This could be due to the fact that the simulated yield with the SWAT model did not consider factors that were included in LSI calculation. For example, the constraints from salinity and pH on growth of the two crops and from higher slope (for example, > 15%) on machine operation were not included in the SWAT model.

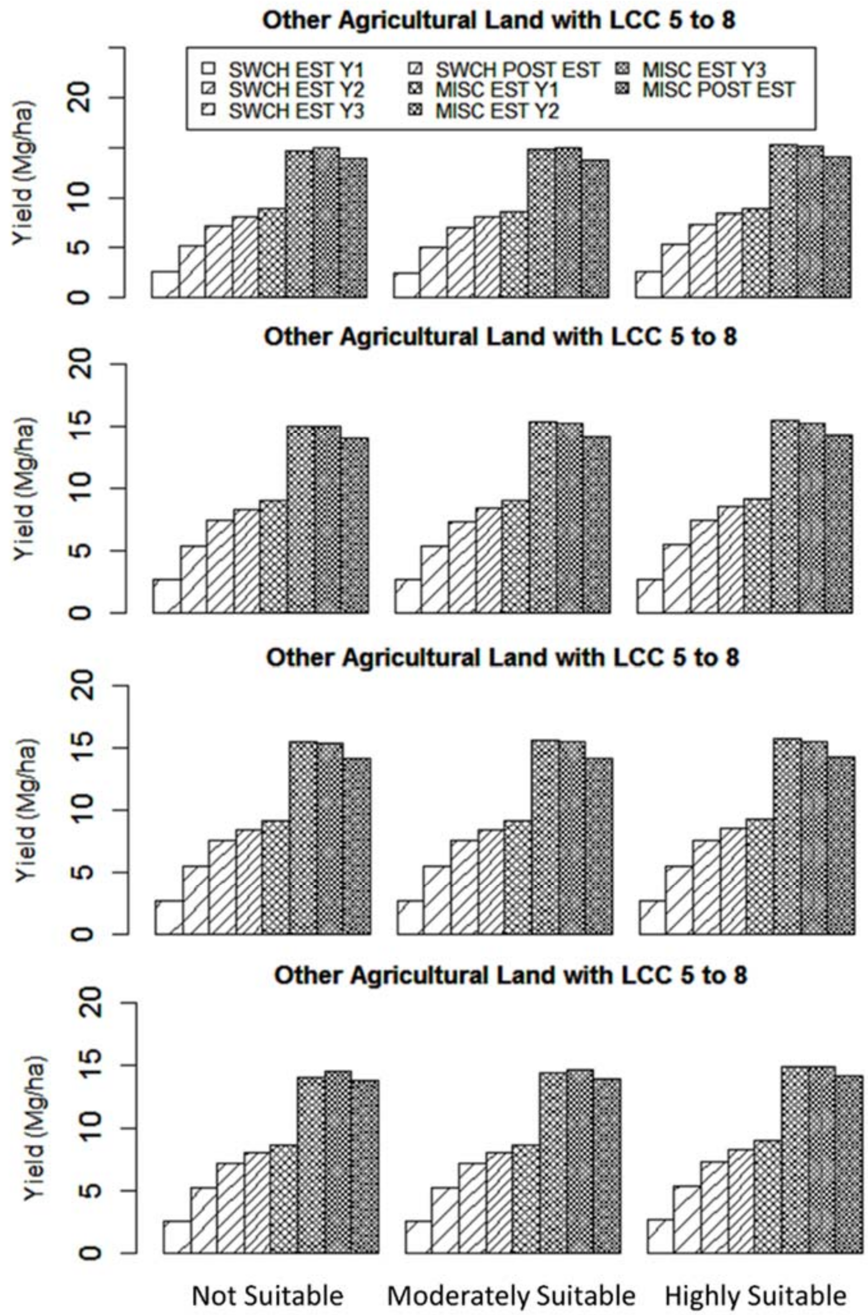
Table 4.3 Average yield of switchgrass and *Miscanthus* and bioethanol potential from the Upper Mississippi River Basin

	Year	Not Suitable ML	Moderately Suitable ML	Highly Suitable ML	Total Biomass (Million Mg)	Total Biofuel (Billion Liter)
Switchgrass	Year 1	2.6	2.6	2.7		
	Year 2	5.4	5.3	5.5		
	Year 3	7.4	7.3	7.5		
	Post Establish	8.3	8.3	8.5	96	29
Miscanthus	Year 1	8.9	8.9	9.1		
	Year 2	14.8	15.1	15.3		
	Year 3	15.0	15.1	15.2		
	Post Establish	13.9	14.0	14.2	160	48

Switchgrass yield during the post establishment period was close to average observed yield (8.3 Mg/ha) from this region (SI Table S1). However, the simulated switchgrass yield was smaller than the average simulated yield (15.8 Mg/ha, 17.4 ton/ha) by Srinivasan *et al.* (2010), mainly due to the fact that the authors used Alamo switchgrass in their simulation which is a lowland variety of switchgrass with relatively greater yields compared to upland switchgrass varieties used in our simulation. For *Miscanthus*, the yield during its post establishment period was much lower than the average observed yield (34 Mg/ha) in the Midwest (SI Table S3). Across years, yield of these two perennial biofeedstock crops showed great variations among HRUs, as shown in SI Figure S1 and S2. During the post establishment period, switchgrass yield ranged from 0 to 11.1 Mg/ha and *Miscanthus* yield ranged from 0 to 16.8 Mg/ha. It took longer for switchgrass to achieve this yield in the majority of the HRUs, even though the assumed establishment period for switchgrass was 2 years. While for *Miscanthus*, some HRUs already produced yields around 20 Mg/ha in the second year, but decreased in the third year and during the post establishment period (SI Figure S2), probably due to environmental stresses. The results reflected the variation of yield for these two perennial grasses in marginal lands. In the model, these variations could be ascribed to one or more of the 4 stresses (temperature, water, nitrogen, and phosphorus). In reality, there could be other additional reasons such as species of these perennial grasses with different growth properties, management practices, and disease and pest pressure.

The total bioethanol that could be produced from marginal land was 29×10^9 liter from switchgrass and 48×10^9 liter from *Miscanthus* (Table 4.3), representing 22% and 37%, respectively, of the biofuel development goal (132×10^9 liter) set in the Energy

Security and Independence Act (EISA) 2007. By converting all agricultural land to switchgrass, the total biomass estimated by Srinivasan *et al.* (2010) was 345 Million Mg (380 Million tons). This could be considered an upper limit of switchgrass as biofeedstock from the UMRB region. Demissie *et al.* (2012) estimated that 15.9×10^9 liter of bioethanol could be produced from corn stover. These results indicated that the UMRB region could contribute a significant amount of cellulosic bioethanol for biofuel development in the



US.

Figure 4.3 Yield of switchgrass and *Miscanthus* averaged over marginal land HRUs with different land suitability levels. SWCH stands for switchgrass and MISC stands for *Miscanthus*. EST stands for establishment period and POST EST stands for post establishment period. Switchgrass have 2 years establishment period (1995 as Y1 in this study) and *Miscanthus* has 3 years establishment periods (1995 as Y1). The value for POST EST is the average ET value of 1998 to 2005 (8 years).

4.4.3 Impacts on hydrologic processes

When marginal land was converted to production of switchgrass and *Miscanthus*, flow at the outlet of the basin was reduced all years (Figure 4.4). The relative change of flow ranged from -3% to -11% when marginal lands were converted to switchgrass and -7% to -15% when converted to *Miscanthus*. The average reduction rates across these 11 years of simulation were 8% and 12% for switchgrass and *Miscanthus*, respectively, indicating that large scale production of perennial grasses on marginal lands may considerably impact water yield in this region. Other researchers have reported that significant impacts on water yield might not occur when *Miscanthus* coverage was less than 50% of the Midwest area (Vanloocke *et al.*, 2010). However, our results indicate that the impact may be considerable and were similar to results reported by other researchers. For example, Demissie *et al.* (2012) predicted a 4.6% reduction of flow when corn production were expanded for biofuel development and Wu *et al.* (2012) predicted about 2% reduction of flow when 10% of pasture land was converted to switchgrass in the same study area.

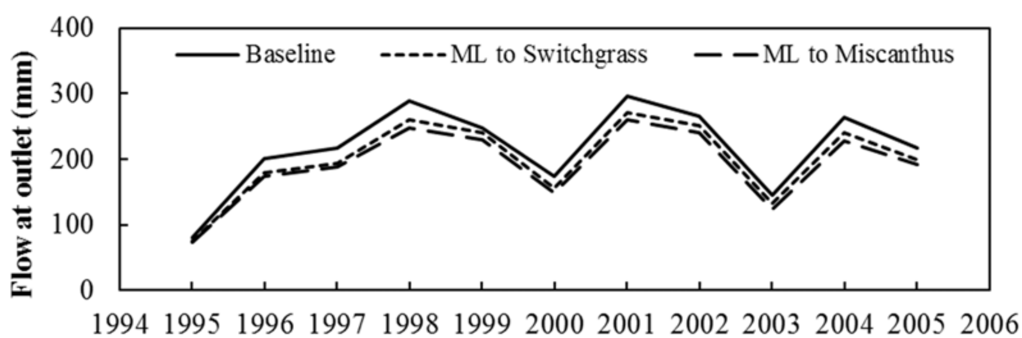


Figure 4.4 Flow at the outlet of the Upper Mississippi River Basin under the baseline, converting Marginal Land (ML) to switchgrass and *Miscanthus* scenarios for 10 year (1995 to 2005) simulation.

