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Economic and Environmental Optimization in the Supply of Switchgrass in Tennessee

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To the Graduate Council:

I am submitting herewith a thesis written by Jia Zhong entitled "Economic and Environmental Optimization in the Supply of Switchgrass in Tennessee." I have examined the final electronic copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Agricultural Economics.

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Vice Provost and Dean of the Graduate School

(Original signatures are on file with official student records.)

Economic and Environmental Optimization in the Supply of Switchgrass in Tennessee

A Thesis Presented for the
Master of Science
Degree
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Jia Zhong
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ABSTRACT

The low efficiency of collection, storage and transportation in the switchgrass supply chain has hindered the commercialization of a switchgrass-based biofuel industry, even given its ecological and environmental advantages in carbon sequestrate, soil quality, water use, and pollution pressure. Thus, designing a switchgrass-based supply chain balancing both environmental and economic performance is important to expedite the development of the cellulosic biofuel industry to meet the national energy plan.

The objectives of this study are to 1) determine economic cost and multiple environmental outcomes in feedstock supply chains and 2) identify the relation between the economic and environmental performances. The first paper considers three objectives: minimization of economic cost, greenhouse gas (GHG) emissions, and soil erosions. The second paper focuses on the relation between economic cost and abated greywater footprint for industrialized supply of cellulosic biofuel in west Tennessee. The improved augmented epsilon method and compromise solution method were applied to high-resolution spatial data to determine the optimal placement of the feedstock supply chains.

Results in the first paper indicated that land change into switchgrass production is crucial to both plant-gate cost and environmental impact of feedstock supply. Converting croplands to switchgrass incurred higher opportunity cost from land use change but stored more soil carbon and generated less soil erosion. Tradeoffs in higher feedstock costs with lower GHG emissions and lower soil erosion on the frontier were captured. Soil erosion was found more cost effective criterion than GHG emission in general. The compromise solution location for the conversion facility generated at 63% increase in feedstock cost but improved the environmental impact in lowering 27 % GHG emission and decreasing soil erosion by 70 times lower in the feedstock supply chain compared with cost minimization location.

Results in the second paper showed that tradeoff between feedstock costs and greywater footprint was mainly associated with the changes of land use, while ambient water quality condition was also influential to the selection of feedstock production area. The average imputed cost of lowering grey water footprint in the most preferred feedstock supply chain in west Tennessee was \$0.94 m⁻³ [per cubic meter].

TABLE OF CONTENTS

| | |
|--|------------|
| CHAPTER I Introduction | 1 |
| Reference | 6 |
| CHAPTER II Analysis of environmental and economic tradeoffs in the design of switchgrass supply chains for biofuel production | 11 |
| Abstract | 12 |
| Introduction..... | 12 |
| Methods and Data | 16 |
| Model structure | 17 |
| Multiple objectives optimization | 21 |
| Data | 25 |
| Results and Discussion | 25 |
| Pareto frontier surface | 26 |
| Individual-optima and compromise solution | 27 |
| Conclusions..... | 31 |
| Reference | 32 |
| Appendix..... | 42 |
| CHAPTER III Grey Water footprint and economic analysis of switchgrass supply chain in west Tennessee | 57 |
| Abstract | 58 |
| Introduction..... | 59 |
| Literature review | 62 |
| Methods and Data | 64 |
| Switchgrass supply chain design | 64 |
| Cost minimization | 66 |
| Grey water footprint minimization | 69 |
| Improved augmented ϵ -constraint method in multi-objective program | 71 |
| Most preferred solution | 72 |
| Data | 73 |
| Results and Discussion | 74 |
| Cost minimization case | 74 |
| TGWF minimization case | 75 |
| Tradeoff relationship and the most preferred solution | 76 |
| Conclusions..... | 78 |
| Reference | 81 |
| Appendix..... | 91 |
| CHAPTER IV Conclusions | 103 |
| Vita | 107 |

LIST OF TABLES

CHAPTER II Analysis of environmental and economic trade-offs in the design of switchgrass supply chains for biofuel production

| | |
|---|----|
| Table 1 Literature review of the operational research on LCB feedstock supply chain | 42 |
| Table 2 Definitions of Subscripts, Parameters and Variables | 44 |
| Table 3 Payoff Table | 46 |
| Table 4 Data sources | 47 |
| Table 5 Summary of yearly itemized cost and environmental metrics | 49 |

CHAPTER III Grey Water footprint and economic analysis of switchgrass supply chain in west Tennessee

| | |
|---|----|
| Table 6 Definitions of Subscripts, Parameters and Variables | 91 |
| Table 7 Data Sources | 92 |

LIST OF FIGURES

CHAPTER II Analysis of environmental and economic trade-offs in the design of switchgrass supply chains for biofuel production

| | |
|---|----|
| Figure 1 Potential feedstock supply area and industrial park sites for conversion facilities ⁴ | 50 |
| Figure 2 System boundary of switchgrass supply chain: field to biorefinery | 51 |
| Figure 3 Regional feasible solutions | 52 |
| Figure 4 Distance scores and objective values for regional efficient solution on Pareto frontier | 53 |
| Figure 5 Placement of the conversion facility and switchgrass draw area under individual-optima and compromise solution cases | 54 |
| Figure 6 Acreage allocation converted to switchgrass | 55 |
| Figure 7 Changes in soil erosion on the feedstock draw area before and after the land was converted to switchgrass | 56 |

CHAPTER III Grey Water footprint and economic analysis of switchgrass supply chain in west Tennessee

| | |
|--|-----|
| Figure 8 Observations of nitrate levels in west Tennessee (1980-2014) | 93 |
| Figure 9 Groundwater System and served population of west Tennessee Aquifers | 94 |
| Figure 10 Flow diagram of switchgrass supply chain from field to biorefinery | 95 |
| Figure 11 Observations of nitrate levels in west Tennessee aquifers (1980-2014) | 96 |
| Figure 12 Placement of switchgrass supply chain for case costs minimization | 97 |
| Figure 13 Placement of switchgrass supply chain for case <i>TGWF</i> minimization | 98 |
| Figure 14 Itemized costs for discussed cases. | 99 |
| Figure 15 Tradeoff relations between <i>TC</i> , <i>TGWF</i> , and nitrate loading change. | 100 |
| Figure 16 Land hectare allocation from crop types in each case | 101 |
| Figure 17 Placement of switchgrass supply chain for solution Mid3 | 102 |

CHAPTER I INTRODUCTION

Concerns over energy security and greenhouse gas (GHG) emissions mitigation are spawning interest in alternative sources to substitute for petroleum-based energy. The Clean Power Plan proposed that biomass-derived fuels can decrease GHG emissions compared to burning conventional fossil fuels (U.S. EPA 2014). The Energy Independence and Security Act (EISA) established the biofuel requirements mandating that 36 billion gallons of ethanol be blended into gasoline and diesel by 2022, of which 16 billion gallons are from LCB feedstock (U.S. EPA 2010). A life cycle GHG emission threshold from cellulosic biofuel must be 60% less than the lifecycle GHG emissions of the 2005 baseline average gasoline or diesel fuel that it replaces. Energy from lignocellulosic biomass (LCB), including short-rotation woody crops, agricultural residues, and herbaceous grasses, had great potential for GHG reduction (Farrell et al. 2006).

Switchgrass (*Panicum virgatum*), one native species in the North American Tallgrass Prairie, has potential of higher productivity on barren soils and greater tolerance to a wide range of environmental conditions compared to other conventional crops and herbaceous species (McLaughlin and Kszos 2005). Research have suggested that switchgrass-based fuel might reduce GHG emissions by 60% to 90% compared with regular fossil fuel sources (Monti et al. 2012). Producing switchgrass can also produce less GHG emissions up to 50% than conventional annual crops rotations (Monti et al. 2009; Ziolkowska 2013). Additional environmental benefits of production switchgrass include less water demand (Dominguez-Faus et al. 2009), less pollution stress (Eranki et al. 2013; Parish et al. 2012), and less structure collapse and organic carbon loss from soil conservation (Khanal et al. 2013; Zenone

et al. 2013). Converting cropland to switchgrass reduces nutrient loading of waterways by reducing sediment, nitrogen and phosphorus respectively (Zhou 2011). Planting switchgrass will also improve the seeding rate of weed species in loess soil and decrease the discharged soil and scattered sediment (Ichizen et al. 2005). In addition to environmental benefits, establishing a switchgrass-based biofuel industry will stimulate rural economies and provide more job opportunities (English et al. 2013).

Despite the potential environmental and social advantage of supplying switchgrass for biofuel production, the technical challenges of switchgrass supply chain and resulting high cost have inhibited the deployment of the switchgrass-based biofuel industry (Khanna et al. 2008; Wesseler 2007). Production cost of a 1 liter of gasoline equivalent from switchgrass was 17.8% higher than that from corn, and 34.4% higher than the cost of gasoline in year 2005 (Pimentel and Patzek 2005; Wesseler 2007). The relative low density of switchgrass increased the harvesting and collecting cost using the conventional hay equipment. Also, a large-scale storage area will be required for the bulky feedstock. Feedstock cost constituted 30%-50% of total switchgrass-based biofuel production cost (Khanna et al. 2008; Yu et al. 2014a; Zhang et al. 2013). The exposure of switchgrass bales to weather during storage might result in dry matter (DM) loss, which might result in additional feedstock cost (Mooney et al. 2012). In addition, the transporting feedstock from supply area to biorefinery is expected to generate significant truck flows due to low feedstock density. Yu et al. (2014b) found about more than 20% of total feedstock plant-gate cost was attributed to feedstock transportation from the field to the potential biorefinery.

Balancing the economic and environmental metrics for switchgrass feedstock supply chain draws recent attention driven by the expectation of creating a sustainable biofuel industry. Various multi-metrics were applied to reduce GHG emissions and improve aquatic environments in the design of the supply chain (Bernardi et al. 2012; Parish et al. 2012; Valdivia et al. 2012; You et al. 2012; Yu et al. 2014b). The multi-objective optimization models were commonly to address the multi-criteria decision question. Resource allocation was determined by the model to achieve economic effectiveness and environmental safeguarding. Most of those studies focused on cost minimization and GHG reduction in LCB feedstock supply chain (Miao et al. 2012; Monti et al. 2012; Sadrul Islam and Ahiduzzaman 2012; Sanderson et al. 2006), while there is also a growing interest in considering broader perspective of environmental benefits, such as reducing water stress and soil erosion (Eranki et al. 2013; Smeets et al. 2009).

To conduct a solid analysis of environmental impact and economic cost of LCB feedstock supply chain, it is crucial to have detailed spatial data in high resolution, such as available land, transportation network, and crop yields for LCB feedstock and other conventional crops (McBride et al. 2011). The accuracy of sustainable assessment was dependent on location- and case-specific data to evaluate biomass availability and feedstock transportation emission (Jäppinen et al. 2011). Observation-calibrated model also enabled a study to better respond to market prices and public policies, and to generate prediction in greater detail than aggregated level models (Egbenewe-Mondzozo et al. 2011). However, most previous studies have not incorporated the high resolution spatial data associated with soil erosion, water usage and

quality into systematic assessment in the optimization decision making with multiple environmental impacts and economic costs, with a few exceptions such as Parish et al. (2012).

The information of multivariate environmental impacts and the associated imputed cost of a LCB feedstock supply chain can provide the farmer, industry, stakeholders and policy-makers better insight into the sustainable design of LCB feedstock supply. Thus, the objectives of this study are : (1) to determine the potential tradeoffs among minimization of feedstock costs, greenhouse gases, soil erosion, water pollution stress for a switchgrass supply chain, and (2) to offer a switchgrass supply chain integrated costs and multiple environmental benefits for a potential commercial scale biofuel conversion facility in Tennessee.

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***CHAPTER II ANALYSIS OF ENVIRONMENTAL AND ECONOMIC TRADEOFFS
IN THE DESIGN OF SWITCHGRASS SUPPLY CHAINS FOR BIOFUEL
PRODUCTION***

Abstract

This study considered the environmental advantages of switchgrass over first-generation feedstock, along with the economic challenges in its logistics, in the development of a sustainable switchgrass supply chain in Tennessee. Applying a multi-objective optimization model using high resolution spatial data, potential tradeoffs among the objectives of minimizing feedstock costs, GHG emissions, and soil erosion were identified on a regional Pareto frontier surface. The tradeoff relationship was primarily driven by type of agricultural land converted to switchgrass. Hay and pasture lands were more cost effective but resulted in higher soil carbon losses and soil erosion. Converting crop lands reduced GHG emissions and soil erosion but resulted in higher feedstock cost primarily due to the higher opportunity cost of land use. The respective average costs of abating GHG emissions and soil erosion on the regional Pareto frontier surface were \$2,378 Mg⁻¹ and \$10 Mg⁻¹. The compromise solution conversion facility site generated 63% higher feedstock cost compared to the cost minimization location, while reduced soil erosion 70 fold, and only diminished GHG emissions by 27%. Soil erosion may be a more cost effective environmental criterion than GHG emissions in the development of a sustainable switchgrass supply chain in Tennessee.

Keywords: Switchgrass, Biofuel, Supply chains, Greenhouse gas, Soil erosion, Trade-off

Introduction

Production of ethanol using corn (*Zea mays* L.) grain as the feedstock has rapidly expanded in the United States. High energy prices and the mandate set forth in the Renewable Fuel Standard (RFS2) as defined in the Energy Independence and Security Act of 2007 (U.S. Congress 2007) have driven the growth in corn-based ethanol production. The surge in U.S. corn ethanol production and the associated changes in agricultural land-use have raised

concerns about increased soil erosion, fertilizer and pesticide pollution, and greenhouse gas emissions with expanded corn production (Larson et al. 2010a). Corn uses more fertilizer ha^{-1} than other major crops and accounted for 46% of all fertilizer use in the United States in 2010 (USDA Economic Research Service 2015). Expansion of corn area on existing cropland area and from converting set aside agricultural lands or grasslands (Gelfand et al. 2011, Hill et al. 2006, Searchinger et al. 2008, Tilman et al. 2009) and the increased use of continuous corn production has exacerbated soil erosion problems (Evers et al. 2013, Vadas et al. 2008) and the loss of nutrients to the environment (Pimentel et al. 1995).

The US Environmental Protection Agency has advocated the production of advanced biofuels to mitigate the potential environmental issues from using starch from grain crops to produce biofuels. The agency requires that life cycle GHG emissions from an advanced biofuel must be 60% less than average lifecycle GHG emissions of gasoline or diesel fuel at 2005 levels (U.S. EPA 2010). The Clean Power Plan proposed by US EPA in 2014 advocates the use of biofuels produced from lignocellulosic biomass (LCB) as a strategy to mitigate GHG emissions (U.S. EPA 2014). Renewable energy produced from LCB, including short-rotation woody crops, agricultural residues, and herbaceous grasses, have great potential for reducing GHG (Farrell et al. 2006). Growing perennial grasses as feedstock for energy could also reduce soil erosion on agricultural lands (Khanal et al. 2013, Zhang et al. 2013a). Reducing soil erosion on agricultural lands has been an important policy objective in U.S agricultural policy since the 1930s (McGranahan et al. 2013).

Switchgrass (*Panicum virgatum*), a herbaceous prairie grass native to North America, requires less fertilizer and chemicals, has better water use efficiency, and has a greater tolerance to a wide range of environmental conditions when compared to field crops and other herbaceous species (Lewandowski et al. 2003, Mitchell et al. 2008). Because switchgrass is a perennial crop with a life span of 10 or more years, it provides year-round

coverage of soils and enhances soils through its extensive root system that reduces water runoff and soil losses and by improving soil organic matter, soil structure, soil water holding capacity, and nutrient holding capacity (Kort et al. 1998). Previous studies have suggested that switchgrass-based biofuels could reduce GHG emissions by 60% to 90% when compared with fossil fuels (Monti et al. 2012) and up to 50% when compared with biofuels produced using corn grain (Monti et al. 2009, Ziolkowska 2013).

Despite the potential environmental and ecological advantages of switchgrass for bioenergy production, the high cost of producing biofuels using it as the feedstock has impeded the development of a switchgrass-based biofuel industry (Khanna et al. 2008, Wesseler 2007). Production cost L^{-1} of gasoline equivalent from switchgrass was 17.8% higher than the cost from corn, and 34.4% higher than the cost of gasoline in 2005 (Pimentel and Patzek 2005, Wesseler 2007). Feedstock procurement costs may constitute 30%–50% of the total cost of producing switchgrass-based biofuel (Khanna et al. 2008, Yu et al. 2014a, Zhang et al. 2013b). Important factors contributing to higher costs include the low bulk density of switchgrass, increasing harvest, storage, and transportation costs, and the losses of feedstock stored outdoors due to weathering if switchgrass is harvested only once a year (Sokhansanj et al. 2006).