Previous studies have reported that the major driver for hydrologic impacts from growing switchgrass and *Miscanthus* was relatively higher ET demands by these two perennial grasses (Demissie *et al.*, 2012; Wu *et al.*, 2012; Yimam *et al.*, 2014; Feng *et al.*, 2015). Thus, the ET levels at HRU level were analyzed under biomass production scenarios in this study (Figure 4.5). Generally, scenarios for production of switchgrass and *Miscanthus* caused more ET than the baseline scenario. ET during the post establishment period of the switchgrass was 60 to 150 mm higher than during the establishment period (Figure 4.5). For *Miscanthus*, ET during the second year was higher than during the first year for all marginal lands. During the post establishment period, ET was lower than the establishment period when marginal land from land for other agricultural crops, corn, soybean, and pasture (Figure 4.5). The higher ET during the second year of *Miscanthus* was due to higher biomass production (SI Figure S2). The lower ET during the post establishment of *Miscanthus* was probably because of relatively lower ET during a few years that reduced the overall average ET for the entire duration of the analysis. During the post establishment period, lower ET happened in dry years including 2012 that lowered the average value. Higher ET from the perennial grass growth was driven mainly by higher biomass production and leaf area index during the growing season (Wu *et al.*, 2012; Feng *et al.*, 2015) and caused the depletion of soil water content, as indicated both in field measurement studies (Yimam *et al.*, 2014) and simulation results in this study (SI Figure S3). The higher yield of *Miscanthus* during both the establishment and post establishment period (Figure 4.3) caused more ET and thus more reduction of flow (Figure 4.4). Perennial grasses also resulted in higher infiltration and consequently reduced runoff.

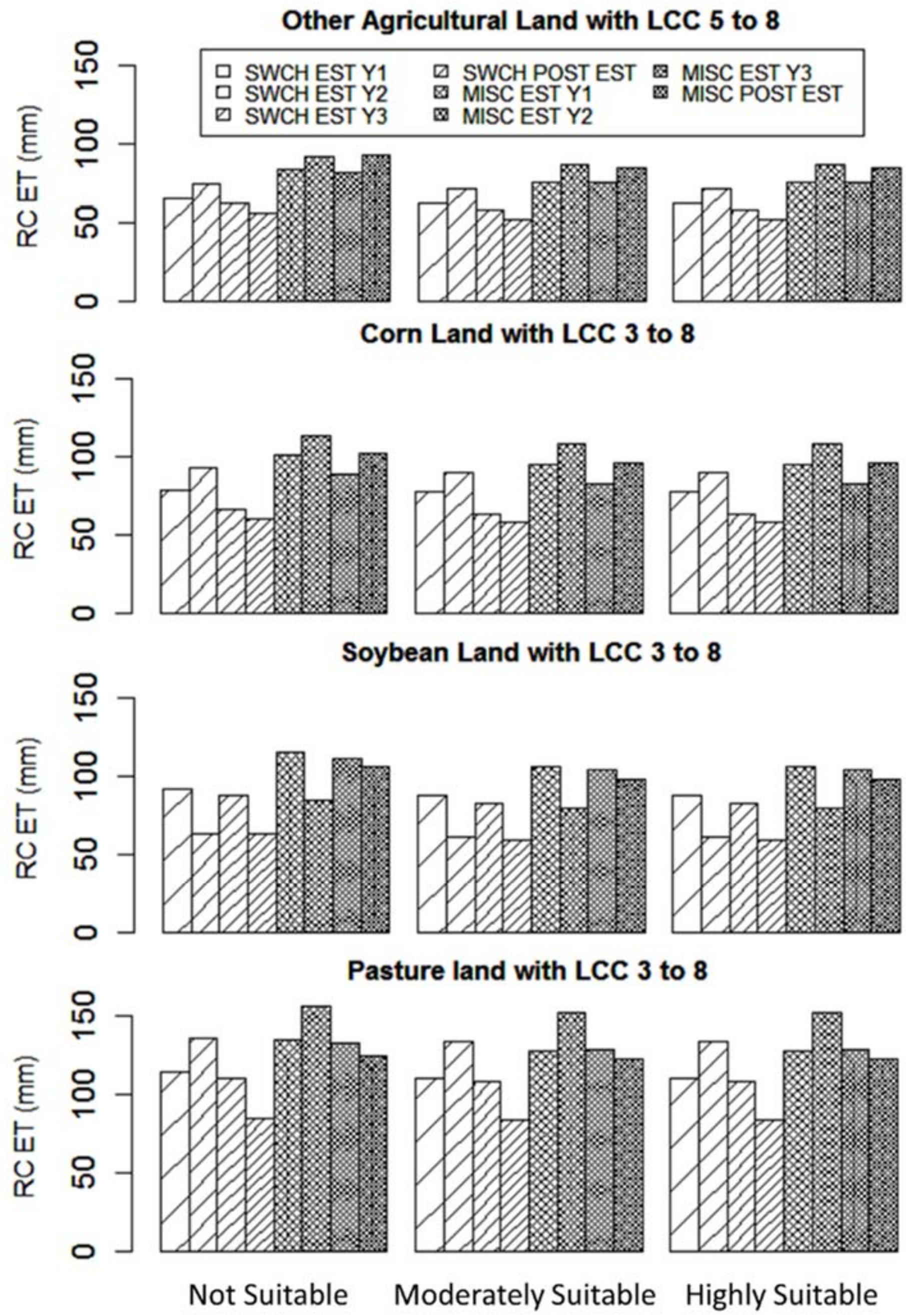


Figure 4.5 Relative changes of Evapotranspiration (ET) to baseline scenario from switchgrass and *Miscanthus* averaged over marginal land HRUs with different land suitability levels. SWCH stands for switchgrass and MISC stands for *Miscanthus*. EST stands for establishment period and POST EST stands for post establishment period. Switchgrass have 2 years establishment period (1995 as Y1 in this study) and *Miscanthus* has 3 years establishment periods (1995 as Y1). The value for POST EST is the average ET value of 1998 to 2005 (8 years). Positive value indicates higher value from SWCH and MISC.

4.4.4 Impacts on soil erosion

Sediment load at the outlet of the UMRB basin was reduced across all simulation years when marginal land was converted to both switchgrass and *Miscanthus* production (Figure 4.6). The relative change of sediment load at the watershed outlet from the baseline ranged from -1 % to -15% when marginal lands were converted to switchgrass and -7% to -20% when converted to *Miscanthus*. The average relative reductions were 8% and 13% for switchgrass and *Miscanthus*, respectively. Similar impacts on sediment loads from growing perennial biofeedstocks were also reported by other researchers. Wu *et al.* (2012) predicted that switchgrass growing on 10% of pasture land in the UMRB caused 2% reduction of total sediment loading. Cibin *et al.* (2015) simulated the growth of switchgrass and *Miscanthus* on corn and soybean land with slopes larger than 2% or in the existing agricultural fields with less than 5% percentile corn/soybean yield. The predicted the reduction of sediment load ranged from 3 to 34% when land was converted to switchgrass or *Miscanthus*.

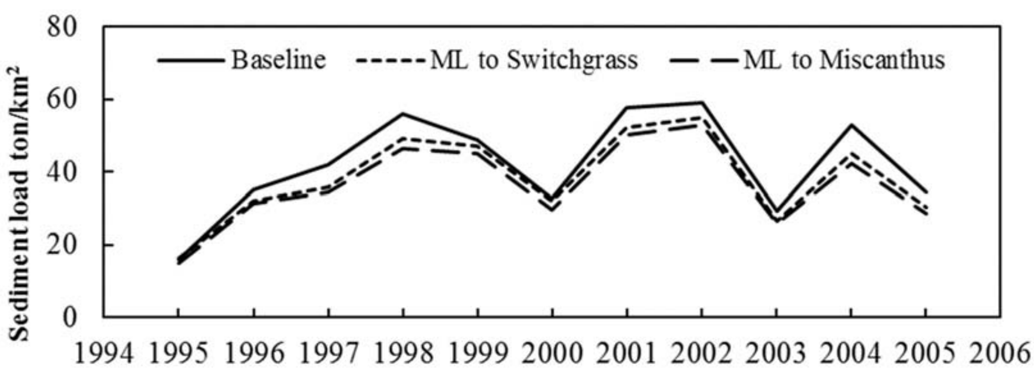


Figure 4.6 Total suspended solid at the outlet of the Upper Mississippi River Basin under the baseline, converting Marginal Land (ML) to switchgrass and *Miscanthus* scenarios for 10 year (2005 to 2014) simulation.

Soil erosion reduction could be mainly caused by two factors: a reduction of runoff and streamflow and/or differences in surface cover for perennial crops. In this study, the conversion of marginal land to two perennial grasses reduced surface runoff. Perennial grasses also had better surface cover and less soil disturbance from tillage equipment typical for annual row crop production. The combined effects of these two impacts resulted in the reduction of soil erosion at the edge of fields and reduced the sediment load at the watershed outlets. At the HRU level (Figure 4.7), soil erosion was reduced when marginal land was converted to both switchgrass and *Miscanthus*. The degree of relative change increased across years during their establishment periods and were highest during their post establishment periods. Across different marginal land types, sediment reduction was the highest when marginal land from other agricultural lands with LCC 5 to 8 were converted. The higher reduction could be due to poor land properties (with LCC 5 to 8) and higher soil erosion under the baseline scenario on marginal land in these areas, with reductions ranging from -5 tons/ha in the first year of establishment period to -13 tons/ha during the post establishment period. The reduction rates were similar on marginal land from corn, soybean and pasture land, which all had reductions ranging from -0.25 tons/ha to -1.3 tons/ha. The reduction rate of soil erosion across all marginal lands were averaged at 99%. Observations at the edge of field showed 63 to 99% reductions in soil erosion when less productive crop and pasture land were converted to switchgrass and *Miscanthus* at various locations (Blanco-Canqui *et al.*, 2006; Thomas, 2011; Dabney & Yoder, 2012; Parajuli, 2012; Wu & Liu, 2012; Cibin *et al.*, 2015).

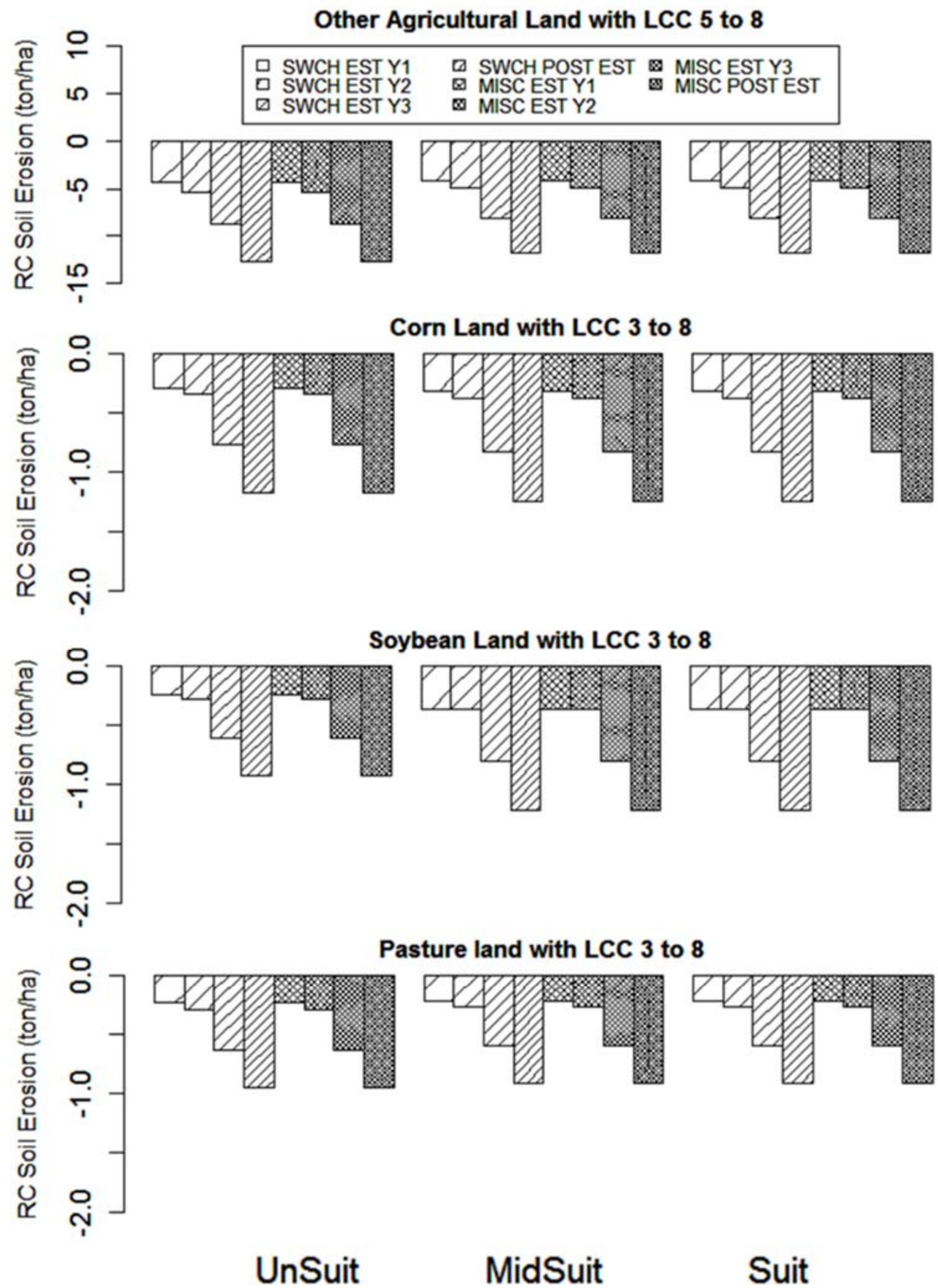


Figure 4.7 Relative changes of soil erosion from switchgrass and *Miscanthus* averaged over marginal land HRUs with different land suitability levels. SWCH stands for switchgrass and MISC stands for *Miscanthus*. EST stands for establishment period and POST EST stands for post establishment period. Switchgrass had 2 years establishment period (1995 as Y1 in this study) and *Miscanthus* had 3 years establishment periods (1995 as Y1). The value for POST EST is the average ET value of 1998 to 2005 (8 years). Positive value indicates higher value from SWCH and MISC compared to baseline.

4.5 Conclusion

This study set up a SWAT model for the UMRB region incorporating marginal lands and their suitability for the growth of two perennial grasses, switchgrass and *Miscanthus*. The model was calibrated and validated at multiple sites for monthly flow and sediment load with observed data. With the calibrated model, the author simulated the growth of the two grasses on marginal lands and explored their production potential and impacts on flow and sediment losses at field and watershed scales. Generally, the results of the study indicated that the perennial biofeedstock production on marginal land in the UMRB region could make important contributions to the biofuel development in the US. Concurrently, the conversion of land use on marginal land will reduce water yield as well as sediment loads from the UMRB.

There are two features that make this study different from other studies in the UMRB region. The first feature is that a much more detailed SWAT model for the UMRB region that included all marginal land fields was developed. Former models generally have smaller number of HRUs in this very large river basin (490,000 km^2). The advantage of having such a detailed model is better representation of the watershed condition, which potentially increased the accuracy and confidence in the model. However, developing such a detailed SWAT model significantly increased simulation time and presented challenges in calibrating the model. In future, similar methods could be applied to other scenarios by having a more detailed representation in interested/targeted regions (such as detailed data for marginal land area) in setting up the model for large river basins. The other feature is that we used a model that could simulate the establishment period of perennial grasses. The simulation results indicated that the establishment period served as a sensitive time period for sediment losses. Even though overall soil erosion was predicted to be reduced, the reduction was much smaller during the establishment period indicating a need to carefully evaluate environmental impacts during this period.

4.6 Acknowledgement

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CHAPTER 5. SUMMARY, CONCLUSIONS AND RECOMMENDATION FOR FUTURE RESEARCH

5.1 Summary

Global interests of biofuel development draw the attention of policy makers and other stakeholders on using marginal lands for the production of biofeedstocks. This is because of the expectation that using the agriculturally unengaged marginal lands could help relieve the pressure of biofeedstock production on the already intensively used highly productive lands. Producing biofeedstock on marginal land, however, is not straightforward since it may cause other unintended consequences, such as impacts on environment, economic/energy cost/benefit trade-offs, life cycle carbon balance, among others. This study focused on evaluating the biomass production and impacts on hydrologic and water quality processes brought potentially by the production of biofeedstock crops on marginal lands. We selected the Upper Mississippi River Basin (UMRB) in the US as our study area. Overall, the study suggested that marginal land in UMRB could provide biofeedstock for producing 14% to 25% of biofuels annually required by the Energy Independence and Security Act 2007. The production of biofeedstock would reduce streamflow by 8% and 12% and sediment load by 8% to 13%, from switchgrass and *Miscanthus*, respectively at the outlet of the UMRB. The results from this study indicated that using marginal is a viable choice in terms of contribution to biofuel development in the U.S. and positive environmental impacts.

5.2 Conclusion

This dissertation started with the evaluation of marginal land for the growth of three prospective biofeedstock crops: switchgrass, *Miscanthus* and Hybrid poplar, as described in Chapter 2. Existing studies on predicting marginal land's contribution to biofuel production generally ignored the heterogeneous quality of marginal lands and used averaged biomass yields for the calculation of total biomass production. This first study developed a Land Suitability Index (LSI) calculated with a fuzzy logic based land suitability evaluation framework. The results indicated that 23% of the UMRB area consisted of marginal lands. Among these marginal lands, 40% of them had relatively lower LSI values and had poor suitability for growth of the three biofeedstock crops. When marginal land suitability information was considered, the total production prediction of biofeedstock was 2/3 of the production made without considering suitability information. These findings confirmed that not all marginal land were suitable for growth of biofeedstock crops and this had to be considered in making biofuel development plans involving these types of lands.

The second study improved the simulation of perennial crop growth during their establishment periods in the Soil and Water Assessment Tool (SWAT) model, as described in Chapter 3. Perennial grasses were widely reported to have an establishment period, during which time their biomass growth increased gradually till their maximum potential. While, in the earlier versions of the SWAT model, simulated biomass and Leaf Area Index during the establishment period were as high as during the post establishment periods.. During this period, plant cover development and uptake of water and nutrient were different from those during post establishment periods. These differences could affect the hydrologic cycle as well as sediment and nutrient loss processes, especially when the production happen at large scale. The improved SWAT model performed well at 5 out of 7 tested sites. Simulations using this model indicated that evapotranspiration tended to be lower during the establishment period than during the post establishment period.

The third study applied the improved SWAT model to evaluate impacts from producing switchgrass and *Miscanthus* on marginal lands in the UMRB region on flow and sediment load at the edge of field and watershed scales. The SWAT model was setup in a way that incorporated the marginal land and their suitability information and calibrated at the multiple gauging stations. The simulation for projected biomass production scenarios suggested that the total biofeedstock produced on marginal land in this region could be converted to biofuels contributing 14% to 25% of the biofuel development goal set in the EISA 2007. The production also would reduce flow by 8% and 12% and sediment load by 8% to 13% at the watershed outlet when all marginal lands were converted to switchgrass or *Miscanthus*.