Operations research methods have been widely used to evaluate the design of LCB feedstock supply chains using cost minimization or profit maximization as the objective of the decision maker (Table 1). An increasing number of studies have examined economic and environmental tradeoffs in the design of a sustainable LCB-based advanced biofuel feedstock supply chain (Bernardi et al. 2012, Parish et al. 2012, Valdivia et al. 2012, You et al. 2012, Yu et al. 2014b). Notwithstanding the growing literature evaluating the environmental tradeoffs of biofuels production, there is a lack of research that explicitly imputes the costs of mitigating environmental degradation or improving environmental quality with LCB-based

biofuel production. The imputed cost represents the proxy value of an externality from mitigating environmental degradation or improving environmental quality that was not captured in the development of a sustainable LCB supply chain (Bernardi et al. 2012, Chan 2011, Parish et al. 2012, Valdivia et al. 2012, You et al. 2012, Yu et al. 2014b).

An assessment of the sustainability of an LCB supply chain depends on the use of high-resolution spatial data to accurately model the characteristics of the supply chain, such as biomass availability, changes in fertilizer and chemical use with LCB production, and feedstock transportation emissions (J äppinen et al. 2011). Models with a high spatial resolution generate more detailed predictions of the footprint of the feedstock supply chain and are more useful for policy analysis and for private and public decision making (Egbendewe-Mondzozo et al. 2011). Most multi-objective studies have not taken into account spatial characteristics, with only a few exceptions having highlighted the value of using geographic data in the economic and/or environmental optimization of the feedstock supply chain (Egbendewe-Mondzozo et al. 2011, Jager et al. 2010, Parish et al. 2012, Yu et al. 2014b). However, a high-resolution geospatial element is still lacking in the systematic assessment of the optimal design of the sustainable LCB feedstock supply chain in previous studies.

The present study aims to add to the literature examining economic and environmental tradeoffs in a feedstock supply chain by utilizing high resolution spatial data in a multi-criteria optimization model. The analysis focuses on the optimal location and design of a switchgrass feedstock supply chain in Tennessee. The state has several characteristics that lend itself to an evaluation of economic and environmental tradeoffs with biofuel production; a humid subtropical climate that is well suited to the production of high yielding switchgrass, agricultural soils that are highly erodible, and a geographically diverse set of agricultural production activities and landscapes. Thus, the objectives of this study are: (1) to determine

the potential tradeoffs among the minimization of feedstock costs, GHG emissions, and soil erosion for a switchgrass supply chain in Tennessee, and (2) to evaluate the imputed cost of abating GHG emissions and soil erosion in the switchgrass supply chain to assist the development of an economically and ecologically viable advanced biofuel project.

Methods and Data

The switchgrass conversion facility was assumed to have a production capacity of 189.3 million liters (L) of ethanol year⁻¹. Switchgrass was assumed to be harvested between November and February after senescence and placed in storage and delivered for processing in the off harvest period from March through October. Feedstock supply chain activities were modeled on a monthly time step. Assuming a conversion rate of 287.7 L of ethanol dry Mg⁻¹ of switchgrass (Wang et al. 1999), the required feedstock for the facility was 600,892 dry Mg year⁻¹. The potential locations for the conversion facility were limited to 150 industrial parks in a Tennessee Valley Authority database (Tennessee Valley Authority Economic Development 2011). Candidate industrial parks had the required space and access to roads and water resources for the facility (Figure 1). The potential feedstock supply area in this study included all agricultural land in Tennessee and a buffer area of 80 km contiguous to the state border. The study area was downscaled to a 13 km² hexagon resolution, defined as the land resource unit, to capture variations in land resources, the transportation network, and other geographic features of the study area. The ratio of crop land to hay and pasture land by land resource unit in Figure 1 indicates that west Tennessee is the major crop production area, while pasture and hay land is primarily located in the eastern region of the state.

The system boundaries for calculating feedstock costs, GHG emissions, and soil erosion produced in the switchgrass supply chain in this study was from the farm field to the conversion facility plant gate (Figure 2). The five main components considered in the design

of the feedstock supply chain were: (i) land resource allocation, (ii) production, (iii) harvest, (iv) storage, and (v) transportation. To determine the most preferred solution of the multi-objective feedstock cost, GHG emission, and soil erosion minimization, the payoff table method was used to develop the most preferred solution (Reeves and Reid 1988). The supply chain model considering the aforementioned factors was solved for each individual objective for each of the 150 industrial park sites in the study area. Optima and nadir values and the ranges obtained from solving for each individual objective were used in an improved augmented ϵ -constraint method (Mavrotas and Florios 2013) to solve the multi-objective function for each potential conversion facility site. The feasible and efficient solutions for all 150 sites in study area were then used to form the regional Pareto frontier surface. The compromise solution method (Ramos et al. 2014) was used to identify the most preferred conversion facility site and the feedstock draw area for the switchgrass supply chain. Costs of abating GHG emissions and soil erosion in the switchgrass supply chain were imputed using the regional Pareto frontier surface solution.

Model structure

Cost minimization

Following Larson et al. (Larson et al. 2015), the objective of minimizing total feedstock cost at the conversion facility plant gate (TC , \$) for a switchgrass supply chain was modeled as:

$$\text{Min } TC = C_{\text{opportunity}} + C_{\text{production}} + C_{\text{harvest}} + C_{\text{storage}} + C_{\text{transportation}}, \quad (1)$$

where $C_{\text{opportunity}}$ was opportunity cost, $C_{\text{production}}$ was production cost, C_{harvest} was harvest cost, C_{storage} was storage cost, and $C_{\text{transportation}}$ was transportation cost, respectively. The definitions of the cost parameters and decision variables are listed in **Table 2**.

Opportunity cost ($C_{\text{opportunity}}$) was defined as the forgone profit from crop, hay, and pasture production activities that took place before the conversion of land to switchgrass

production. Farmers were assumed to require a profit from switchgrass production that was at least as much as the existing agricultural production activity. Thus, opportunity cost in Equation (2) was defined as the higher of net revenue from the prior land use or the market rental rate for the land (Larson et al. 2015):

$$C_{opportunity} = \begin{cases} \sum_{ip} [(Price_{ip} \times Yield_{ip} - PC_{ip}) \times AH_{ip}], & \text{if } (Price_{ip} \times Yield_{ip} - PC_{ip} - LR_{ip}) \geq 0 \\ \sum_{ip} (LR_{ip} \times AH_{ip}) & , \text{if } (Price_{ip} \times Yield_{ip} - PC_{ip} - LR_{ip}) < 0 \end{cases} \quad (2)$$

Costs for production, harvest, storage, and transportation in Equation (1) included equipment ownership, maintenance, labor, fuel, and materials used for farm field to plant gate activities in the switchgrass supply chain:

$$C_{production} = \sum_{mip} ((Est + AM) \times AH_{mip}), \quad (3)$$

$$C_{harvest} = \sum_{ip} (\sigma_i \times AH_{ip}), \quad (4)$$

$$C_{storage} = \sum_{mi} (\gamma_i \times NXS_{mi}), \text{ and} \quad (5)$$

$$C_{transportation} = \sum_i (\theta_i \times (\sum_m XTN_{mi} + \sum_m XTO_{mi})) / (1 - DML^{trans}). \quad (6)$$

The cost of switchgrass production ($C_{production}$) in Equation (3) included the annualized establishment cost and annual maintenance cost of the switchgrass stand. Harvest cost ($C_{harvest}$) in Equation (4) models switchgrass harvested using a large rectangular bale system. Storage cost for switchgrass (γ_i) in Equation (5) included costs of materials, equipment, and labor for rectangular bale staging and storage operations. Transportation costs (θ_i) in Equation (6) assumed the use of semi-trailer trucks and trailers to transport switchgrass from storage to the conversion facility. Costs for transportation were determined by the time for each activity. Loading and unloading times for bales were taken from a study by Duffy (Duffy 2007). Distance and truck speeds based on highway speed limits were used to

determine transportation time. Maximum travel distance to transport switchgrass to the conversion facility was assumed to be 121 km.

The cost minimization was subject to constraints based on practical operations requirements and rules of mass balance:

$$\text{Available area for production: } \sum_m AH_{mip} \leq Aa_{ip}, \forall i, p \text{ Nov} \leq m \leq \text{Feb.} \quad (7)$$

$$\text{Available harvest working hours: } Numb_m^k \times Avehour_m - \sum_i (MTB_i^k \times AH_{mip}) \geq 0, \forall k, m. \quad (8)$$

Harvest to shipment and storage balance:

$$\sum_p AH_{mip} \times Yield_i^{swg} = XTN_{mi} / (1 - DML^{trans}) + NXS_{mi}, \forall m, i. \quad (9)$$

Cumulative storage balance during harvest season:

$$XS_{(m+1)i} = (1 - DML_m^{stor}) \times XS_{mi} + NXS_{(m+1)i}, \forall m, i \text{ Nov} \leq m \leq \text{Feb.} \quad (10)$$

Cumulative storage balance during off-harvest season:

$$XS_{(m+1)i} = (1 - DML_m^{stor}) \times XS_{mi} - XTO_{(m+1)ip} / (1 - DML^{trans}), \forall m, i \text{ March} \leq m \leq \text{Oct.} \quad (11)$$

$$\text{Ethanol production requirement: } \lambda (\sum_i XTN_{mip} + \sum_i XTO_{mi}) - Q_m = 0, \forall m. \quad (12)$$

$$AH, XTN, NXS, XS, XTO, \text{ and } Numb_m^k \geq 0 \quad (13)$$

Equation (7) restricts available land area based on switchgrass yields for LCB feedstock production in each land resource unit. Equation (8) constrains machine hours month⁻¹ based on available harvest days due to weather during harvest season, while Equation (9) requires feedstock harvested equals the summation of direct delivery after adjusting for transportation dry matter losses during harvest season and the amount of feedstock sent to storage. In addition, Equations (10) and (11) maintain the balance of the cumulative storage of switchgrass after taking into account storage dry matter losses. Feedstock deliveries to the conversion facility in each month need to meet the demand for biofuel production in Equation (12). All parameters and variables in the model are nonnegative as required in Equation (13).

GHG emissions minimization

A modified version of the framework presented by Yu et al. (Yu et al. 2014b) was used to calculate GHG emissions in the model. Equations (14) through (18) model the minimization of total GHG emissions (TE , kg yr^{-1}) from supply chain activities:

$$\text{Min } TE = E_{luc} + E_{energy} + E_{transportation} + E_{ind}. \quad (14)$$

$$E_{luc} = \sum_p \left(\sum_{mi} AH_{mip} \times (\Delta LUCO_{2,P} + \Delta LUCH_{4,P} + \Delta LUN_{2O,P}) \right), \quad (15)$$

$$E_{energy} = \sum_{mip} AH_{mip} \times (ProE + HarE) + \sum_{mip} AH_{mip} \times Yield_i^{swg} \times StorE, \quad (16)$$

$$E_{transportation} = \sum_{mi} TransE_{mip} \times (XTN_{mi} + XTO_{mi}) / (Loadwt \times (1 - DML^{trans})), \text{ and} \quad (17)$$

$$E_{ind} = \sum_{mip} (FertE + ChemE + SeedE) \times AH_{mip} + \sum_{mb} Numb_{mb}^k \times machE^k. \quad (18)$$

The definitions for the emission parameters are listed in Table 2. The major sources of changes in emissions were from adjustments in land use (E_{luc}), energy consumption from switchgrass production, storage, and harvest (E_{energy}), transportation ($E_{transportation}$), and from the energy used in the manufacture of seed, fertilizer, chemicals, and machinery (E_{ind}) inputs used in the supply chain. Emissions caused by changes in land use were calculated by multiplying the emission factors of three biogenic greenhouse gases (CO_2 , CH_4 , and N_2O) by the changes crop area with switchgrass production [Equation (15)]. Energy consumption for switchgrass production and storage activities were calculated through the summation of land area times the farm operations emission factors and storage tonnage times the storage emission factor [Equation (16)]. Transportation emissions were calculated through the multiplication of the emission factor per truck per route times the truck loads for all the transported biomass [Equation (17)]. Indirect emissions are from the manufacture of fertilizer, chemicals, seed, and machinery inputs used in the production of switchgrass [Equation (18)].

Soil erosion minimization

For the soil erosion minimization objective, changes in water-induced soil erosion from converting crop, hay, and pasture lands to switchgrass production were estimated using the Revised Universal Soil Loss Equation (RUSLE) (Kokkinidis 2014, Renard et al. 1997, Wischmeier and Smith 1978). Water-induced soil erosion is influenced by the land use activity (crop, hay, and pasture production), tillage method, landscape, and precipitation factors in the RUSLE model. Equation (19) models the long-term average annual soil loss soil loss (T_{SoilE} , $Mg\ ha^{-1}\ yr^{-1}$) minimization objective:

$$\text{Min } T_{SoilE} = \sum_i \{(R_i \times K_i \times LS_i \times P_i) \times \sum_p [(\Delta Cf) \times \sum_b AH_{ipb}]\}, \quad (19)$$

where R was rainfall and runoff factor, K was soil erodibility factor, LS was length and steepness of slope factor, P was support practice factor, and ΔCf was crop vegetation and management factor. The R , K , LS , and P factors in each land resource unit were obtained using the ArcGIS intersect geoprocessing method and pivot table in Excel to estimate weighted average values for each factor for each land resource unit in Equation (19).

To evaluate the impact on soil erosion of land conversion to switchgrass, the estimates of T_{SoilE} before and after the conversion of land to switchgrass production were compared with USDA NRCS estimates of soil loss tolerance (T , $Mg\ ha^{-1}\ yr^{-1}$) by land resource unit (United States Department of Agriculture). Soil loss tolerance, T , is defined in the RUSLE2 database as “the maximum amount of soil loss in [$Mg\ ha^{-1}\ yr^{-1}$], that can be tolerated and still permit a high level of crop productivity to be sustained economically and indefinitely.” (U.S. Department of Agriculture Natural Resources Conservation Service 2014). The frequency of land resources where $T_{SoilE} > T$ before and after the conversion of crop, hay, and pasture lands into switchgrass production were evaluated to ascertain the effects of switchgrass production on soil erosion within the switchgrass supply chain area.

Multiple objectives optimization

Improved augmented ε -constraint method in multi-objective program

The improved augmented ε -constraint method, AUGMECON2 (Mavrotas and Florios 2013) was applied to derive the tradeoff relationship among the three competing objectives for each potential conversion facility location. The tradeoff relationship among objectives indicates that the performance of one objective could not be improved without degrading the performance of the other objectives. Applying the procedure to all 150 potential industrial park locations for conversion facilities in the study area generated the regional tradeoff frontier surface. The details of AUGMECON2 method are available in Mavrotas and Florios (Mavrotas and Florios 2013).

The AUGMECON2 method was applied to formulate the three objectives of a potential conversion facility:

$$\text{Min. } (TC - \varepsilon \times (s_2 / r_2 + 10^{-1} \times s_3 / r_3)), \quad (20)$$

Subject to:

$$TE + s_2 = e_2, \text{ and} \quad (21)$$

$$TSoilE + s_3 = e_3, \quad (22)$$

where TC , TE , and $TSoilE$ are the three competing objectives defined in Equations (1), (14), and (19), ε is a small number (in this study ε was set to be 10^{-3}), s is the non-negative slack variable, r_2 and r_3 are the range of the objective function of TE and $TSoilE$, e is the constraint applied to the TE and $TSoilE$ through interpolating four grid points to create five equal intervals in the value range (r). The slack variable s was added to the objective function in Equations (20) – (22) to produce only efficient solutions. The lexicographic optimization (Mavrotas and Florios 2013) assumed that minimization of total feedstock cost was the primary objective of conversion facility decision makers. High feedstock costs have been identified as an important impediment to the development of a switchgrass-based biofuel

industry for private investors interested in maximizing profits (Khanna et al. 2008, Wesseler 2007). The two environmental criteria, minimization of GHG emissions, TE , and minimization of soil erosion, $TSoilE$, are driven by US EPA and USDA policies aimed at reducing their levels (U.S. EPA 2014),(McGranahan et al. 2013).

To determine the nadir values and generate the range of the TE and $TSoilE$ objective functions, a 3×3 payoff table, illustrated in Table 3, was generated by considering each of the objectives as a single objective problem. The diagonal of the payoff table provides the optima values for each of the three objectives. For the TE and $TSoilE$ objectives, the optima were also the lower bound values (l_2) and (l_3), respectively. The nadir value of TE and $TSoilE$, u_2 and u_3 , respectively, were the maximum values in the TE and $TSoilE$ columns of Table 3. The ranges of the objective value for TE and $TSoilE$ were obtained from the differences between upper and lower bound values: $r_2 = u_2 - l_2$; $r_3 = u_3 - l_3$.