5.3 Assumptions, limitations and recommendations for future research

5.3.1 Assumptions made in the dissertation

A list of assumptions made within this dissertation was summarized below for better understanding of the results:

1. The fuzzy membership functions that described the value of limiting factors and their belongingness to suitability class were assumed to be linear.

2. The average yields of perennial grasses were assumed to be achieved when marginal land suitability index (LSI) value was 100.
3. The lower boundary of pH for *Miscanthus* was assumed based on the value for hybrid poplar.
4. The leaf area index (LAI) of perennial grasses were assumed to be stable during the post establishment period.
5. The Radiation Use Efficiency (RUE) of perennial grasses was assumed to change following the pattern of LAI, which increased during the establishment period and stayed stable during the post establishment period.
6. The establishment period of switchgrass at the CBSI site was assumed to be 2 years.

5.3.2 Limitations and recommendations for future research

This study utilized a quantifiable definition of marginal land based solely on biophysical land properties. However, marginal land is a complex definition that also requires consideration of economic trade-offs, crop growth performance under current land cover types, technology impacts land property and crop growth, and intended or potential land use types, in identifying and mapping these areas. Due to the lack of data for these aspects of land, they are not considered. In reality, a land could be considered as marginal due to various reasons, making it hard to give a certain, clear, and uniformly applicable definition that could consider all of the aforementioned considerations. One possible solution to this problem would be provide a matrix of factors and apply a subset of factors specifically for lands at a relative smaller scale, such as a county.

Land suitability evaluation in study was conducted with a fuzzy logic based evaluation methods, which provided important insights to the growth of perennial crops. However, this information still contains large uncertainty due to the fact that plant growth was affected by more factors than those considered in the analysis. As found in the third study, yields of perennial crops did not show significant difference among marginal lands with different suitability levels indicated by the LSI values. One reason could be that the SWAT model and the fuzzy logic based methods considered different groups of factors that would affect crop growth. For example, the SWAT model did not consider the impacts of pH and salinity on plant growth and restrictions of slope on machine operation safety and the potential risk of soil erosion. While, the fuzzy logic methods is an empirical model, which does not reflect the physical growth processes of perennial crops. Future research efforts are required to solve the limitations of SWAT model to include more consideration for agricultural production. Other efforts might also be taken to increase the understanding of relationships among land suitability and crop growth restriction factors and reduce the uncertainty of fuzzy logic based land suitability evaluation methods.

In the improvement of the SWAT model for establishment period simulation, the model performed well mainly in the WQFS and TPAC. The poorer performances of the model at other tested sites were explained. The reasons of these performances included parameter uncertainties, the missing of crop module in simulating some properties of switchgrass tiller growth, and the lack of plant death representation by the model. Another reason might be that all simulation results were uncalibrated and the default values were for crop growth under the growing condition of WQFS and TPAC, two sites being very close to each other than other sites. The uncalibrated model was used in order to explore the model improvement effects, which might be affected during the calibration processes. These drawbacks found in the SWAT model suggested a need for further understanding the processes of perennial crop growth and improving their representation in the model. For the sake of better understanding these processes and model development/calibration/validation, this study also proposed that more data are needed during the establishment period. The yield data for the first year was almost all missing in the dataset collected in this study. Besides, data for LAI, biomass partitioning ratio, and RUE were rarer.

The setup of SWAT model for the UMRB region was conducted using ArcSWAT. One feature of the SWAT model for UMRB region in this study among other existing SWAT models for the same region is the including of Hydrologic Response Unit (HRU) for marginal land, which resulted to 113,226 HRUs in the final model setup. Other existing SWAT models for the same region had much smaller number of HRUs, at most 18,000 number of HRUs in Jha *et al* (2006). The increase of HRU numbers greatly increased the time to run the model, thus difficulties in managing the files, calibrating and validating the model. Fortunately, the input files prepared default model provided good simulation results as an easy starting point. The flow simulation was calibrated with small efforts. However, the calibration of sediment load and nutrient variables was not easy. For larger areas, longer time for simulation might be necessary due to the large number of HRUs to be created. While, there is still possibility of increasing the efficiency for preparing the input tables and of modifying the structure of the model to reduce the time and efforts needed by the users to use the model. Even though this study used a validated model simulation to predict the impacts from perennial growth on hydrologic and nutrient loss processes, it still suggested that these effects needs more measured data to validate these predictions.

APPENDIX

Appendix A Supporting Information for Chapter 2

Contents in the supporting information:

SI-I: Additional figures and tables, including 6 tables (Tables S1-S6) and 4 figures (Figures S1-S4)

SI-II: Data sources and Fuzzy logic modeling

Table S1: Data sources used in determining marginal land types

Marginal land types and protected area	Data sources
Type 1: Cropland and grassland with land capability class (LCC) 3 and 4	Cropland, grassland, and other agricultural land were identified based on Cropland Data Layer (CDL) 2013 prepared by National Agricultural Statistics Service (NASS). This dataset provided detailed land cover information for the whole U.S. continent at the resolution of 30 by 30 m. The dataset was downloaded from http://nassgeodata.gmu.edu/Cr opScape/. Cropland included land for corn, soybean and wheat (CDL code: 1, 5, 22, 23, 24, 26, 225, 241). Grassland included land grassland/pasture, alfalfa, other hay/non alfalfa and switchgrass (CDL code: 36, 37, 60, 176). Other agricultural land included all other types of land engaged in agricultural production, such as for pumpkin, clover, etc. LCC groups soils based on degree and types of limitations, the risk of damage if used for crops, and the response to management on the land for most kind of crops (Agriculture Handbook No. 210, http://www.nrcs.usda.gov/Internet/FSE_DOCUMENTS/nrcs142p2_052290.pdf. Classes 1 to 4 were considered suitable for traditional annual crop cultivation, while classes 5 to 8 were considered unsuitable for traditional annual crop cultivation. LCC data were available in the Gridded Soil Survey Geographic Database (gSSRUGO). The gSSURGO dataset for the conterminous U.S. with a resolution of 30 by 30 m was provided by Larry Theller, GIS specialist in the Department of Agriculture and Biological Engineering, Purdue University.
Type 2: Land located within 10 meter along streams and roads, where forest and developed land were excluded	The stream data was downloaded from the National Hydrography Dataset available at http://viewer.nationalmap.gov/viewer/nhd.html?p=nhd. The road dataset was downloaded from the Topologically Integrated Geographic Encoding and Referencing (TIGER) available at (https://www.census.gov/geo/maps-data/data/tiger.html). The primary and secondary road was used in the analysis. Forest and developed land was identified according to the CDL2013 dataset.
Type 3:idle, barren, fallow land	These three land were categories of land in CDL2013. They were directly identified from the dataset.
Protected area	The dataset was downloaded from Protected Area Database (http://gapanalysis.usgs.gov/padus/data/download/). This dataset described national public land ownership, management and conservation lands. In this study, the land were removed when the Gap Analysis Program (GAP) code was 1 and 2, which indicated areas that were permanently protected for conservation of natural land.

Table S2: Slope values used in land suitability evaluation studies for traditional and perennial crops under non-irrigation condition

Literature	Targeted crop	Threshold of slope (%)	
		Lower bound of highest suitability class	Higher bound of not suitable class
Nisar *et al.*, 2000[1]	Finger millet	3	10
	Paddy	1	5
	Ground nut	3	10
Kalogirou, 2002[2]	Conventional crops	3	18
Shalaby *et al.*, 2006[3]	Olive	4	16
	Guava	2	8
	Date palm	4	16
Tienwong *et al.*, 2009[4]	Sugarcane	12	35
	Cassava	12	35
Anderberg *et al.*, 2010[5]	Sugar beet	2	8
Walke *et al.*, 2012[6]	Cotton	1	3
Elsheikh *et al.*, 2014[7]	tropical crops	6	20
Average		4.4	15.3

Table S3: Fuzzy membership functions and their shapes for each environmental variable that could potentially limit growth of switchgrass in Upper Mississippi River Basin

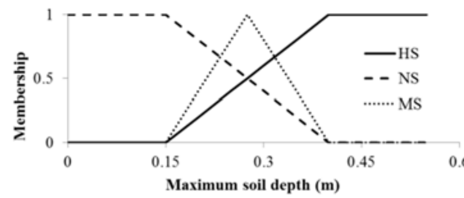
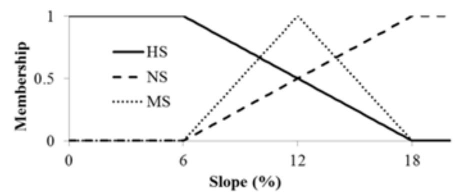
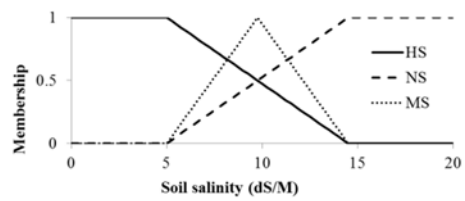
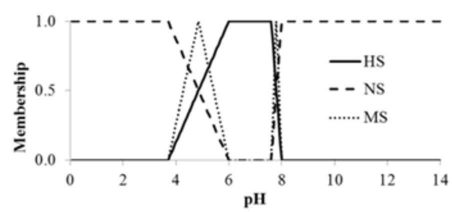
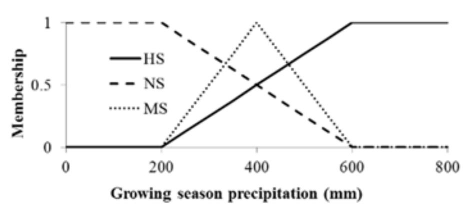
Variable	Membership functions for high suitability	Shapes
Maximum soil depth	$S_{depth}(x) = \begin{cases} 0, \; x < 0.15 \\ \frac{x - 0.15}{0.4 - 0.15}, \; 0.15 \leq x < 0.40 \\ 1, \; x \geq 0.40 \end{cases}$	
Slope	$S_{depth}(x) = \begin{cases} 1, \; x < 6 \\ \frac{18 - x}{18 - 6}, \; 6 \leq x < 18 \\ 0, \; x \geq 18 \end{cases}$	
Salinity	$S_{depth}(x) = \begin{cases} 1, \; x < 5.0 \\ \frac{14.5 - x}{14.5 - 5}, \; 5.0 \leq x < 14.5 \\ 0, \; x \geq 14.5 \end{cases}$	
pH	$S_{depth}(x) = \begin{cases} 0, \; x \leq 3.7 \; or \; x \geq 8.0 \\ \frac{x - 3.7}{6 - 3.7}, \; 3.7 < x < 6.0 \\ 1, \; 6.0 \leq x < 7.6 \\ \frac{8.0 - x}{8.0 - 7.6}, \; 7.6 \leq x < 8.0 \end{cases}$	
Growing season precipitation	$S_{depth}(x) = \begin{cases} 0, \; x < 200 \\ \frac{x - 200}{600 - 200}, \; 200 \leq x < 600 \\ 1, \; x \geq 600 \end{cases}$	

Table S4: Measured switchgrass yield in the US used in suitability map accuracy validation and the calculation of average biomass yield

ID	County	State	Average yield (Mg/ha)	Yield Standard deviation	Land Suitability Index	Literature
1	Ames	Iowa	9.7	2.97	0.90	Vogel *et al.,* 2002
2	Chariton	Iowa	8.5	1.28	0.68	Lemus, 2002
3	Dickinson	North Dakota	4.6	1.28	0.39	Berdahl *et al.,* 2005
4	Mandan	North Dakota	6.9	3.46	0.50	Berdahl *et al.,* 2005
5	Brookings	South Dakota	4.2	0.86	0.62	Casler and Boe, 2003
6	Morgantown	West Virginia	11.4	0.78	0.08	Fike *et al.,* 2006;
7	Arlington	Wisconsin	10.8	0.84	0.78	Casler *et al.,* 2007
8	Arlington	Wisconsin	11.3	3.34	0.78	Casler and Boe, 2003
9	Spooner	Wisconsin	7.4	0.04	0.70	Casler *et al.*, 2007

Table S5: Measured *Miscanthus* yield in the US used in the calculation of average biomass yield

ID	County	State	Average yield (Mg/ha)	Yield Standard deviation	Literature
1	Shabbona	Illinois	27.8	3.0	Heaton *et al.*, 2008[10]
2	Urbana	Illinois	46.7	5.7	Heaton *et al.*, 2008
3	Dixon Springs	Illinois	48.5	10.8	Heaton *et al.*, 2008
4	West Lafayette	Indiana	19.8	--	Woodson, 2011[11]
5	Elsberry	Missouri	27.5	12.0	Kiniry *et al.*, 2011[23]
6	Gustine	Texas	16.32	4.23	Kiniry *et al.*, 2011

Table S6: Measured hybrid poplar yield used in the calculation of average biomass yield

ID	County	State	Average yield[1] (Mg/ha)	Literature
1	RhineLander	Wisconsin	9.4	Strong and Hansen, 1993[24]
2		Kentucky	11.3	Hansen, 1991[25]
3		Pennsylvania	7.0	Hansen, 1991
4		Washigonton	16.8	Hansen, 1991
5		Whisconsin	11.7	Hansen, 1991
6		Iowa	10.0	Hansen, 1991
7	Ashland	Wisconsin	3.8	Netzer *et al.*, 2002[26]
8	Cloquet	Minnesota	5.4	Netzer *et al.*, 2002
9	Fairmont	Minnesota	6.8	Netzer *et al.*, 2002
10	Granite Falls	Minnesota	6.6	Netzer *et al.*, 2002
11	Mondovi	Wisconsin	7.0	Netzer *et al.*, 2002
12	Sioux Falls	South Dakota	4.4	Netzer *et al.*, 2002

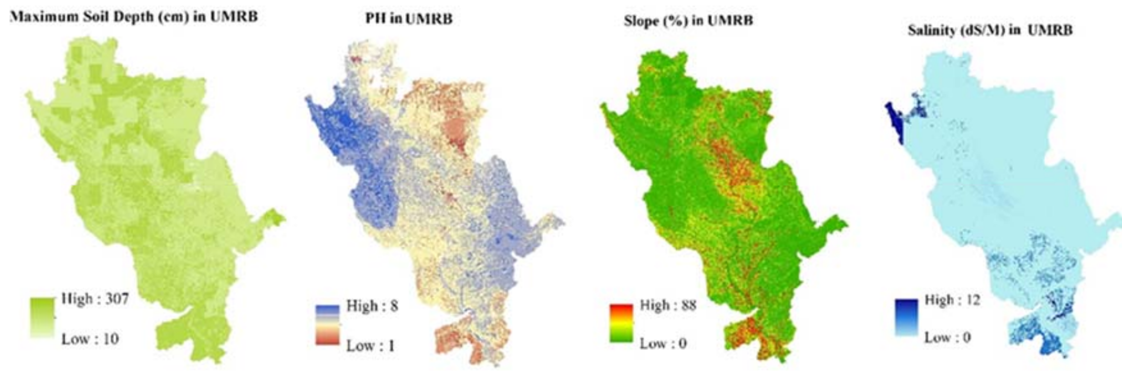


Figure S1: Actual range of maximum soil depth in cm, salinity in dS/m, slope in %, and pH within UMRB region based on SSURGO database

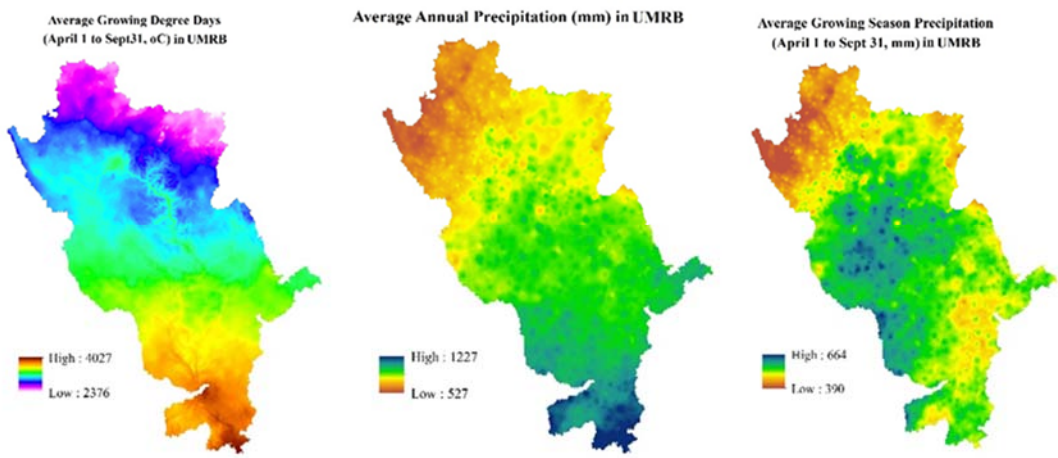


Figure S2: Actual range of average annual and growing season precipitation in mm and average growing degree days in ºC within UMRB region based SSURGO database. Growing season started from April 1st to September 30th. These data was calculated as 30 year average data downloaded from the PRISM Climate Group (http://www.prism.oregonstate.edu/) from 19810101 to 20111231. The data was originally at the resolution of 4 km, and resampled in ArcGIS 10.2.2 to 30 m as input for the fuzzy logic modeling. Growing degree days was calculated with the base temperature of 10 ºC.

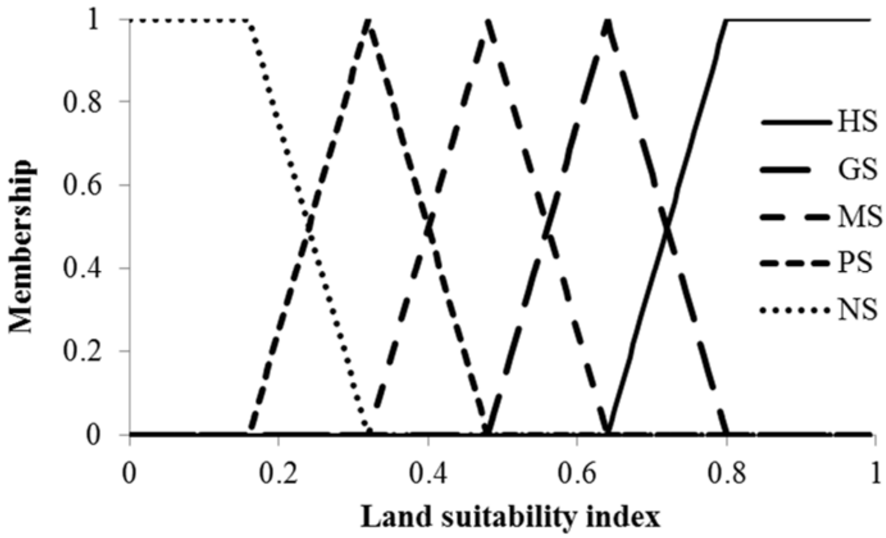


Figure S3: Membership functions of Land Suitability Index for each of five suitability levels used in defuzzification step. HS: Highly Suitable, GS: Good Suitable, MS: Moderately Suitable, PS: Poorly Suitable, NS: Not Suitable.