The AUGMECON2 method identifies weakly efficient points and bypasses the surplus grid points, reducing computation time (Mavrotas and Florios 2013). The combination of two sets of grid points for other objectives started from looping through the inner most objective (TE) first from the nadir value grid to the optima value grid, followed by the exterior grid point ($TSoilE$) after each iteration of the inner objective loop. The feasible solution can be obtained with the first round of relaxed exterior constraints. The rolling computation for the exterior grid point could be saved to reduce computation time if no alternative optima were generated from the prior settings of lexicographic optimization objective in Equation (20). In this study, the algorithm for solving the three competing objectives was further improved by eliminating the iteration of the grid points for $TSoilE$ given that the solutions did not vary from those obtained from iterating the grid points of the TE objective. Thus, the iteration in constrained objectives for a conversion facility candidate node was reduced from 36 (6×6)

to 6 in the solving process, which consequently improved the computation efficiency and reduced computation time by more than 80%.

Compromise solution method

The regional Pareto frontier surface was developed to evaluate the potential tradeoffs among the three competing objectives. The most preferred solution point on the regional Pareto surface was identified using the compromise solution method (Ramos et al. 2014). The compromise solution optimal point was determined by the minimum distance (D(S)), measured by Tchebycheff norms (Olson 1993), to the ideal point (z^*) on the regional Pareto frontier surface:

$$D(S) = \max_{j=1,\dots,3} \{ \lambda_j |z_j(S) - z_j^*| \} \quad (23)$$

where j was the index for the objective functions, λ_j was the normalized weight for each objective function, and S was the efficient set of points on the Pareto surface. The normalized weight, λ_j , was defined as:

$$\lambda_j = 1/r_j \times [\sum_{j=1}^3 (1/r_j)]^{-1}, \quad (24)$$

where r was the previously defined objective value range. The ideal point (z^*) was defined according to the individual minima of each objective ($z^* = [l_1, l_2, l_3]$) from the payoff tables. To further illustrate the relative relationship between each point on the Pareto surface and the compromise solution point, a D score was calculated as the relative value of the D(S) of each point to the D(S) of the compromise optimal solution (i.e. the min. D(S)):

$$D \text{ score} = [D(S) / \min. D(S)]. \quad (25)$$

The regional Pareto frontier surface was used to impute the costs of mitigating GHG emissions and soil erosion in the switchgrass supply chain [31]. Two measures of the tradeoffs in higher feedstock costs with lower GHG emissions and soil erosion were

calculated using the model solution for the efficient set of conversion facilities on the regional Pareto frontier surface. The first approach was to calculate the marginal rate of substitution (MRS) between feedstock cost and GHG emissions and feedstock cost and soil erosion to provide the average costs Mg^{-1} of reducing the two aforementioned pollutants for the efficient solution (Clemen and Reilly 1999). The second approach was to calculate the costs of reducing GHG emissions and soil erosion for the compromise solution conversion facility location versus the cost minimization solution conversion facility location. Cost comparisons were also made for the GHG emission and soil erosion minimization conversion facility locations versus the cost minimization solution conversion facility location.

Data

The data sources and models used to estimate feedstock cost, GHG emissions, and soil erosion for the determination of the most preferred switchgrass supply chain solution are summarized in Table 4. The data and derived parameters were all associated with geospatial characteristics at the land resource unit in Tennessee. The DAYCENT model (Schimel 1986), a daily time-step biogeochemical model for plant-soil system, was adopted to simulate the soil carbon uptake and CH_4 and N_2O emission factors. The change in soil carbon stock was calculated using IPCC guidelines (Aalde et al. 2006). Differences in geography and soils between east, middle and west Tennessee were considered in the estimation of soil carbons (Tennessee General Assembly 2014). Emission factors for energy combustion from farm equipment operations and the indirect emission factors for the manufacturer of agricultural machinery, fertilizer, chemicals, and seed were estimated using the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) Model (Argonne National Laboratory 2013). Emissions from feedstock transportation were estimated using the Motor

Vehicle Emissions Simulator (MOVES) version 2010b (U.S. EPA 2013), considering travel distance, local weather, travel speed and the slopes of road.

Results and Discussion

Pareto frontier surface

Figure 3 presents the relationships among the three competing objectives for a single conversion facility site (Figure 3-i), all 150 potential sites (Figure 3-ii), and the regional Pareto frontier surface (Figure 3-iii). The following describes the key components in the development of the regional Pareto frontier surface that are illustrated in each panel of the chart and the economic implications of the frontier surface. First, GHG emissions and soil losses were mitigated in the LCB feedstock supply chains when feedstock costs increased; whereas, GHG emissions and soil erosion were positively correlated with each other (Figure 3-i). The model converted more cropland to accommodate the tradeoffs in lower levels of GHG emissions and soil erosion for higher feedstock costs. Crop lands have higher opportunity costs, larger fertilizer and chemical expenditures, and greater soil erosion relative to hay and pasture lands.

Second, GHG emissions and soil erosion in the switchgrass supply chain had a smaller dispersion with low feedstock costs (Figure 3-ii). The ranges of GHG emissions and soil erosion expanded as feedstock costs were increased in the model to facilitate tradeoffs in the cost and environmental objectives. Low feedstock costs were associated with the conversion of hay and pasture lands. Abatement of GHG emissions and soil erosion were achieved through the conversion of crop land leading to a wider dispersion in feedstock costs.

Third, a total of 881 feasible solution points were found in the optimization (Figure 3-iii) for the 150 potential conversion facility sites. Black dots on the regional Pareto frontier surface are the final conversion facility site solution points given that the value of one objective could not be improved upon without degrading the values of the other two

objectives. Among those 150 sites, there were a total of 40 feasible and efficient potential conversion facility sites on the regional frontier surface. The individual-optima solution points for feedstock costs (A), GHG emissions (B), and soil erosion (C) are identified as blue dots on the Pareto surface. The compromise solution point (O) is identified as a red dot.

Finally, tradeoffs in higher feedstock costs with lower GHG emissions and lower soil erosion on the frontier surface illustrated in Figure 3-iii were imputed using the MRS. For the 40 conversion facilities on the frontier, the average cost of abating one Mg of GHG emissions was \$2,378. GHG emission abatement cost was considerably more expensive than the \$10.00 average cost to reduce soil erosion by one Mg. Results indicated that soil erosion may be a more cost effective environmental criterion than GHG emissions in the development of a sustainable switchgrass supply chain in Tennessee.

Figure 4 further illustrates the tradeoffs among the three competing objectives. D scores for the 40 conversion facilities on the regional Pareto frontier surface and the geographic locations of the efficient facilities are shown on a map of Tennessee. The color of each circle is related to the D score and the size of the circles represents the level of each objective: feedstock cost (panel i), GHG emissions (panel ii), and soil erosion (panel iii). For example, the compromise solution point (O) had larger feedstock costs and GHG emissions but lower soil erosion relative to many of the other sites on the Pareto frontier surface.

Individual-optima and compromise solution

The feedstock draw areas for each individual-optima conversion facility site and for the compromise solution conversion facility site are displayed in Figure 5. The feedstock draw area for the cost minimization solution (A) was the most geographically compact, while the draw areas for the GHG emission, soil erosion, and compromise solutions (B, C, and O) were more geographically dispersed. Feedstock cost is related to the density of switchgrass

production in conversion facility draw area which impacts feedstock transportation costs (Larson et al. 2015). Crop production is more concentrated in West Tennessee while hay and pasture production is more prevalent in Middle and East Tennessee. With the two environmental objectives, the model traded off feedstock costs to convert highly erodible crop land to switchgrass in Middle and East Tennessee for the compromise solution (O). Thus, the choice of conversion facility location and feedstock draw area was primarily related to the availability of land resources and existing agricultural production.

Figure 6 shows the land coverage change for switchgrass production. Hay and pasture lands were primarily selected in the cost minimization solution (A), whereas crop lands were mostly utilized for switchgrass production in the GHG minimization (B) and soil erosion minimization (C) solutions. Converting crop lands to switchgrass resulted in higher opportunity cost from land use selection, increased soil carbon storage, and reduced soil erosion. The opportunity costs for converting hay and pasture lands to switchgrass were lower but resulted in higher soil carbon and soil erosion losses (Cherubini and Jungmeier 2009, Monti et al. 2012). Thus, a combination of crop, hay, and pasture lands were utilized in the compromise solution (O) to achieve the integrated multi-objective goal embodied in the compromise solution.

The percentage of land area with soil erosion exceeding USDA NRCS tolerance levels *ex ante* and *ex post* land converted to switchgrass for the individual-optima and compromise solutions are shown in Figure 7. Prior to converting land to switchgrass production, nearly 50% of the switchgrass feedstock draw area for the cost minimization (A) exceeded tolerance levels. Whereas, all of the land area for the GHG emission (B) and soil erosion (C) minimization cases had soil erosion exceeding the tolerance level. For the compromise solution (O), almost all (97%) of switchgrass draw area prior to land conversion also had soil erosion that exceeded the tolerance rate. However, less than 1% of all land areas *ex post*

switchgrass production exceeded the soil erosion tolerance levels for all four solutions. The reduction in soil losses mostly resulted from the year-round ground cover and deep root system provided by perennial switchgrass.

Itemized costs for each of the individual-optima and compromise solutions are summarized in Table 5. The cost minimization solution (A) had a total plant-gate feedstock cost of \$43.4 million. Harvest cost accounted for 51.6% of total feedstock cost, followed by production cost which made up 19.8% of total costs. Opportunity cost of \$1.3 million for the cost minimization solution was the lowest among the three objectives because low cost hay and pasture lands were primarily converted to switchgrass production. For the environmental objectives, the two primary factors influencing cost differences were increased opportunity costs, caused by conversion of crop lands that had higher GHG emissions and soil erosion, and increased feedstock transportation costs caused by a wider dispersion switchgrass production area. Total feedstock cost increased to \$60.5 million for the GHG minimization solution (B). Opportunity cost for the GHG solution was 11.8 times greater and transportation cost was 27.7% larger than for the cost minimization solution (A). Soil erosion minimization (C) had the highest total cost among all individual optima cases of \$85.4 million with considerably higher opportunity (\$35.6 million) and feedstock transportation (\$16.1 million) costs. Total feedstock cost for the compromise solution (O) was \$70.7 million, 62.9% higher than the cost minimization solution, but 20.7% lower than the soil erosion minimization solution (C).

The cost effectiveness of switchgrass production in reducing GHG emissions and soil erosion was further evaluated through an examination of cost and abatement amount differences among the four solutions (Table 5). The GHG emission minimization (B) solution reduced total net GHG emissions by 59%, from 44.9 thousand Mg to 18.6 thousand Mg, but at an increased feedstock cost of \$17 million when compared to feedstock cost minimization

(A) solution (Table 5). The imputed cost of abating GHG emissions was \$648 Mg⁻¹ (\$17 million /26.3 thousand Mg) between the two solutions. Reduction in total emissions resulted from converting crop lands to switchgrass that sequestered more soil carbon and used fewer inputs than the crops it replaced (Cherubini and Jungmeier 2009, Monti et al. 2012). For the feedstock cost minimization (A) and soil erosion minimization (C) comparisons, the imputed cost of GHG emission sequestration was almost \$2,765 Mg⁻¹ given that feedstock cost nearly doubled and GHG emissions were reduced by only 33%. Similarly, a high imputed cost of GHG emissions abatement of \$2,270 Mg⁻¹ was incurred when comparing the feedstock cost minimization solution (A) to the compromise solution (O). Consistent with the earlier results for the Pareto surface, targeting GHG emissions as an objective in the development of a sustainable switchgrass supply chain in Tennessee may not be cost effective.

With respect to the soil erosion minimization (C) solution, 7.5 million Mg in soil erosion was averted at an additional feedstock cost of \$15.2 million when compared with the feedstock cost minimization (A) solution. The imputed cost of reduced soil erosion was \$5.60 Mg⁻¹ for the soil erosion minimization (C) solution. Contrasting the GHG emission minimization (B) solution with the cost minimization (A) solution resulted in 3.4 million Mg less soil erosion with an imputed cost of abatement of \$5.00 Mg⁻¹. Finally, about 7.4 million Mg soil erosion was averted with an increase in total feedstock cost of \$12 million with the compromise solution (O). The imputed cost for conserving soil in the feedstock draw area was the lowest among the four model optimal solutions at \$3.70 Mg⁻¹. The Pareto frontier surface and compromise solution results indicate that targeting soil erosion as an objective in the development of a sustainable switchgrass supply chain in Tennessee may be more cost effective than targeting GHG emissions.

Conclusions

This study identified an efficient Pareto frontier surface for multiple-objective model to optimize the feedstock cost along with two environmental benefits, GHG emissions and soil erosion mitigation, for a switchgrass supply chain. Results show that the type of agricultural land converted to switchgrass production is crucial to determining feedstock costs and environmental impacts of the feedstock supply chain. Converting crop lands to switchgrass incurred higher opportunity cost from land use change but stored more soil carbon and generated less soil erosion. The opportunity cost of converting hay and pasture lands to switchgrass was lower but likely released more soil GHG emissions and caused higher soil losses. A mix of crop, hay, and pasture lands could help to achieve the goal of integrating three objectives in the switchgrass supply chain.

Given the tradeoffs among minimization of feedstock costs, GHG emissions and soil erosion on the regional Pareto frontier surface, the imputed cost of abating GHG emissions and soil erosion on was derived by the approach of marginal rate of substitution. The average imputed cost of abating GHG emissions and soil erosion on the Pareto frontier surface was \$2,378 and \$10, respectively. This finding suggests that soil erosion could be a more cost effective environmental criterion than GHG emissions in the development of a sustainable switchgrass supply chain in Tennessee. Also, the compromise solution location for the conversion facility generated 63% higher feedstock cost compared to the cost minimization location, but reduced soil erosion up to 70 times and GHG emissions by 27%. The derived imputed cost of abating GHG emissions and soil erosion in switchgrass supply chain in Tennessee could provide policy makers important information to expedite the development of a sustainable switchgrass biofuel industry.

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Appendix

Table 1 Literature review of the operational research on LCB feedstock supply chain

| Source | Purpose | Models | System | Spatial unit | Findings |
|-----------------------|---|--|---|---|---|
| Dunnett et al. (2007) | Min. Cost | State-Task-Network (STN) approach | LCB feedstock stock supply chain from field to conversion facility | Single land grid of 994 ha area | Land, cultivation and harvesting accounted for the major portion of the total cost |
| Zhang et al. (2013b) | Min. Cost | Mixed Integer Linear Programming | Switchgrass supply chain from field to biofuel consumption | County-level | 61% of the marginal agricultural land was converted to meet the demand of fuel. |
| English et al. (2013) | Min. Cost | Linear Programming (LP) | Plant-gate switchgrass feedstock supply chain | 13 km ² hexagon | The least-cost configuration of the feedstock supply chain influenced the levels and types of economic impact of biorefinery |
| An et al. (2011) | Max Profit | A time-staged, multi-commodity, production/distribution system model | Switchgrass based lignocellulosic biofuel supply system | Not spatially explicit | Ethanol price was the most significant factor in the economic viability of a lignocellulosic biofuel supply chain. |
| Larson et al. (2015) | Min Cost | MILP | Plant-gate switchgrass feedstock supply chain | 13 km ² hexagon | The conversion facility can optimize the feedstock inventory and delivery management through coordinating the timing and location of switchgrass harvest with storage and delivery. |
| Eranki et al. (2013) | Max. production Min erosion Max SOC Min N loss Min P loss Min GHGs | Watershed-scale Optimized and Rearranged Landscape Design Model | Cellulosic feedstock (perennial grasses, riparian buffers and double crops) | Seven-digit hydrologic unit (greater than county-level) | 60-77% of landscape altered to feedstock with significant energy yields and improve impacts in environmental categories. |

Table 1 Continued

| Source | Purpose | Models | System | Spatial unit | Findings |
|-----------------------------|--|---|---|------------------------------|---|
| Yu et al. (2014b) | Min Cost Min GHG | Multi-objective optimization | Plant-gate switchgrass feedstock supply chain | 13 km ² hexagon | Tradeoff between cost and GHG emissions for the switchgrass supply chain is primarily driven by the type of land converted. |
| Bernardi et al. (2012) | Min. Cost Min. GHG Min. Water footprint | multi-period multiple objective MILP problem | Upstream of typical biofuels supply chain | Not spatially explicit | Increase efficiency in agricultural irrigation water consumption scenario by 31% and 49% of total water footprint |
| Tenerelli and Carver (2012) | agricultural and environmental objectives: Land capacity; Ecological Consideration | GIS based multi-criteria approach | Land conversion scenario of perennial energy crops: including perennial grasses, short rotation coppice and short rotation forestry (SRF) | 25 km ² grid cell | Perennial grass best suited the most relevant environmental conditions. |
| Parish et al. (2012) | Min. Cost Min. Water Pollution | Biomass Location for Optimal Sustainability Model (BLOSM) | Switchgrass land use conversion scenarios | Sub-basin (HRU) | 1.3% of watershed planted with perennial switchgrass with 5.5% of pasture/hay land converted to switchgrass |
| Ziolkowska (2013) | Multiple Objectives of economic, environment, and social benefit | Multi-objective PROMETHEE method; expert elicitation approach; fuzzy set theory | Comparison of multiple biofuels production and technologies | Not spatially explicit | Switchgrass was the most suitable and sustainable feedstock for biofuels production; Corn has the lowest sustainability potential among the analyzed feedstock. |

Table 2 Definitions of Subscripts, Parameters and Variables

| | Unit | Definition |
|--|--|--|
| Subscripts | | |
| <i>i</i> | | land resource units |
| <i>j</i> | | industrial park sites for conversion facility |
| <i>m</i> | | Month |
| <i>p</i> | | crops (hay and pasture, corn, soybean, wheat, sorghum, cotton) |
| <i>k</i> | | type of machinery (tractor, mower, loader, rake, baler) |
| Parameters | | |
| <i>Price_{ip}</i> | \$ Mg ⁻¹ | crop prices |
| <i>Yield_{ip}</i> | Mg ha ⁻¹ | crop yields |
| <i>PC_{ip}</i> | \$ ha ⁻¹ | Crop production costs |
| <i>Yield^{swg}_i</i> | Mg ha ⁻¹ | switchgrass yields |
| <i>LR_{ip}</i> | \$ Mg ha ⁻¹ | land rent |
| <i>Est</i> | \$ ha ⁻¹ | Switchgrass establishment cost |
| <i>AM</i> | \$ ha ⁻¹ | Annual maintenance cost |
| <i>σ_i</i> | \$ ha ⁻¹ | cost of harvesting switchgrass |
| <i>γ_i</i> | \$ ha ⁻¹ | cost per unit of storing switchgrass |
| <i>θ_i</i> | \$ ha ⁻¹ | cost per unit of transporting switchgrass |
| <i>DML^{trans}</i> | % | dry matter loss during transportation |
| <i>Aa_{ip}</i> | Ha | crop land available in each land resource unit |
| <i>Avehour_m</i> | Hour | average working hours of machinery in each month |
| <i>DML^{stor}_m</i> | % | dry matter loss during storage |
| <i>MTB^k_i</i> | hours ha ⁻¹ | machine time ha ⁻¹ for each machinery |
| <i>λ</i> | L Mg ⁻¹ | switchgrass-ethanol conversional rate |
| <i>Q_m</i> | L month ⁻¹ | monthly demand for ethanol |
| <i>ΔLU_{CO₂,p}</i> | CO ₂ e kg ha ⁻¹ | CO ₂ emission from land conversion |
| <i>ΔLU_{CH₄,p}</i> | CO ₂ e kg ha ⁻¹ | CH ₄ emission from land conversion |
| <i>ΔLU_{N₂O,p}</i> | CO ₂ e kg ha ⁻¹ | N ₂ O emission from land conversion |
| <i>ProE</i> | CO ₂ e kg ha ⁻¹ | GHG emissions factor from energy use during production |
| <i>HarE</i> | CO ₂ e kg ha ⁻¹ | GHG emissions factor from energy usage during harvest |
| <i>StorE</i> | CO ₂ e kg ha ⁻¹ | GHG emissions factor from energy usage during storage |
| <i>MachE</i> | CO ₂ e kg unit ⁻¹ | GHG emissions factor from machinery production |
| <i>TransE_{mip}</i> | CO ₂ e kg route ⁻¹ | GHG emissions from energy usage during transportation |
| <i>Loadwt</i> | Mg truck ⁻¹ | switchgrass delivered per truck |
| <i>FertE</i> | CO ₂ e kg Mg ⁻¹ | GHG emissions factor from fertilizer production |
| <i>ChemE</i> | CO ₂ e kg Mg ⁻¹ | GHG emissions factor from chemical production |
| <i>SeedE</i> | CO ₂ e kg Mg ⁻¹ | GHG emissions factor from seed production |
| Variables | | |
| <i>AH_{mip}</i> | ha | area of switchgrass harvested monthly |
| <i>XTN_{mi}</i> | Mg | switchgrass transported directly to the biorefinery |
| <i>NXS_{mi}</i> | Mg | switchgrass stored during harvest season |

Table 2 Continued

| | Unit | Definition |
|------------|------|---|
| XS_{mi} | Mg | switchgrass stored monthly |
| XTO_{mi} | Mg | switchgrass transported from storage to the biorefinery |
| $Numb_m^k$ | Unit | number of equipment used during harvest |
| u | | Upper bound values for certain objective |
| l | | Lower bound values for certain objective |
| r | | Range of certain objective |

Table 3 Payoff Table

| Objective | Total Feedstock Cost (TC) | Total GHG Emissions (TE) | Total Soil Erosion ($TSoilE$) |
|---------------|-------------------------------|------------------------------|---------------------------------|
| Min. TC | TC optima | | |
| Min. TE | | TE optima (l_2) | |
| Min. $TSoilE$ | | | $TSoilE$ optima (l_3) |

Table 4 Data sources

| | Economic Cost | GHG Emissions | Soil Erosion |
|---|---|--|---|
| Land conversion from crop land to switchgrass | <p>Opportunity cost: Crop yields:USDA, SSURGO (U.S. Department of Agriculture Nature Resources Conservation Service 2012); Crop price and acreage: USDA NASS (U.S. Department of Agriculture 2014; U.S. Department of Agriculture 2011); Crop production cost: USDA ERS (U.S. Department of Agriculture 2014), POLYSIS(De La Torre Ugarte and Ray 2000) Switchgrass plantation: Yield: Jager et al. (Jager et al. 2010) Production and harvest Cost: Larson et al. (2010), the University of Tennessee (2015)</p> | <p>Land use change (Daycent(Schimel et al. 2001)): Weather data: DayMET¹.; Soil texture: USDA SSURGO(U.S. Department of Agriculture Nature Resources Conservation Service 2012) Management practice for crops: UT extension budget (University of Tennessee 2015) Hay/pasture management: (Bowling et al. 2006; Fribourg and Loveland 1978) Switchgrass management: (Muir et al. 2001)</p> | <p>R factor: USDA RUSLE2² K factor: USDA SSURGO³ C factor: USDA RUSLE2, TN bulletin(Jent et al. 1967), and (Hayes 2014) P factor: TN bulletin(Jent et al. 1967) LS factor: Drained area method(Mitasova et al. 2001; Mitasova et al. 1996).</p> |
| Production | <p>Establishment: American Agricultural Economics Association (2000)</p> <p>Annual maintenance: American Society of Agricultural and Biological Engineers (2006).</p> | <p>Fuel usage: GREET(Argone National Laboratory 2013) Fertilizer, herbicide, seed: GREET(Argone National Laboratory 2013) Machine production: GREET(Argone National Laboratory 2013)</p> | |

¹<http://daymet.ornl.gov/>

²RUSLE2 model website: http://fargo.nserl.purdue.edu/rusle2_dataweb/RUSLE2_Index.htm

³SSURGO database: http://www.nrcs.usda.gov/wps/portal/nrcs/detail/soils/survey/geo/?cid=nrcs142p2_053627

Table 4 Continued

| | Economic Cost | GHG Emissions | Soil Erosion |
|----------------|---|--|--------------|
| Harvest | Fuels and labors: University of Tennessee (2015): | Fuel: GREET(Argone National Laboratory 2013) Machine production: GREET(Argone National Laboratory 2013) | |
| Storage | Covers and pallets: University of Tennessee (2015) | | |
| Transportation | Trailer, fuel and labor: University of Tennessee (2015) | MOVES modeling(U.S. EPA 2013); Indirect emission from truck production: GREET | |

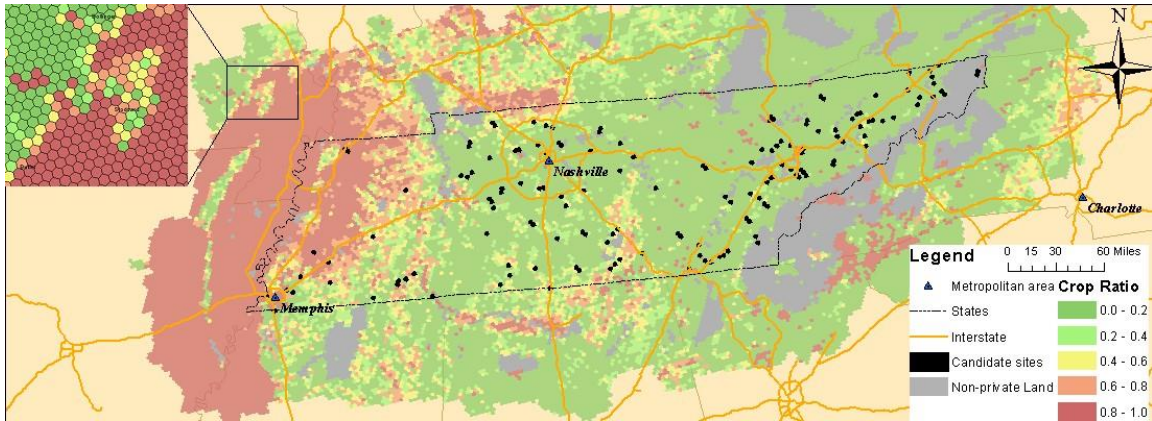


Figure 1 Potential feedstock supply area and industrial park sites for conversion facilities ⁴

⁴. Crop ratio is the ratio of crop land to hay and pasture lands.

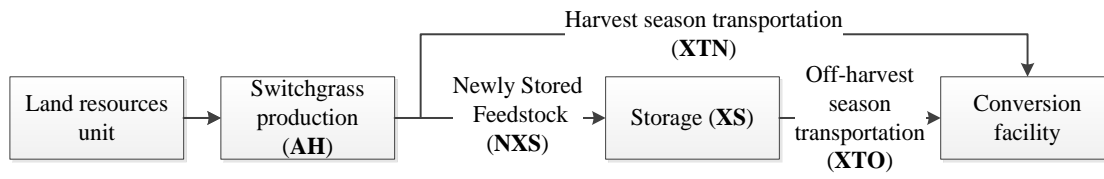
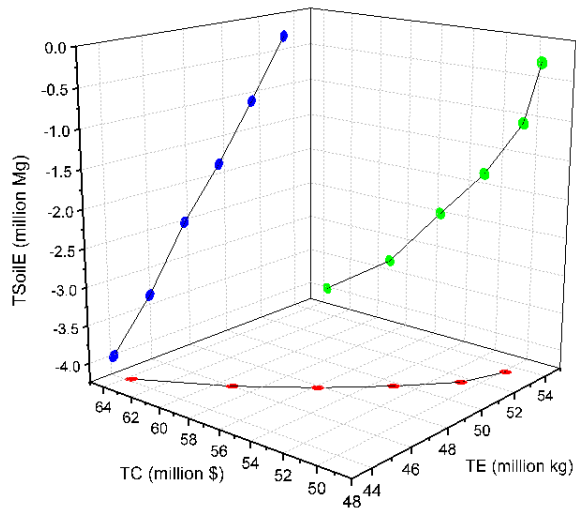
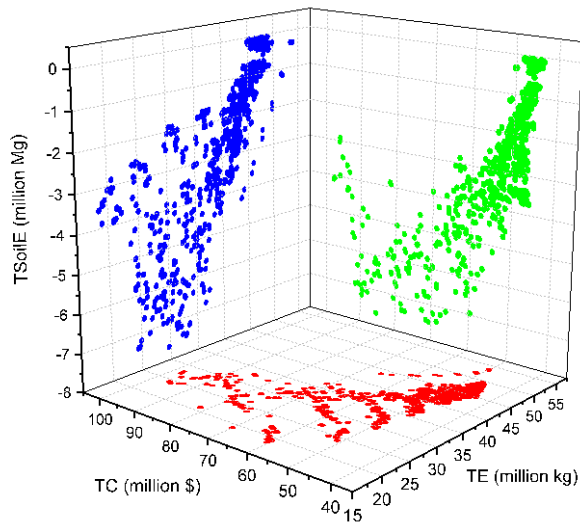


Figure 2 System boundary of switchgrass supply chain: field to biorefinery

3-i: Solution projection on each coordinator panel for one candidate site



3-ii: Solution projection on each coordinator panel



3-iii: Pareto surface embracing feasible points

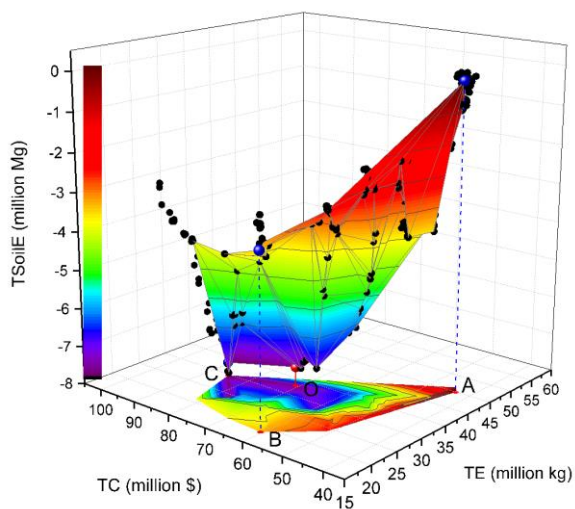
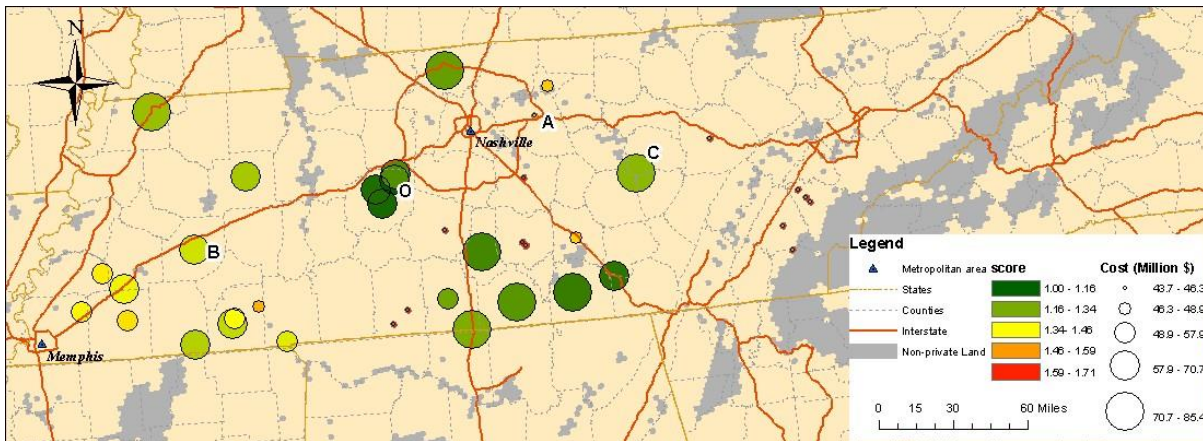
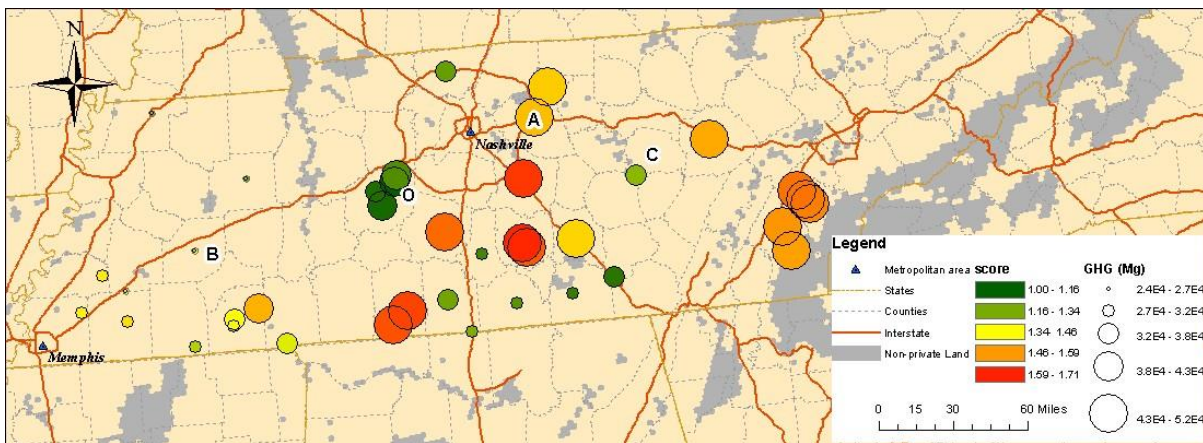


Figure 3 Regional feasible solutions (A: total cost minimization, B:GHG minimization, C: soil erosion minimization, O: compromise solution)