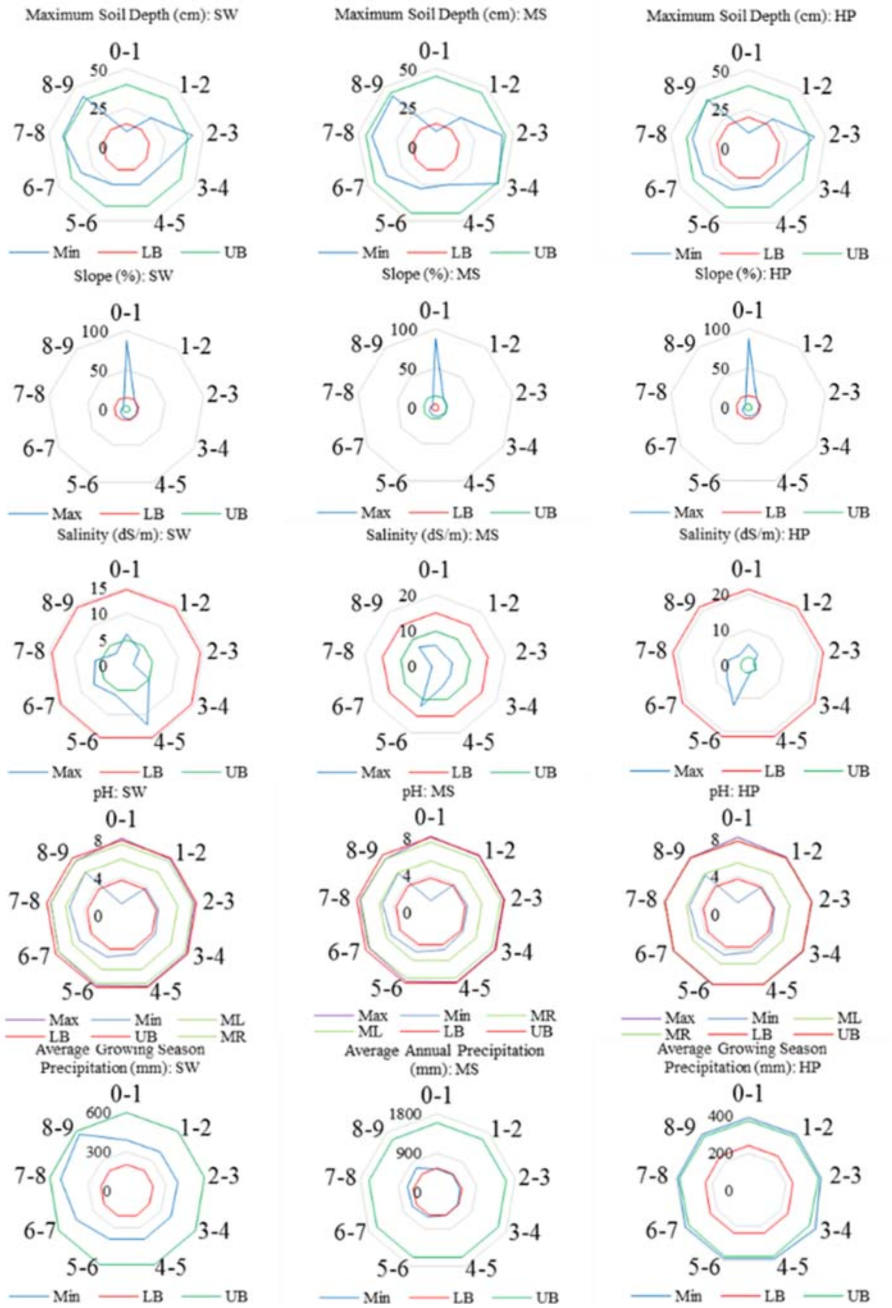


Figure S4: Values of Maximum Soil Depth (cm), slope (%), Salinity (dS/M), pH, and Average Annual and Growing Season Precipitation (mm) within each range of LSI values for ***switchgrass (SW), Miscanthus (MS) and Hybrid Poplar (HP)*** in marginal land of UMRB region. The red line represents the lower bound (LB) for high suitability membership function, beyond which land is not suitable, and green line represents the upper bound (UB) high suitable membership function, beyond which land is completely suitable. The blue line is the value of soil properties. The closer the point to the red line, the poorer suitability the land will have.

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Appendix B Supporting Information for Chapter 3

Contents in the supporting information:

SI: Additional figures and tables, including 7 tables (Tables S1-S7)

Table S1. Definition of plant growth parameters appeared in the paper.

Parameter	Parameter Definition[1]
BIO_E	Radiation Use Efficiency in ambient CO_2
T_BASE	Base Temperature
T_OPT	Optimal Temperature
EXT_COEF	Light Extinction Coefficient
BLAI	Maximum Leaf Area Index (LAI)
DLAI	Point in growing season when LAI declines
FRGRW1	Fraction of growing season coinciding with LAIMX1
LAIMX2	Fraction of BLAI corresponding to second point on optimal leaf area development curve
FRGRW2	Fraction of growing season coinciding with LAIMX2
LAIMX1	Fraction of BLAI corresponding to first point on optimal leaf area development curve
CNYLD	Plant nitrogen fraction in harvested biomass
PLTNFR3	Plant nitrogen fraction at maturity (whole plant)
GSI	Maximum stomatal conductance
PLTNFR1	Plant nitrogen fraction at emergence (whole plant)
PLTNFR2	Plant nitrogen fraction at 50% maturity (whole plant)
CHTMX	Maximum Canopy Height
FRGMAX	Fraction of GSI corresponding to the second point on the stomatal conductance curve
VPDFR	Vapor pressure deficit
RSDCO_PL	Plant residue decomposition coefficient
PLTPFR3	Plant phosphorus fraction at maturity (whole plant)
CPYLD	Plant phosphorus fraction in harvested biomass
USLE_C	Minimum Crop Factor for Water Erosion
RDMX	Maximum Rooting Depth
PLTPFR1	Plant phosphorus fraction at emergence (whole plant)
PLTPFR2	Plant phosphorus fraction at 50% maturity (whole plant)

Table S2.Studies that have switchgrass longer than 2 years

Location	Planting year	Data availability	References
		Alamo	
Virginia, US	2011	2011-2013	(Smith *et al.*, 2015)
Kentucky, US	2011	2011-2013	
Texas, US	2007	2008-2010	(Kiniry *et al.*, 2011)
Oklahoma, US	1993	1994-2000	(Fuentes & Taliaferro, 2002)
Texas, US	1992	1993-1996	(Sanderson *et al.*, 1999)
		Kanlow	
Oklahoma, US	1993	1994-2000	(Fuentes & Taliaferro, 2002)
Oklahoma, US	1996	1997-2000	(Thomason, 2005)
	1998	1998-2000	
		Shawnee	
North Dakota	2000	2001-2003	(Berdahl *et al.*, 2005)
	1999	2000-2002	
South Dakota, US	1997	1998-2001	(Casler & Boe, 2003)
Wisconsin, US	1997	1998-2001	
Indiana, US	2007	2008-2014	Unpublished
		Other upland	
Oklahoma, US	1993	1994-2000	(Fuentes & Taliaferro, 2002)
North Dakota	2000	2001-2003	(Berdahl *et al.*, 2005)
South Dakota, US	1997	1998-2001	(Casler & Boe, 2003)
Wisconsin, US	1997	1998-2001	
Texas, US	1992	1993-1996	(Sanderson *et al.*, 1999)

Table S3. Studies that have *Miscanthus* yield longer than 3 years

Location	Planting year	Data availability	References
		Miscanthus in Europe	
Denmark	1990	1993-1995	(Jørgensen, 1997)
United Kingdom	1993	1993-2006	(Christian *et al.*, 2008)
United Kingdom	1994	1995-2000	(Price *et al.*, 2004)
Turkey	1999	1999-2001	(Acaroğlu & Şemi Aksoy, 2005)
Germany	1997	1997-2010	(Gauder *et al.*, 2012)
Italy	1992	1992-2003	(Angelini *et al.*, 2009)
United Kingdom	1993	1993-2002	(Powlson *et al.*, 2005)
Sweden, Denmark, England, Germany, Portugal	1996	1997-1999	(Clifton-Brown *et al.*, 2001)
		fe in US	
Indiana, US	2008	2009-2014	Unpublished
	2011	2012-2014	
Illinois, US	2002	2004-2011	(Arundale *et al.*, 2014)

Table S4. Studies providing annual maximum LAI values for switchgrass and *Miscanthus*

Location	Planting year	Data availability	References
		Switchgrass	
Canada	1994	1995-1996	(Madakadze *et al.*, 1998)
Missouri, Oklahoma, Arkansas, Texas, US	2009	2010-2011	(Kiniry *et al.*, 2013)
		Miscanthus	
Missouri, Oklahoma, Arkansas, Texas, US	2009	2010-2011	(Kiniry *et al.*, 2013)
United Kingdom	1992	1992-1993	(Beale & Long, 1995)
Italy	1993	1993-1995	(Cosentino *et al.*, 2007)

Table S5. Studies providing annual biomass partitioning ratios at plant maturity for switchgrass and *Miscanthus*

Location	Planting year	Data availability	References
		Switchgrass	
Canada	1994	1995-1996	(Madakadze *et al.*, 1998)
Missouri, Oklahoma, Arkansas, Texas, US	2009	2010-2011	(Kiniry *et al.*, 2013)
Indiana, US	2007	2009-2011	Unpublished
		Miscanthus	
Sweden, Denmark, England, Germany, Portugal	1996	1997-1999	(Clifton-Brown *et al.*, 2001)
United Kingdom	1992	1992-1993	(Beale & Long, 1995)
England	1993	1995-1997	(Christian *et al.*, 2006)
Indiana, US	2008	2009-2011	Unpublished

Table S6. Changes to source code of SWAT (revision 635)

File	Code	Comment
Grow.f	`real :: rto_per`	Added a new local variable that represent the ratio of LAI to BLAI at each year during the establishment period.
	`rto_per = 1.`	Initialization of the variable.