4-i: Total cost



4-ii: GHG emission



4-iii: Soil erosion

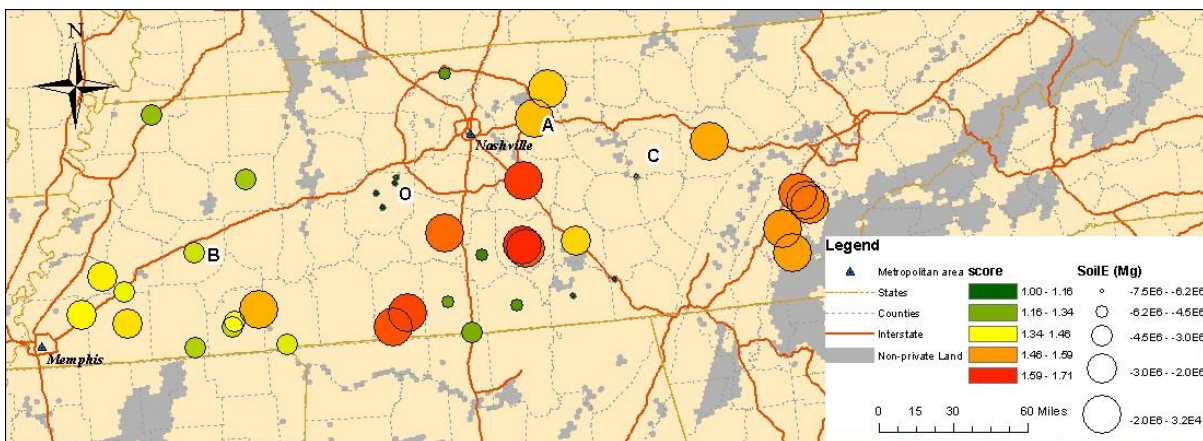
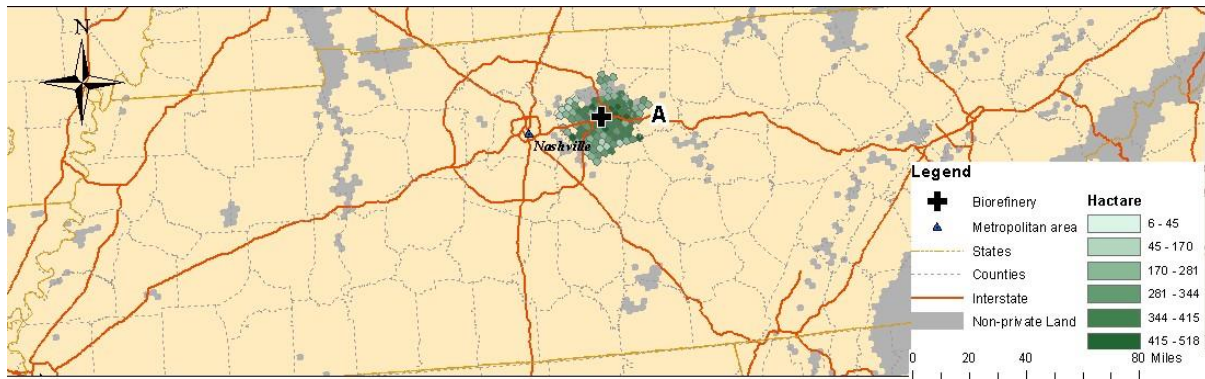
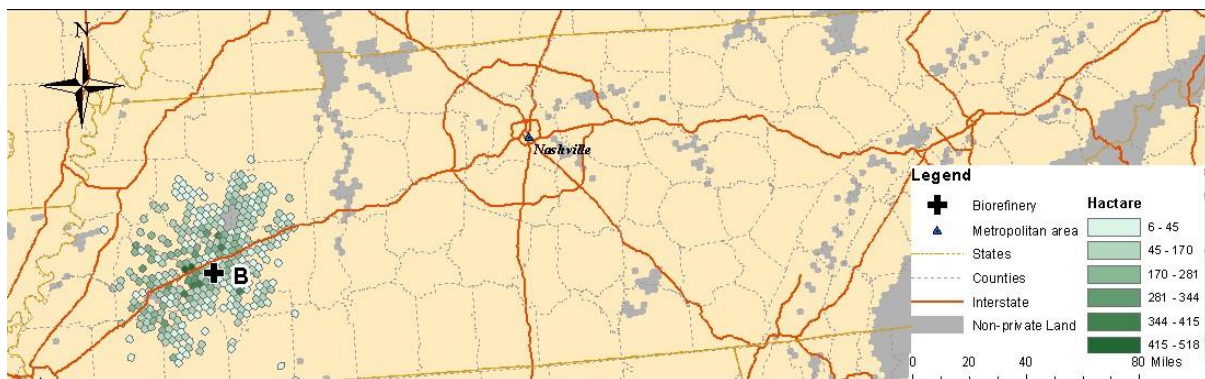


Figure 4 Distance scores and objective values for regional efficient solution on Pareto frontier. (A: total cost minimization, B:GHG minimization, C: soil erosion minimization, O: compromise solution)

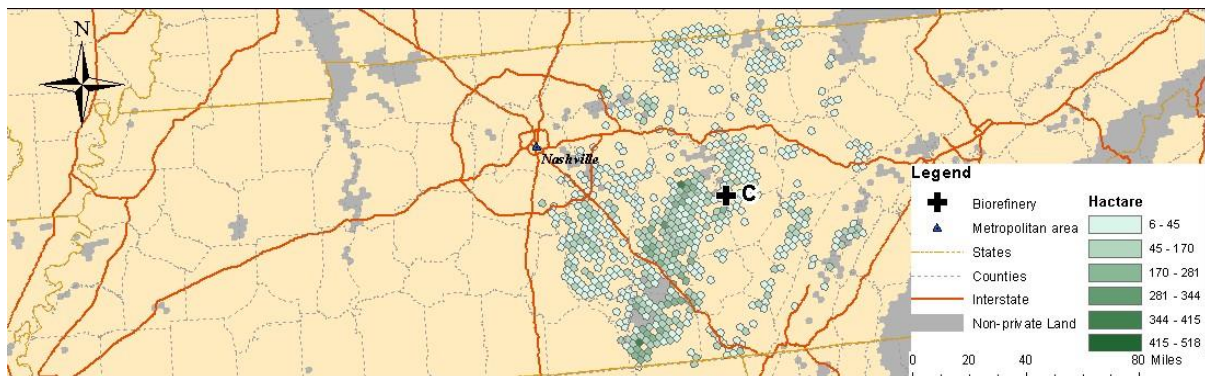
5-i: Individual optima for total cost minimization (A)



5-ii: Individual optima for GHG emission minimization (B)



5-iii: Individual optima for soil erosion minimization (C)



5-iv: Compromise solution (O)

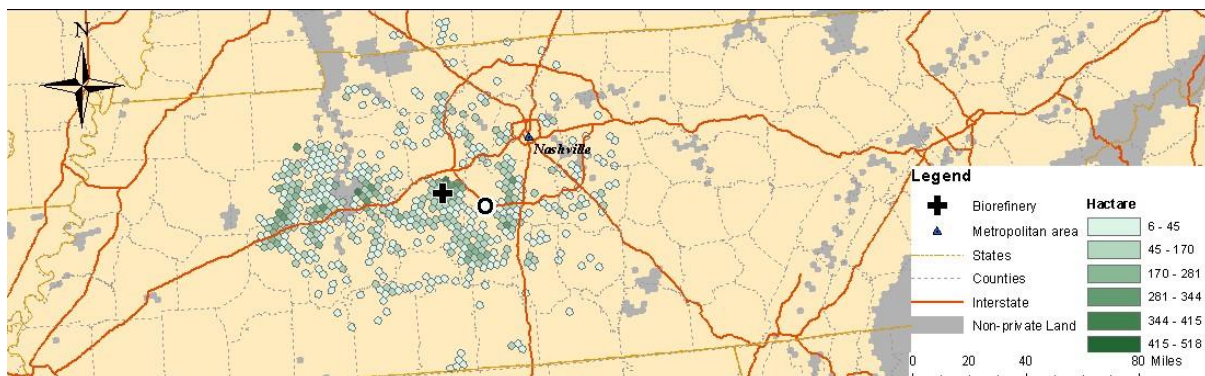


Figure 5 Placement of the conversion facility and switchgrass draw area under individual-optima and compromise solution cases

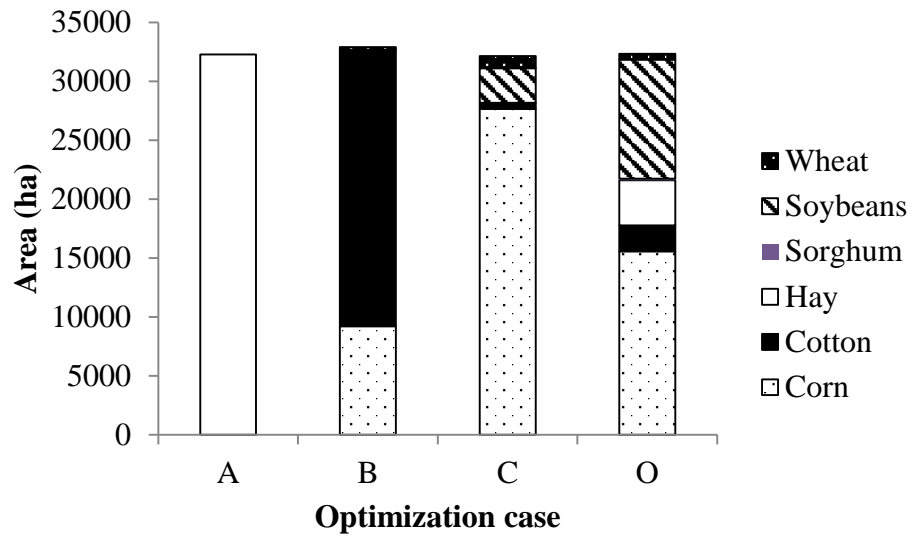


Figure 6 Acreage allocation converted to switchgrass (A: total cost minimization, B:GHG minimization, C: soil erosion minimization, O: compromise solution)

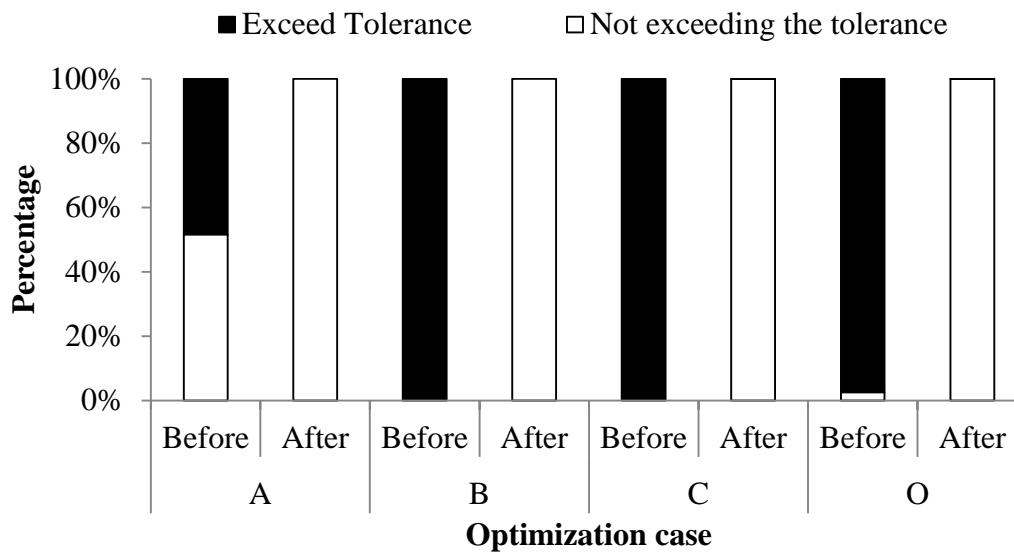


Figure 7 Changes in soil erosion on the feedstock draw area before and after the land was converted to switchgrass (A: total cost minimization, B:GHG minimization, C: soil erosion minimization, O: compromise solution)

***CHAPTER III GREY WATER FOOTPRINT AND ECONOMIC ANALYSIS OF
SWITCHGRASS SUPPLY CHAIN IN WEST TENNESSEE***

Abstract

Displacing partial crop land with production of switchgrass as a biofuel feedstock could reduce nitrate loadings to groundwater and lower the risk of groundwater contamination in west Tennessee. However, the low efficiency of collection, storage and transportation in feedstock supply chain hinders the commercialization of a switchgrass-based biofuel industry. The objectives of this study were to: i) determine grey water footprint (GWF) used for nitrate dilution to meet ambient water quality standards from producing switchgrass in west Tennessee, and ii) identify the potential tradeoff relationship between the costs of supplying switchgrass and the associated GWF. A multi-objective optimization model was applied to high-resolution spatial data in determining the most preferred case of the feedstock supply chain. Results suggest that ambient water quality condition and the types of cropland converted to switchgrass production were influential to both feedstock cost and aquatic environment in the switchgrass supply chain. The average imputed cost of reducing grey water footprint in the most preferred feedstock supply chain was \$0.94 m⁻³ in the region. A tradeoff relation between switchgrass feedstock costs and reduced nitrate loading in groundwater was observed, mainly attributed to land use selection.

Keywords: biofuel, switchgrass, supply chain, grey water footprint

Introduction

Groundwater has been one of the major water resources in west Tennessee. Nearly 96% of all citizens in the region utilize groundwater for drinking in year 2014, primarily from their private wells and springs (US EPA 2015). The City of Memphis had one of the largest groundwater withdrawals of any municipality in the southeastern United States (Steele et al. 2011). The safety of the groundwater sources in west Tennessee was inextricably linked to the land use and quality in highly mobile and directional groundwater flow in the region's karstic aquifers (Tennessee Department of Environment and Conservation 2012). The unconfined sand aquifers in west Tennessee vulnerable to contamination from aboveground activities were identified as the critical issues of groundwater pollution prevention and management in the region (Tennessee Department of Environment and Conservation 2012).

Nearly 1.1 million ha of crop production were located in west Tennessee in 2014, which accounted for 73% of total cropland in Tennessee (USDA National Agricultural Statistics Service Cropland Data Layer 2014). Nitrate concentrations in shallow groundwater underlying agricultural and urban areas are commonly higher in west Tennessee than other areas because of human activities in Mississippi embayment aquifer system (Kingsbury et al. 2014; Welch et al. 2009). Between 1980 and 2014, three wells exceeded the maximum contaminant level (MCL) of nitrate concentration (10 mg L^{-1}) issued by US Environmental Protection Agency (EPA) in west Tennessee (U.S. EPA 2009). Additional 11 wells also exceeded 5 mg L^{-1} that were under more frequent monitoring in the region. Those wells were

primarily located at the Mississippi embayment aquifer system (see Figure 8) (U.S. Geological Survey Water Resources 2000-2013).

Many studies have showed that application of commercial fertilizers was the largest single nonpoint source of nutrients loading and contributed nitrate to water bodies, causing problems of low-oxygen zone and eutrophication (Dubrovsky et al. 2010; Keeney and Follett 1991; Nolan and Hitt 2006; Turner and Rabalais 2003). Fertilizer application to the low-nitrogen-uptake-efficiency crop results in additional nitrogen loadings discharged to runoff into surface waters, to be retained in the soil, or leached into groundwater. Households using domestic shallow wells near existing or former agricultural settings as source of drinking water have a potential human health concern with elevated nitrate concentrations (Dubrovsky et al. 2010).

Displacing partial crop land with production of switchgrass as a biofuel feedstock could reduce nitrate loadings to groundwater (Parish et al. 2012); hence lowering the risk of groundwater contamination in west Tennessee. Switchgrass is a native species in the North American, which has been suggested as a potential feedstock for renewable energy to reduce greenhouse gas (GHG) emissions relative to petroleum-based energy (Schmer et al. 2008; Wu et al. 2006). In addition, switchgrass has many advantages as compared to row crops: e.g. higher biomass yield (Parrish and Fike 2005; Sanderson et al. 2006; Zhuang et al. 2013), greater climate and soils adaptability (McLaughlin and Kszos 2005) , and lower fertilization requirement with high nutrient uptake efficiency (Monti et al. 2012; Parrish and Fike 2005). These bionomic attributes facilitate better ecosystem performance with less water demand

(Dominguez-Faus et al. 2009; Hendrickson et al. 2013) and less pollution pressure from fertilization (Eranksi et al. 2013; Nelson et al. 2006; Parish et al. 2012) than field crops.

Despite its environmental benefit as a biofuel feedstock, the high cost of producing low density switchgrass relative to its energy value, along with the low efficiency of feedstock collection, storage and transportation, hindered commercialization of a switchgrass-based biofuel industry. Biofuel production cost L^{-1} of gasoline equivalent from switchgrass was 17% higher than corn-based ethanol cost (Haque and Epplin 2012; USDA Economic Research Service 2015). Feedstock procurement costs could constitute 30%–50% of the total cost of producing switchgrass-based biofuel (Khanna et al. 2008; Yu et al. 2014; Zhang et al. 2013). The high cost of feedstock had impeded the development of a switchgrass-based biofuel industry (Khanna et al. 2008; Wesseler 2007).

Considering the externality of positive aquatic impact of switchgrass production can potentially prompt the commercialization of switchgrass biofuel industry in west Tennessee, hence mitigating the nitrate loading issue in regional groundwater. To capture the externalities associated with groundwater quality, one could analyze the differences between how nitrate accumulates in groundwater if land is used for feedstock instead of crop production over some period of time and how these differences affect the risk of exceeding ambient groundwater quality standards over that period of time. However, the data on aquifer boundaries and volumes, along with modeling of the fate of N and N levels in groundwater aquifers over time, is difficult to obtain and manage. An alternative approach was through the concept of *grey water footprint* (GWF, Gerbens-Leenes et al. 2009; Wu et al. 2012). GWF is

defined as the volume of water needed to sufficiently dilute pollutant loadings to meet ambient water quality standards, given background pollutant concentrations. The GWF used to dilute the leachate from the surface crop management could also be considered as the volume of polluted water resulting from aboveground activities. In addition, as groundwater has become an increasingly important water supply source (Richey et al. 2015), measuring the amount of groundwater used for agricultural leachate provides crucial information to evaluate regional water source availability in the future.

Quantifying the positive externalities associated with reductions in nitrate loadings and GWF can provide the stakeholders the proxy value of environmental benefits from supplying switchgrass. Also, incorporating both economic and environmental performance in switchgrass supply chain can potentially accelerate the development of a sustainable biofuel industry in west Tennessee. Thus, the objectives of this study were twofold: i) determining GWF of various switchgrass supply chains in west Tennessee, and ii) identifying the potential tradeoff relationship between the costs of supplying switchgrass as a biofuel feedstock and the associated GWF in west Tennessee.

Literature review

Water quality impact of biofuel feedstock production have been widely studied over the past decade, with the primary focus on surface water runoff conditions (e.g.(Einheuser et al. 2013; Nelson et al. 2006; Parish et al. 2012; Zhou 2011). The leachate of nitrate loadings to groundwater body and consequent water quality impact of biofuel feedstock production

system has also received increasing attention, e.g. (Rios et al.). (Welch et al. 2010) studied the impact of corn ethanol boom on water quality and found rising concentration of nitrate contamination of groundwater in Mississippi Delta due to high fertilizer chemical application rate to corn. Also, increases in fertilizer inputs and nitrate leaching potentials from the expanded cultivation of corn and soybeans for biofuel production resulted in growing vulnerability of the groundwater (Li and Merchant 2013).

Water footprint assessment was one approach used for evaluating the environmental impact on water bodies recently. Most of the water footprint analysis for biofuel crop production focused on consumptive water of green water and blue water footprint, which represented the water demand by evapotranspiration in the form of rainwater and irrigation water, respectively (Gerbens-Leenes et al. 2009; Mishra and Yeh 2011). Analysis of GWF in the application of groundwater quality was still limited nowadays. Mekonnen and Hoekstra (2010) estimated water footprints for 126 crops including conventional crops for ethanol of corn, soybeans, sorghum in a global-scale and spatially-explicit way and found the surface GWF of those crops ranged from 200-500 m³ ton⁻¹ of the biomass for bioenergy feedstocks. Recent studies have estimated GWF from nitrogen runoff in biofuels life cycle analysis of ethanol from corn stover (29,000 – 1,098,355 L ha⁻¹) (Wu et al. 2012), ethanol from corn grain, stover, wheat straw, and biodiesel from soybean (30 – 1,508 L L⁻¹ biofuel) (Chiu and Wu 2012), and biofuels from forest wood residues (400 - 443 L L⁻¹ biofuel) in the United States (Chiu and Wu 2013). The estimated GWF from nitrogen runoff of producing switchgrass for biofuel is still lacking though.

Mathematical programming models are commonly used by researchers to determine the optimal design of biofuel feedstock supply chains (Sharma et al. 2013). A few applications of optimizing switchgrass supply have particularly considered water quality from land use selection. Eranki et al. (2013) minimized the N and P losses and maximized the water use efficiency when determining the land cover change for switchgrass production. Their results showed that the perennial grass and riparian buffers plantation reduced N and P losses and improved water use efficiency, soil erosion, and GHG emission by 20% to 100%. Parish et al. (2012) considered multiple objectives, including minimizing N, P and sediment in water and maximizing the profit for production of switchgrass, in the decision of producing switchgrass-based transportation fuel at Lower Little Tennessee watershed. Since the estimation of GWF associated with switchgrass production is still lacking in the literature, the multiobjective optimization of the biomass feedstock supply chain considering both feedstock cost and GWF from converting different types of agricultural land to switchgrass production is thus not available. The present study offered a case study considering both economic cost and GWF of switchgrass in the design of biomass supply chain at west Tennessee to fill the gap in the literature.

Methods and Data

Switchgrass supply chain design

The system boundary for calculating costs and GWF produced in the switchgrass feedstock supply chain in this study was from farm to the conversion facility (Figure 10). Six main components considered in the design of the feedstock supply chain were: (i) land

resource allocation, (ii) biomass production, (iii) harvest management, (iv) biomass storage, (v) biomass transportation, and (vi) conversion facility investment and operations.

Switchgrass production area (AH) was located based on the availability of agricultural land, opportunity cost of land use change, and distance to conversion facilities. After being harvested, some switchgrass harvests are directly delivered to the conversion facility (XTN) for biofuel production in harvest season, while remained harvests are brought to storage at the side of the fields (NXS). The stored switchgrass (XS) is then transported to a conversion facility (XTO) every month during the off-harvest season.

The annual biofuel production in west Tennessee was set at 946 million L year⁻¹, which was derived from the assumption of replacing 20% of transportation fuel use (606 trillion Btu energy in 2012) in Tennessee (U.S. energy Information Administration 2012) along with the share of population in west Tennessee. A conversion rate of 300 L of ethanol Mg⁻¹ of switchgrass was assumed (Wang et al. 1999). The potential locations for conversion facilities were assumed to be among 18 industry parks (Tennessee Valley Authority Economic Development 2011). Two capacity scale of conversion facility, 189 million L of ethanol year⁻¹ (MLY) or 378 MLY, were considered and the economy of scale in the investment of the larger capacity was based on (Tembo et al. 2003). Only one conversion facility was allowed at each site.

The potential feedstock supply area in this study included all agricultural land in west Tennessee and a buffer area of 80 km contiguous to the state border. It was assumed up to 50% of the hay/pasture land could be used for land conversion to maintain the feedstock

source for local livestock industry. Switchgrass was harvested after senescence between November and February using square balers. The dry matter loss in square bales with protection of tarp and pallet during storage was from Mooney et al. (2012).

The multi-objective optimization considering economic cost and GWF minimization in the switchgrass supply chain were conducted in several steps. First, the supply chain model was solved for each individual objective in the study area. Next, the optima and nadir values and the range obtained from the first step were used as additional constraints using improved augmented ε -constraint method (Mavrotas and Florios 2013). The mixed integer linear program (MILP) model of supply chain design considering multiple objectives of cost and GWF minimization was solved for the multi-objective function with inserted middle points. Finally, the average imputed cost of environmental aspects and compromise solution method (Ramos et al. 2014) was used to identify the most preferred design of the feedstock draw area and conversion facility placement for the industrial-scaled switchgrass supply chain.

Cost minimization

Based on Larson et al. (2015), the objective of minimizing total feedstock cost (\$) for a switchgrass supply chain was extended by including both upper stream (fields) and middle stream (conversion facilities) components:

$$\text{Min } TC = C_{\text{opportunity}} + C_{\text{production}} + C_{\text{harvest}} + C_{\text{storage}} + C_{\text{transportation}} + C_{\text{investment}} + C_{\text{operation}} \quad (26)$$

where $C_{\text{opportunity}}$ was opportunity cost, $C_{\text{production}}$ was production cost; C_{harvest} was harvest cost, C_{storage} was storage cost; $C_{\text{transportation}}$ was transportation cost of switchgrass; $C_{\text{investment}}$

was the conversion facility construction cost; and $C_{operation}$ was the operational cost for biofuel production. The definitions of the parameters and decision variables were listed in Table 6. The cost minimization case was considered as private industry decision standpoint, which was taken as a benchmark solution.

Opportunity cost ($C_{opportunity}$) was defined as the forgone profit from crop, hay, and pasture production activities that took place before the conversion of land to switchgrass production. Farmers were assumed to receive the profit from switchgrass production that has to at least match the existing agricultural production activity. Thus, opportunity cost in Equation 27 was defined as the net revenue from the prior land use or the land rent, whichever is higher (Larson et al. 2015):

$$C_{opportunity} = \begin{cases} \sum_{ip} [(Price_{ip} \times Yield_{ip} - PC_{ip}) \times AH_{ip}], & \text{if } (Price_{ip} \times Yield_{ip} - PC_{ip} - LR_{ip}) \geq 0 \\ \sum_{ip} (LR_{ip} \times AH_{ip}) & , \text{ if } (Price_{ip} \times Yield_{ip} - PC_{ip} - LR_{ip}) < 0 \end{cases} \quad (27)$$

The cost of switchgrass production ($C_{production}$) in Equation 28 included the establishment of switchgrass and annual maintenance costs. Harvest cost ($C_{harvest}$) in Equation 29 modeled switchgrass harvested using a large rectangular bale system. Storage cost for switchgrass (γ_i) in Equation 5 included costs of materials, equipment, and labor for bale staging and storage operations. Transportation costs (θ_i) in Equation 31 assumed the use of semi-trailer trucks and trailers to transport switchgrass from storage to the conversion facility. Costs for transportation were determined by the time for each activity. Loading and unloading times for bales were from Duffy (2007). Distance and truck speeds based on posted highway limits determined transportation time. Maximum travel distance to transport switchgrass to the

conversion facility was 121 km. The amortized investment cost of the conversion facility by capacity (ω_{cap}) (Humbird et al. 2011) was multiplied by the number of conversion facility in Equation 32. The operational cost of producing biofuel in each conversion facility was calculated given the facility capacity in Equation 33.

$$C_{production} = \sum_{mip} ((Est + AM) \times AH_{mip}) \quad (28)$$

$$C_{harvest} = \sum_{ip} (\sigma_i \times AH_{ip}) \quad (29)$$

$$C_{storage} = \sum_{mi} (\gamma_i \times NXS_{mi}) \quad (30)$$

$$C_{transportation} = \sum_i (\theta_i \times (\sum_m XTN_{mi} + \sum_m XTO_{mi}) / (1 - DML^{trans})) \quad (31)$$

$$C_{investment} = \sum_i (\omega_{cap} \times CBB_{cap,i}) \quad (32)$$

$$C_{operation} = \sum_{cap,i} (\alpha \times Q_{cap} \times CBB_{cap,i}) \quad (33)$$

A set of constraints were imposed given practical operations requirements and rules of mass balance. Equation 34 restricted available land area based on switchgrass yields for LCB feedstock production in each land resource unit. Equation 35 constrained machine hours month⁻¹ based on available harvest days due to weather during harvest season. Equation 36 required feedstock harvested during harvest season equals the summation of direct delivery after adjusting for transportation dry matter losses and indirect transportation to storage. In addition, Equations 37 and 38 maintained the balance of the cumulative storage of switchgrass after taking into account storage dry matter losses. Lastly, feedstock deliveries to the conversion facility in each month needed to meet the demand for biofuel production in Equation 39. All parameters and variables in the model were nonnegative (Equation 40).

Production constraint:

$$\sum_m AH_{mip} \leq Aa_{ip}, \forall i, p \text{ Nov} \leq m \leq \text{Feb} \quad (34)$$

Harvest machine hours constraint:

$$Numb_m^k \times Avehour_m - \sum_i (MTB_i^k \times AH_{mip}) \geq 0, \forall k, m \quad (35)$$

Harvest to shipment and storage balance constraint:

$$\sum_p AH_{mip} \times Yield_i^{swg} = XTN_{mi} / (1 - DML^{trans}) + NXS_{mi}, \forall m, i \quad (36)$$

Cumulative storage balance in harvest season:

$$XS_{(m+1)i} = (1 - DML_m^{stor}) \times XS_{mi} + NXS_{(m+1)i}, \forall m, i \text{ Nov} \leq m \leq \text{Feb} \quad (37)$$

Cumulative storage balance during off-harvest season:

$$XS_{(m+1)i} = (1 - DML_m^{stor}) \times XS_{mi} - XTO_{(m+1)ip} / (1 - DML^{trans}), \forall m, i \text{ March} \leq m \leq \text{Oct} \quad (38)$$

Ethanol demand constraint:

$$\lambda (\sum_i XTN_{mi} + \sum_i XTO_{mi}) - Q_m = 0, \forall m \quad (39)$$

Nonnegative constraint:

$$AH_{mip}, XTN_{mi}, NXS_{mi}, XS_{mi}, XTO_{mi}, Numb_m^k \geq 0 \quad (40)$$

Grey water footprint minimization

Conceptually, *GWF* was defined as the volume of freshwater that was required to assimilate the load of nutrients/chemicals (Aldaya et al. 2012) on the basis of water quality standards established by the U.S. Environmental Protection Agency (EPA) (Tennessee Water Quality Control Board 2008).

$$GWF = \frac{Nload \times Acre}{Nutrinet_{\text{permit}} - C_{\text{nitrate}}} \quad (41)$$

where $Nload$ was the estimated nitrate loading per ha; $Nutrinet_{permit}$ was the concentration in the ambient water quality standards set by EPA regulated as 10 mg L^{-1} for drinking water, which was the highest level of contamination; and $C_{nitrate}$ was the natural background nitrate concentration in the water body. Aquifer-level background nitrate concentration was disaggregated to spatial unit through ArcGIS intersect geoprocess and Excel pivot table.

The nitrate loadings output of each crop in west Tennessee were simulated by DayCent model (Parton et al. 1994; Schimel et al. 2001). DayCent is a biogeochemical model focusing on the management schedule of plant-soil system in the simulation of the exchanges of carbon and nutrients for crops on a daily basis. Plant growth simulation is a function of soil texture and nutrient, water availability, temperature, and plant specific parameters such as biomass C:N ratio, and above- and below-ground N allocation. Inorganic N availability from atmospheric deposition and fixation, fertilizer, plant uptake, and soil penetration related to land use changes or different aboveground activities can be captured by DayCent model (Li et al. 2004; Robertson et al. 2011; Zhang 2012).

In this study, simulation of leaching losses from each crop was conducted from 2010 to 2040 with two paths: the first one assumed the cropland to be converted to switchgrass; while the second scenario assumed the land to be used for the original crop over the same period. The nitrate leachate underground per year was calculated by taking an average of 30 years output for each crop type and switchgrass. Pollutions into groundwater from vehicle transportation and operations in the fields and inside conversion facility were hard to capture and assumed to be negligible. Thus, the objective of GWF consumption ($TGWF$) in a given

spatial unit i was to minimize the net GWF (m^3) from converting different types of agricultural land to switchgrass (i.e. $GWF_{swg} - GWF_p$)

$$\text{Min. } TGWF = \sum_i \frac{Nload_{i,swg} \times \sum_p AH_{ip}}{10\text{mg/L} - C_i} - \sum_{ip} \frac{Nload_{i,p} \times AH_{ip}}{10\text{mg/L} - C_i} \quad (42)$$

Under this sole objective, the cost of switchgrass supply chain was assumed not to be considered.

Improved augmented ε -constraint method in multi-objective program

An improved augmented ε -constraint method was applied to derive the tradeoff relationship between the objectives of TC and $TGWF$ minimization by interpolating grid points between the individual optima and nadir values (Mavrotas and Florios 2013). The logic of the improved augmented ε -constraint method (AUGMECON2) was to optimize the primary objective while binding the other objective to constrained values (Mavrotas 2009). Solutions generated forms the tradeoff curve, indicating that the performance of one objective could not be improved without degrading the performance of the other objective.

The improved AUGMECON2 was applied to formulate the two objectives as:

$$\text{Min. } (TC - \varepsilon \times (s/r)) \quad (43)$$

$$\text{Subject to: } TGWF + s = e_g \quad (44)$$

where TC was the total cost (\$), ε was a small number (in this study ε was set to be 10^{-3}), s was the non-negative slack variable, r was the value range of $TGWF$. The value of e_g were determined by interpolating a set of 3 grid points (i.e. Mid 1, Mid 2 and Mid 3) evenly within

the range of r , where g was the index of grid point. The slack variable s was added to the objective function (43) to prevent weak efficient solutions.

Most preferred solution

The most preferred case among those efficient solutions on the tradeoff curve between TC and $TGWF$ was determined by two selection criteria: a) imputed average cost of GWF, and b) compromise solution method (Ramos et al. 2014). The imputed average cost of GWF of each case was derived by dividing its TC by associated $TGWF$, which suggests the imputed cost of every unit of saved GWF. The solution with the minimum imputed average cost was selected as the most preferred case.