	`select case(idc(idp))`
	`case(6)`
	`if (curry> nyskip) then`
	`rto_per = 1/(1+`
	`Exp((bio_leaf(idp)-`
	`float(curyr-nyskip))`
	`/(bmx_trees(idp)/1000)))`
	`end if`
	`end select`
		Calculate the ratio of BLAI development according to the equation provided by Miguez *et al.* (2008)

	`if (co2(hru_sub(j)) > 330.) then`
	`beadj = ((100. * co2(hru_sub(j))`
	`/ (co2(hru_sub(j)) +`
	`Exp(wac21(idp)-`
	`co2(hru_sub(j))`
	`* wac22(idp)))))*rto_per`
	`else`
	`beadj = bio_e(idp)*rto_per`
	`end if`
		Bio_E was also assumed to be reduced proportionally according to the ratio used for BLAI. Thus the Bio_E was multiplied with “rto_per”.

	`select case (idc(idp))`
	`case (1,2,3,4,5)`
	`laimax = blai(idp)`
	`case (6)`
	`laimax = blai(idp)*rto_per`
	`case (7)`
	`laimax = rto * blai(idp)`
		Modified the BLAI calculation choices, to include the case of perennial grasses and reduce BLAI according to “rto_per”.

Table S7. Data sources for setting up the SWAT model at four locations

Data type	Data Source	Links	Location
DEM	USGS Geodata Gateway	https://gdg.sc.egov.usda.gov/	For all four locations, Water quality field station, Throckmorton Purdue Agriculture Center, Brookings, and Arlington.
Soil	gSSURGO		
Land use	NASS2014		
Climate	NOAA-NCDC	http://gis.ncdc.noaa.gov/map/viewer/#app=cdo&cfg=cdo&theme=daily&layers=111	

Table S8. Management practices input for switchgrass and *Miscanthus* at 7 testing locations

Crop	Planting	Harvest	Fertilizer	References
Water Quality Field Station (WQFS) & Throckmorton Purdue Agriculture Center (TPAC), IN				
Switchgrass *Miscanthus*	April 1	Oct 31	112 kg Urea/ha (April 15)	Cibin *et al.*, 2015
Brooking, SD and Arlington, WI reported in Casler and Boe (2003) (CBSD)				
Switchgrass	May 1	Aug 15 Sept 15 Oct 15	243 kg Urea/ha (May 15)	Casler *et al.*, 2005
Northeast Purdue Agriculture Center (NEPAC), IN				
Switchgrass *Miscanthus*	April 27	Oct 31	217 kg Urea/ha (May 1 from second year)	Unpublished
Schochoh, KY				
Miscanthus	April 27	Oct 31	109 kg Urea/ha (May 2)	Unpublished
Lafayette, IN				
Miscanthus	April 27	Nov 15	163 kg Urea/ha (May 1)	Unpublished

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Appendix C Supporting Information for Chapter 4

Contents in the supporting information:

SI: Additional figures and tables, including 1 tables (Tables S1) and 2 figures (Figure S1 to S2)

Table S1: Field sites for switchgrass inside or within 50 km around the boundary of the Upper Mississippi River (UMRB) Basin

ID	County	State	Average yield (Mg/ha)	Yield Standard deviation	Land Suitability Index	Literature
1	Ames	Iowa	9.7	2.97	0.90	Vogel *et al.,* 2002
2	Chariton	Iowa	8.5	1.28	0.68	Lemus, 2002
3	Dickinson	North Dakota	4.6	1.28	0.39	Berdahl *et al.,* 2005
4	Mandan	North Dakota	6.9	3.46	0.50	Berdahl *et al.,* 2005
5	Brookings	South Dakota	4.2	0.86	0.62	Casler and Boe, 2003
6	Morgantown	West Virginia	11.4	0.78	0.08	Fike *et al.,* 2006;
7	Arlington	Wisconsin	10.8	0.84	0.78	Casler *et al.,* 2007
8	Arlington	Wisconsin	11.3	3.34	0.78	Casler and Boe, 2003
9	Spooner	Wisconsin	7.4	0.04	0.70	Casler er al., 2007

References for Table S1

Berdahl JD, Frank AB, Krupinsky JM, Carr PM, Hanson JD, Johnson HA (2005) Biomass yield, phenology, and survival of diverse switchgrass cultivars and experimental strains in Western North Dakota. *Agronomy Journal*, **97**, 549.

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Table S2 Parameters used in calibrating the SWAT model

Parameters	Definition(unit)	Default value	Calibrated value
		Hydrologic	
CN2.mgt	Initial SCS CN II value	Varies	Reduced by 0% to 25% at different subbasins
Alpha_BF.gw	Baseflow alpha factor (days)	0.048	Varies at different subbasins
DEP_IMP.hru	Depth of impervious layer (mm)	6000	6000 for non-tiled HRUs, 1500 for tiled hrus
DDRAIN.mgt	Depth to drains (mm)	0	1000 for HRUs with soil of somewhat poor, poor, and very poor drainage classes based on SSURGO and STATSGO database on corn and soybean land of <2% slopes
TDRAIN	Time to drain soil to field capacity (hr)	0	24 on tiled drained HRUs
GDRAIN	Drain tile lag time (hr)	0	48 on tile drained HRUs
SMFMX.bsn	Melt factor for snow on June 21 (mm H2O/ºC-day)	4.5	2.5
SMFMN.bsn	Melt factor for snow on December 21 (mm H2O/ºC-day)	4.5	2.5
Surlag.bsn	Surface runoff lag time (days)	4	0.2
		Sediment load	
RES_NSED/res	Equilibrium sediment concentration in the reservoir (mg/L)	Varies	Varies for different reservoir
USLE_P.mgt	USLE equation support practice factor	1	Determined based on slope and Table 20-4 of Chapter 20 in the Input Output Document for SWAT2009.

Tble S3 Field sites for *Miscanthus* around the boundary from the Midwest US

ID	County	State	Average yield (Mg/ha)	Yield Standard deviation	Literature
1	Shabbona	Illinois	27.8	3.0	Heaton *et al.*, 2008
2	Urbana	Illinois	46.7	5.7	Heaton *et al.*, 2008
3	Dixon	Illinois	48.5	10.8	Heaton *et al.*, 2008

	Springs				
4	West Lafayette	Indiana	19.8	--	Unpublished
5	Lafayette	Indiana	26.8	5.5	Unpublished

References for Table S2

Heaton EA, Dohleman FG, Long SP (2008) Meeting US biofuel goals with less land: the potential of Miscanthus. *Global Change Biology*, **14**, 2000–2014.