Alternatively, the compromise solution method located the most preferred solution that was closest to the ideal point (Ramos et al. 2014). The ideal point (z^*) was defined as a case that has the individual minima of each objective ($z^* = [l_{TC}, l_{TGWF}]$). The compromise optimal solution was determined by identifying the efficient point with the minimum distance ($D(S)$), measured by Tchebycheff norm (Olson 1993), to z^* on the Pareto surface. The D score was the ratio of the $D(S)$ of each efficient point to the $D(S)$ of compromise optimal:

$$D(S) = \max_{j=1,\dots,3} \left\{ \lambda_j \left| z_j(S) - z_j^* \right| \right\} \quad (45)$$

where S stood for the efficient points on the Pareto Frontier, λ_j was the normalized factor for each objective function, and j was the index for the objective functions:

$$\lambda_j = 1 / r_j \times \left[\sum_{i=1}^3 (1 / r_i) \right]^{-1} \quad (46)$$

Data

Data collected was listed in Table 7. Spatial data was typically important when analyzing the economic and environmental impacts in a biofuel feedstock supply chain (Archer and Johnson 2012). Thus, the study area was downscaled to a 13-km² hexagon resolution (defined as the spatial unit) to highlight geospatial variation in land resources, the transportation network, and other geographic features of the study area. The biomass yield, production cost, and hectare available for conversion from all crop lands and switchgrass were collected and adjusted with the resolution of the spatial unit. The nitrogen input and its leachate loadings to underground simulated by Daycent model was also adjusted to the spatial unit.

There were 204 nitrate monitoring sites with historical records for groundwater nitrate level from 1980 to 2014 from west Tennessee, 90% of which were in the Mississippi embayment aquifer system (Figure 1). More than 30% of all the sampling wells exceed the national average level of 1.00 mg L⁻¹. The maximum, minimum, and mean of observed nitrate concentrations at each aquifer are illustrated in Figure 11. The Mississippi embayment aquifer system had the highest average nitrate level of 1.42 mg L⁻¹ and the diverse range of nitrate level, followed by the Mississippi aquifer. The background nitrate concentration of groundwater quality was applied to spatial unit using the average value from the observations for all the spatial units within the same aquifer.

Results and Discussion

Cost minimization case

Total three conversion facilities were selected in the cost minimizing case: one 189-MLY (at Fayette County) and two 378-MLY conversion facilities (at Carroll and McNairy County) that were served by nearly 161 thousand ha of switchgrass production. About 94% of total converted lands were from hay/pasture lands. The opportunity cost of hay/pasture land was the lowest among all the other crop types hence it was the dominant source for switchgrass production. Since up to 50% of hay/pasture land in the total agricultural land were used for conversion, some croplands were gathered near the conversion facility site for ease of transportation (Figure 12). The wellheads served for drinking water covered in this area that regulated routinely by EPA (US EPA 2015). Results show that 73 sites of public water system relying on groundwater were within feedstock draw area, and approximate 301 thousand people potentially benefited from switchgrass production and consequent improved groundwater sources with less nitrate-loading.

The total cost of switchgrass supply chain in the cost minimization case was more than \$743 million. Conversion facility investment cost accounted for nearly 40% of total cost, followed by conversion facility operational cost (31%), and harvest cost (15%). Transportation cost of feedstock made up to 7% of total cost, while opportunity cost only took a small portion (1%) of the total cost since the dominant land sources were from the most economic hay and pasture lands.

The *TGWF* that considered as water usage and quality impact from converting agricultural land use into switchgrass was at -125,225,976 m³. The negative number

represents the offset or avoided *TGWF* when the land was changed to switchgrass production from the use of other fertilizer intense crop types. That is, total 125,225,976 m³ of GWF were saved when those lands were converted to switchgrass under the cost minimization case. The average *TGWF* per hectare for switchgrass was 774,834 Lha⁻¹, much lower than the current cropland for feedstock draw area of 1,483,040 L ha⁻¹. The total nitrate loadings leachate underground reduced from 2,292 Mg to 1,144 Mg after the lands were converted to switchgrass.

TGWF minimization case

The *TGWF* minimization case selected total six conversion facilities with 189-MLY of capacity when industry cost was not concerned. The selected sites were not fully utilized and scattered over the region and some were not adhere to feedstock draw area, since the land conversion priority was given to the area of N intense crops and aquifers with higher nitrate concentration. The total converted area included 168 thousand ha for switchgrass production mainly from corn and soybeans, whereas hay/pasture lands were not selected for switchgrass production. The feedstock area (Figure 13) had a scattered pattern and located mainly at the Mississippi embayment aquifer system, which was one of the main aquifer serving public water supply in the western shallow groundwater system (Gonthier 2000; Welch et al. 2009).

Given the sole objective of *TGWF* minimization, an estimated cost of \$1,035 million was incurred to develop the switchgrass supply chain, 39% higher compared to the cost minimization case. As shown in Figure 14, a great increase in facility investment cost was

imposed because of six 189-MLY conversion facilities were selected instead of three facilities (two 378-MLY and one 189-MLY). Opportunity cost soared up as the second largest cost component (15%) because of converting more valuable lands of corn and soybeans. The transportation cost increased by 46% compared to cost minimization case because of the scattered feedstock draw area pattern.

The reduced *TGWF* of 1,040,659,845 m³ was 8.3 times more than that in the cost minimization case. This great saved volume of GWF was mainly from the displacement of corn and soybeans production because of their higher nitrogen input loadings. The nitrate loading was 10,232 Mg discharged by corn and soybeans but only 1,198 Mg from switchgrass.

Tradeoff relationship and the most preferred solution

The *TC* minimization and *TGWF* minimization cases along with three middle grid points between two minimization cases (Mid 1 through Mid 3) showed a tradeoff relationship between *TC* and *TGWF*. The three middle points had similar itemized cost as the *TC* minimization case excepting for the opportunity cost of land use change. The converted land was primarily from hay and pasture land in the *TC* minimization case, while more preference were given to croplands when moving toward the *TGWF* minimization case (Figure 16). Preferred crop lands to be replaced by switchgrass mainly came from soybeans and corn because of the higher potential to reduce nitrate loadings and *TGWF*. The *TGWF* and nitrate loadings showed a gradual increase when the total cost lowered, suggesting greater *TGWF*

and nitrate offset from conversion by switchgrass. The relationship between *TC* and *TGWF* followed a concave pattern with a diminishing marginal change of *TC* in terms of *TGWF*.

The GWF per hectare of switchgrass production on groundwater system were 774,834 L ha⁻¹ under the TC minimization case, 781,035 L ha⁻¹ under Mid 1 case, 782,098 L/ha under Mid 2 case, 781,853 L ha⁻¹ under Mid 3 case, and 819,046 L/ha under the *TGWF* min case. The variation in *TGWF* was mainly attributed to the variation in groundwater condition across the study area. The estimated GWF were within the range of GWF of other cellulosic biofuel feedstock, including corn stover and wheat straw (Wu et al. 2012; Wu and Chiu 2014). The average GWF per Mg of switchgrass was 38–42 m³ Mg⁻¹, much lower than 200–500 m³ Mg⁻¹ of row crops used for biofuel (Mekonnen and Hoekstra 2010).

The imputed average costs of reduction in *TGWF* for five cases were: \$0.99/m³ (*TGWF* min), \$0.94 m⁻³ (Mid3), \$1.31 m⁻³ (Mid2), \$2.12 m⁻³ (Mid3), and \$5.94 m⁻³ (TC min).

Although the *TGWF* min case saved the most *TGWF*, the surging investment cost of made it inefficient in terms of imputed average cost. The most preferred point with minimum imputed average cost was Mid3 case. The imputed cost of *TGWF* abatement information developed in this tradeoff analysis may be useful to policymakers and LCB-based energy investors seeking to develop a sustainable bioenergy sector in the region while improve the groundwater quality. The Mid 3 case was also chosen in the compromise solution method given its lowest Distance score. Total three conversion facilities (one 189 MLY and two 378 MLY of capacity) were located in the south of west Tennessee (Figure 17). Covered area embraced 53 public groundwater systems serving largest 1,031,613 populations. The total cost increased

by 3.5% from the cost minimization case while *TGWF* reduced by 6.5 times at -811,801,378 m³. In addition, about additional 6.4 times less nitrate loading was discharged compared to the cost minimization case.

Conclusions

Aquifers in west Tennessee are at risk of contamination from the 1.1 million ha of crop production in the area, which jeopardized the primary drinking water sources. Displacing crop production with large-scale production of switchgrass as a biofuel feedstock could reduce nitrate loadings to groundwater and lower the risk of groundwater contamination in west Tennessee. The advantages of switchgrass in ecological and environmental performance allowed less demand fertilizer by switchgrass will alleviate the groundwater quality pressure especially in groundwater-dependent public water supply in west Tennessee. However, the low efficiency of storage and transportation in the feedstock supply chains has hindered the commercialization of a switchgrass-based biofuel industry. Thus, the objective of this study is to identify the relationship between the cost of supplying switchgrass as a biofuel feedstock and reduced grey water footprint used for nitrate dilution to meet ambient water quality standards. In this study, a MILP multi-objective optimization model was applied to high-resolution spatial data in determining the optimal placement of the feedstock supply chain.

Result found that in west Tennessee, where most of aquifers underwent groundwater quality deteriorating processes with pressures from both public water supply and agricultural use, the industrial bioenergy feedstock supply chain design was heavily influenced by the

type of land converted for switchgrass production based on different objectives. Combination of multiple sites on different capacity scales with allocation of surrounding feedstock production land made it possible to accomplish the different goals. Findings that (1) The selections of hay/pasture lands with lowest opportunity determine the performance of total cost; (2) The economic crops of corn/soybeans affect significantly the *TGWF* and nitrate loadings; (3) Higher nitrate concentration in Mississippi embayment aquifer system was prior to get converted for purpose of *TGWF* minimization, were the basic logic behind this MILP model. Their tradeoff relation between TC and GWF therefore was also obtained by using the improved augmented ϵ -constraint method.

GWF factor for switchgrass in the groundwater system was firstly obtained from this study. Both two methods of imputed cost and compromise solution method that found Mid 3 case was the most preferred solution by balancing the 2 metrics. This optimal solution showed the relatively stable imputed cost of decreasing *TGWF* at $\$0.94 \text{ m}^{-3}$ GWF, while increasing the total cost by 3.5%. However, the *TGWF* was reduced by 6.5 times with additional 6.4 times less nitrate loading was discharged compared to the cost minimization case.

The results from this study provide important information for policy makers and researchers interested in the sustainable development of the cellulosic biofuel industry in the U.S. For future research, the analysis can be extended to whole Tennessee and set up supply chain serving for biofuel demand from whole state. More discussion about crop yield compensation may be required from displacing crop production with feedstock production in

west Tennessee either by increasing cultivated land expansion or exportation of the fertilizer-intensive crop production to another area.

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Appendix

Table 6 Definitions of Subscripts, Parameters and Variables

| | Unit | Definition |
|-----------------------------------|-----------------------|--|
| Subscripts | | |
| i | | locations of switchgrass production field |
| j | | location of the biorefinery |
| m | | month |
| p | | crops (hay/pasture, corn, soybean, wheat, sorghum, cotton) |
| k | | type of machinery (tractor, mower, loader, rake, baler) |
| cap | | capacity scale (50 MGY, 100 MGY) |
| Parameters | | |
| Price _{ip} | \$ per unit | traditional crop price |
| Yield _{ip} | Mg area ⁻¹ | tradition crop yield |
| PC _{ip} | \$ ha ⁻¹ | production cost of traditional crop |
| Yield ^{swg} _i | Mg ha ⁻¹ | yield for switchgrass in each hexagon |
| LR _{ip} | \$ ha ⁻¹ | land rent of traditional crop |
| Est | \$ ha ⁻¹ | establishment cost in the first year |
| AM | \$ ha ⁻¹ | annual maintenance cost |
| σ _i | \$ ha ⁻¹ | cost of harvesting switchgrass |
| γ _i | \$ Mg ⁻¹ | cost per unit of storing switchgrass |
| θ _i | \$ Mg ⁻¹ | cost per unit of transporting switchgrass |
| ω _{cap} | \$ per unit | amortized biorefinery investment cost |
| α | \$ kL ⁻¹ | operation cost per kL of biofuel production |
| DML ^{trans} | % | dry matter loss during transportation |
| Aa _{ip} | ha | cropland available in each hexagon for each crop |
| Avehour _m | hour | average working hours of machinery in each month |
| DML ^{stor} _m | % | dry matter loss during storage |
| MTB ^k _i | hour ha ⁻¹ | machine time per ha for each machinery |
| λ | L Mg ⁻¹ | switchgrass-ethanol conversional rate |
| Q _m | L month ⁻¹ | monthly demand for ethanol |
| Loadwt | Mg per truck | tonnage of switchgrass delivered per truck |
| Nload | Mg ha ⁻¹ | nitrate loading of inorganic N leachate |
| C | mg L ⁻¹ | nitrogen concentration in the ambient groundwater |
| Variables | | |
| AH _{mip} | ha | ha of switchgrass harvested monthly |
| XTN _{mi} | Mg | switchgrass transported directly to the biorefinery |
| NXS _{mi} | Mg | switchgrass stored during harvest season |
| XS _{mi} | Mg | switchgrass stored monthly |
| XTO _{mi} | Mg | switchgrass transported from storage to the biorefinery |
| Num ^k _m | unit | number of equipment used during harvest |
| CBB _{cap,i} | unit | binary index of biorefinery selection |
| u | | upper limit of objective value |
| l | | lower limit of objective value |
| r | | range of objective value |

Table 7 Data Sources

| | Economic Cost | Grey water footprint |
|---|--|---|
| Land conversion from crop land to switchgrass | Opportunity cost: Crop yields: USDA SSURGO (U.S. Department of Agriculture Nature Resources Conservation Service 2012); Crop price and hectare: USDA NASS (U.S. Department of Agriculture 2014; U.S. Department of Agriculture 2011); Crop production cost: USDA ERS (U.S. Department of Agriculture 2014), POLYSIS(De La Torre Ugarte and Ray 2000) Switchgrass plantation: Yield: Jager et al. (Jager et al. 2010) Production and harvest Cost: Larson et al. (2010), University of Tennessee (2015) | Farm management of crops and switchgrass: University of Tennessee (2015) Nitrate leachate from soil-plant system: Daycent (Schimel et al. 2001); Nitrate level underground: USGS Water Resources (2015) |
| Production | Establishment: American Agricultural Economics Association (2000) Annual maintenance: American Society of Agricultural and Biological Engineers (2006) | |
| Harvest | Fuels and labors: University of Tennessee (2015): | |
| Storage | Covers and pallets: University of Tennessee (2015) | |
| Transportation | Trailer, fuel and labor: University of Tennessee (2015) | |