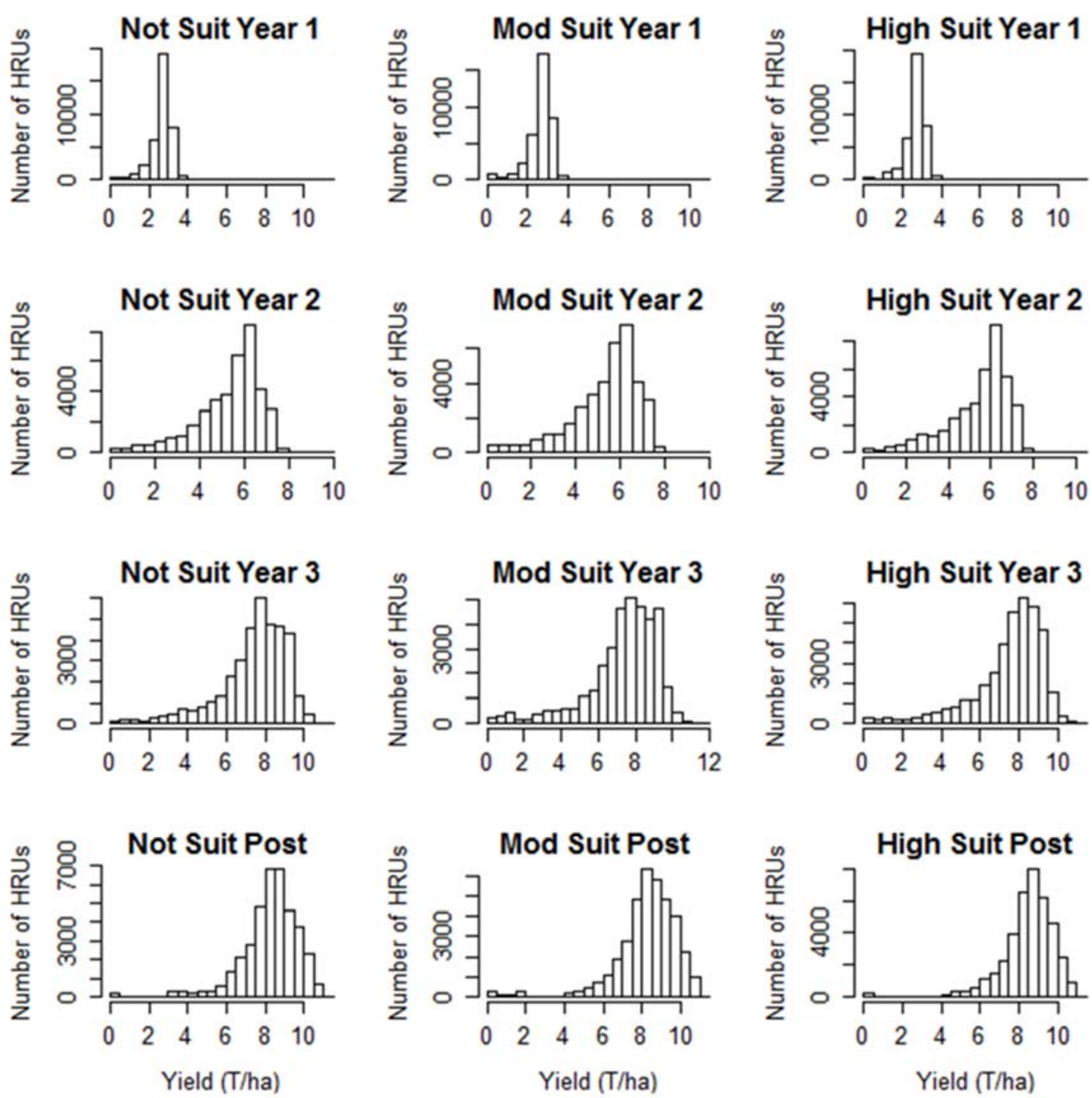

Figure S1: Distribution of switchgrass and *Miscanthus* on marginal land with different land suitability (evaluated by Land Suitability Index, LSI) levels.

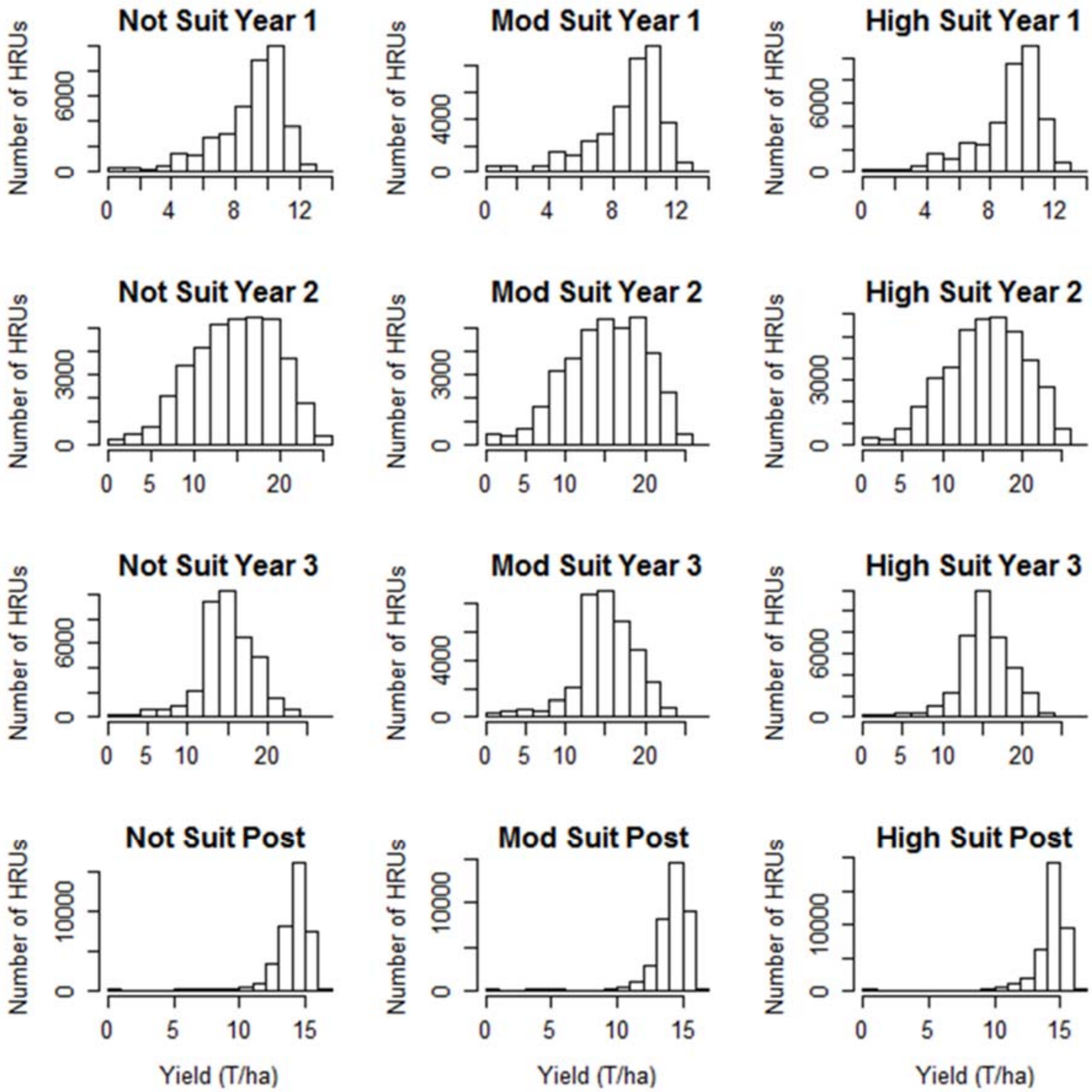

Figure S2: Distribution of Miscanthus on marginal land with different land suitability (evaluated by Land Suitability Index, LSI) levels.

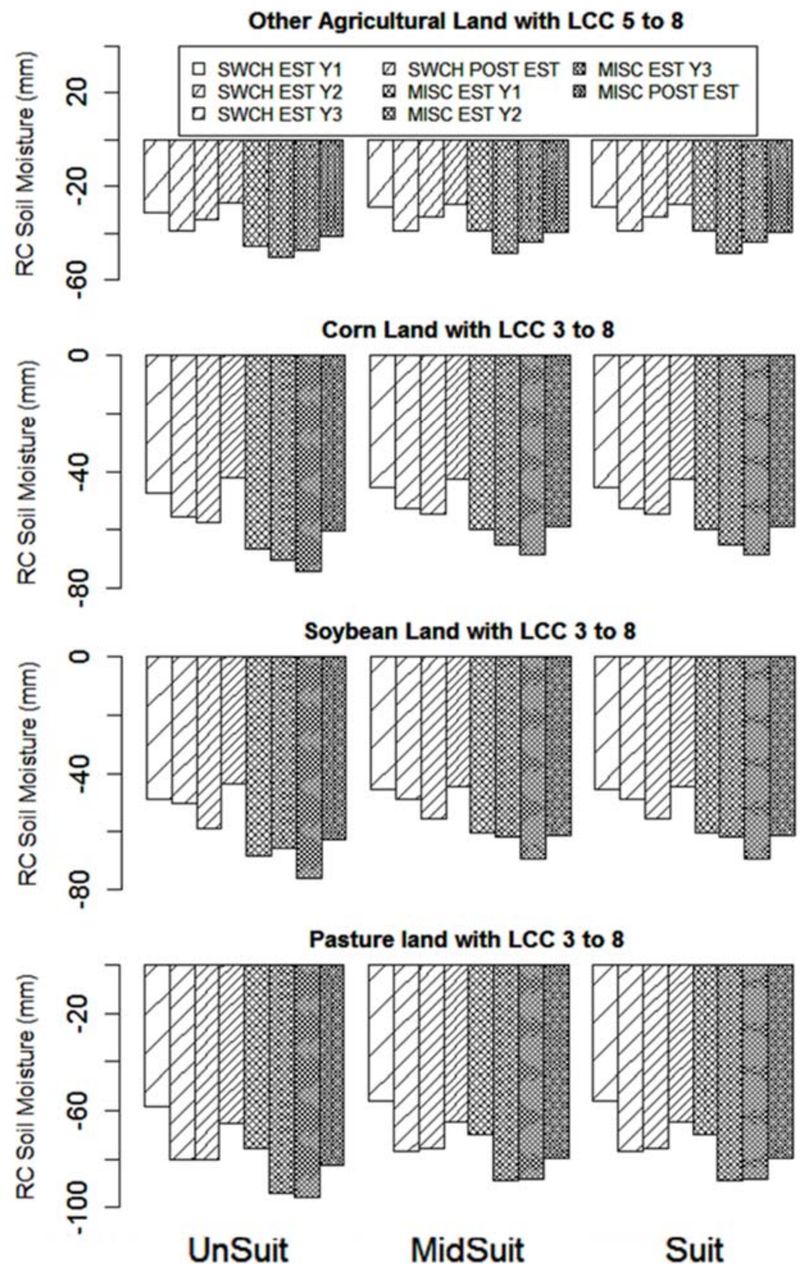

Figure S2 Soil water content changes under switchgrass and Miscanthus averaged over marginal land HRUs with different land suitability levels. SWCH stands for switchgrass and MISC stands for Miscanthus. EST stands for establishment period and POST EST stands for post establishment period. Switchgrass have 2 years establishment period (1995 as Y1 in this study) and Miscanthus has 3 years establishment periods (1995 as Y1). The value for POST EST is the average ET value of 1998 to 2005 (8 years). Positive value indicates higher value from SWCH and MISC.

VITA

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PUBLICATION

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