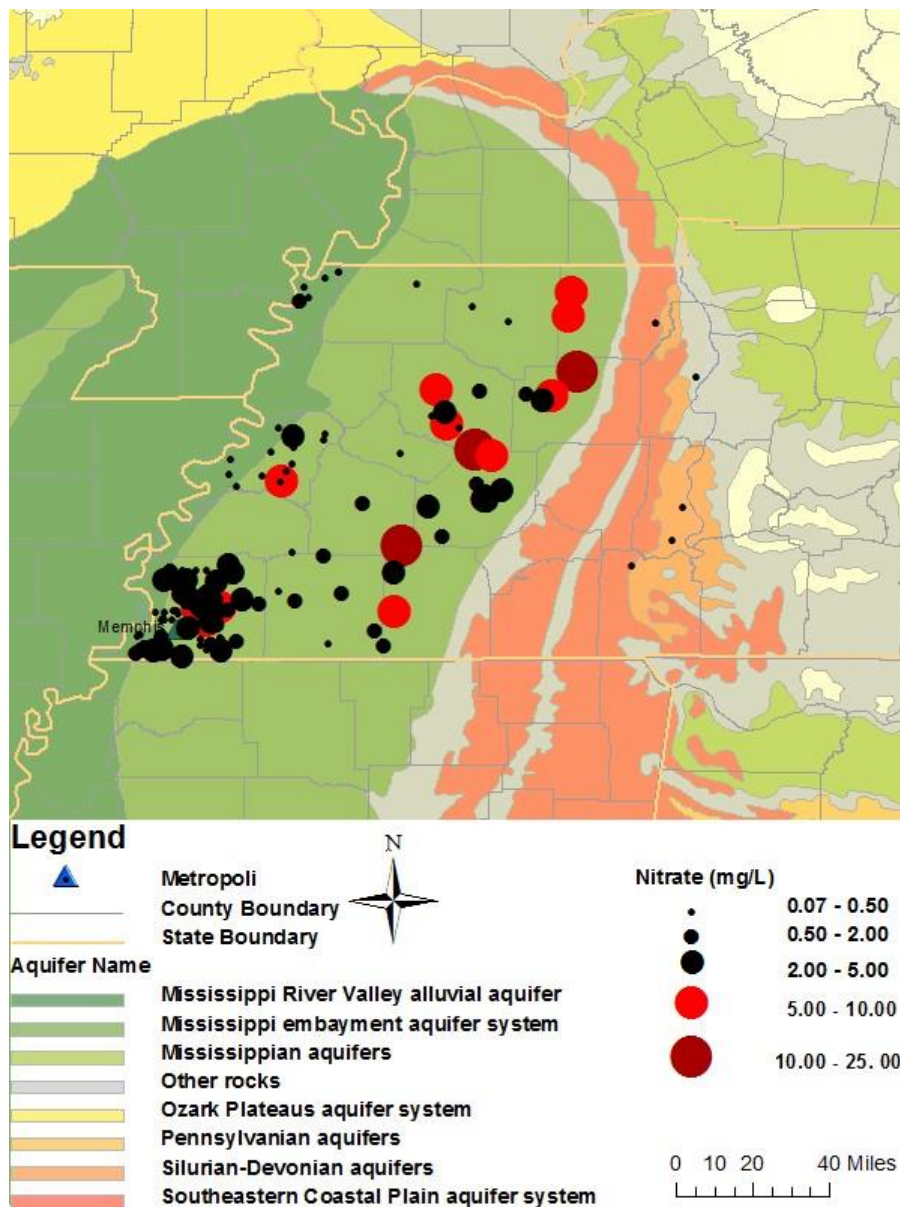
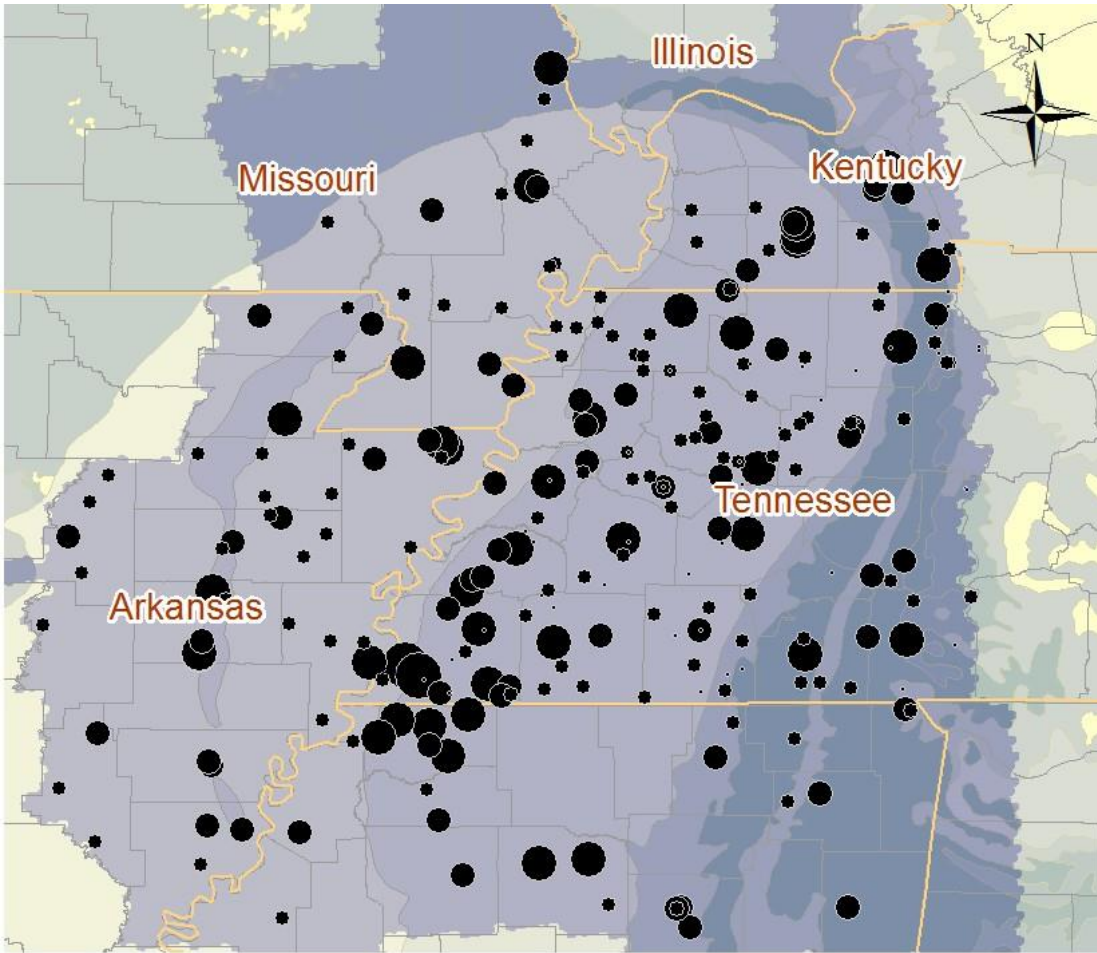


Figure 8 Observations of nitrate levels in west Tennessee (1980-2014)
 Data was from USGS Water Resources (2015)



Legend

| | |
|---------------------------------|---|
| Groundwater Water System | Study Area |
| Serving Population | Aquifer Name |
| · Very Small (0-500) | Mississippi River Valley alluvial aquifer |
| * Small (500-3,300) | Mississippi embayment aquifer system |
| ● Medium (3,301-10,000) | Mississippian aquifers |
| ● Large (10,001-100,000) | Other rocks |
| ● Very Large (100,000+) | Ozark Plateaus aquifer system |
| ▲ Metropoli | Pennsylvanian aquifers |
| — County Boundary | Silurian-Devonian aquifers |
| — State Boundary | Southeastern Coastal Plain aquifer system |
| | 0 20 40 80 Miles |

Figure 9 Groundwater System and served population of west Tennessee Aquifers
 Data was from US EPA (2015)

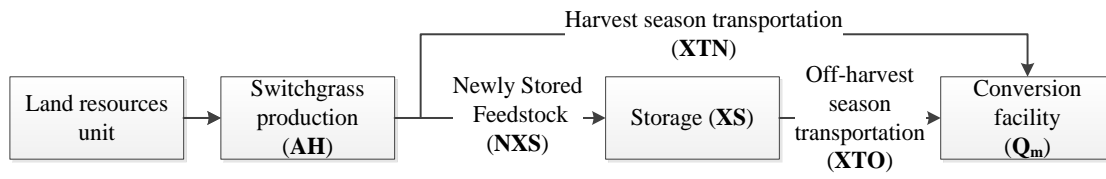


Figure 10 Flow diagram of switchgrass supply chain from field to biorefinery
 Data was from USGS Water Resources (2015)

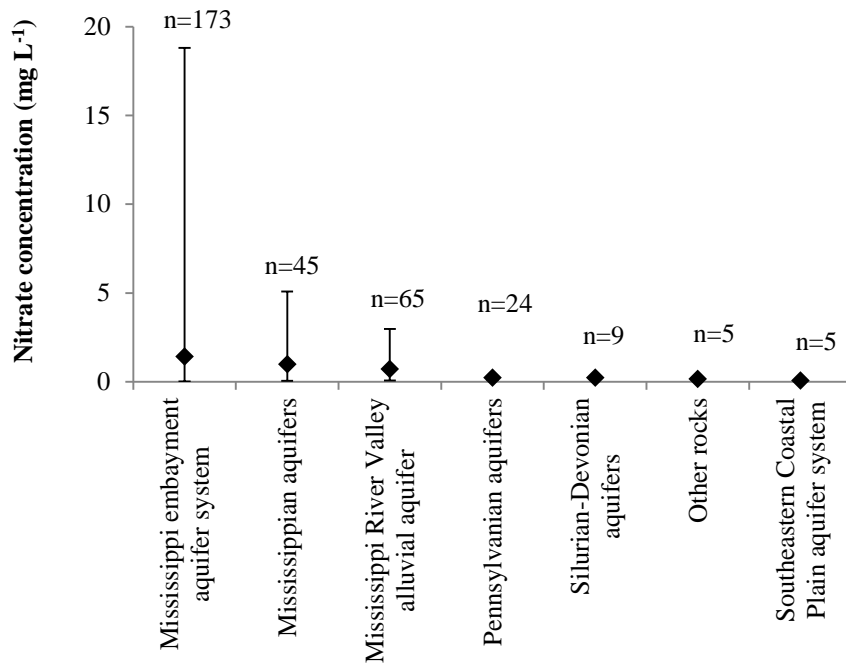


Figure 11 Observations of nitrate levels in west Tennessee aquifers (1980-2014)
 Note: n represent the number of observation in each aquifer

Observation data was from USGS Water Resources (2015)

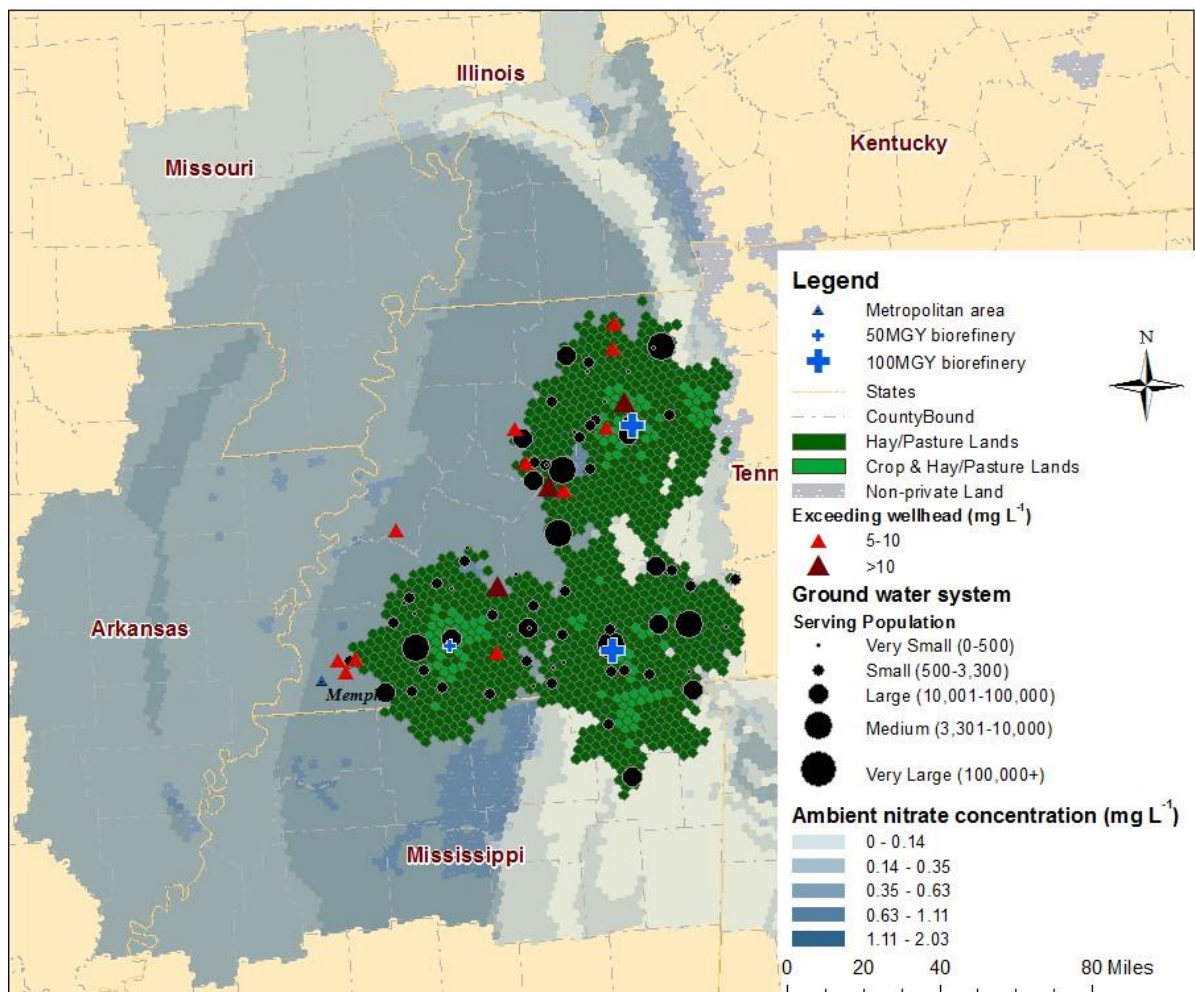


Figure 12 Placement of switchgrass supply chain for case costs minimization

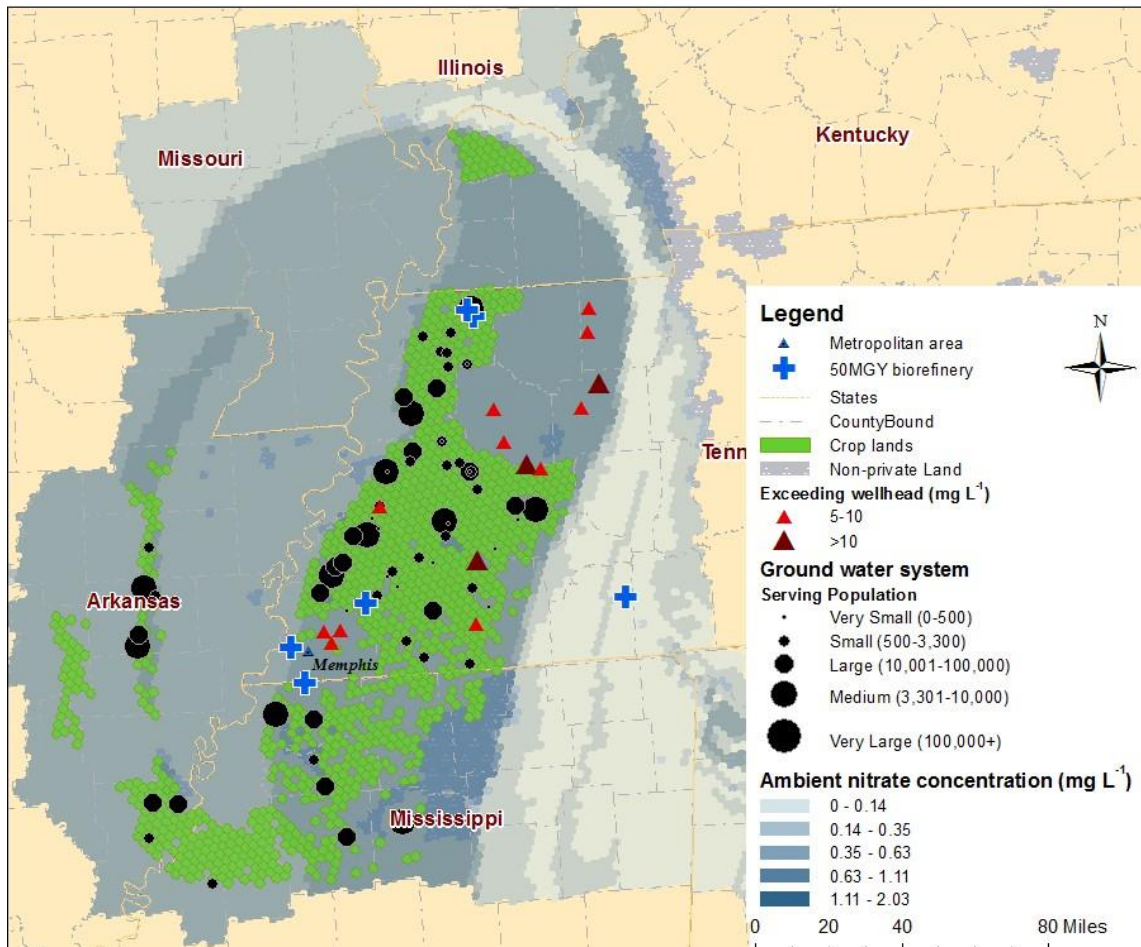


Figure 13 Placement of switchgrass supply chain for case *TGWF* minimization

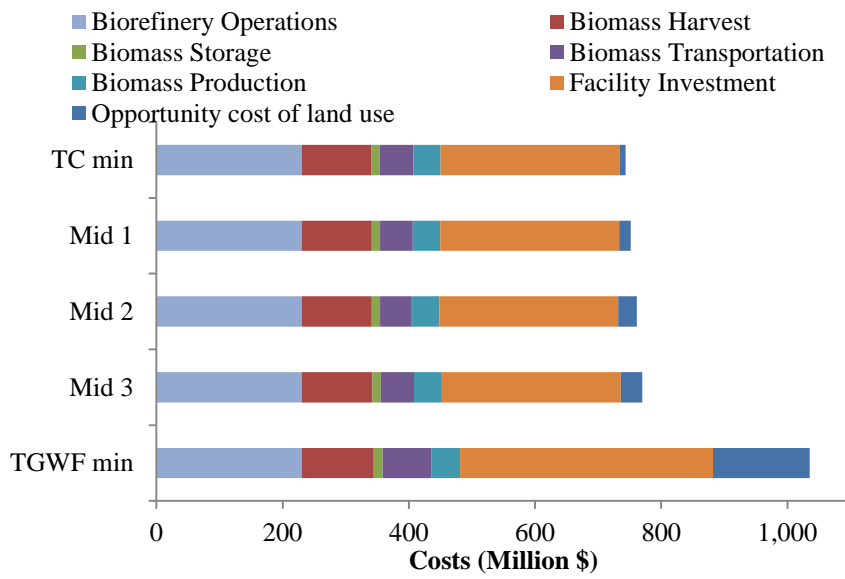


Figure 14 Itemized costs for discussed cases.

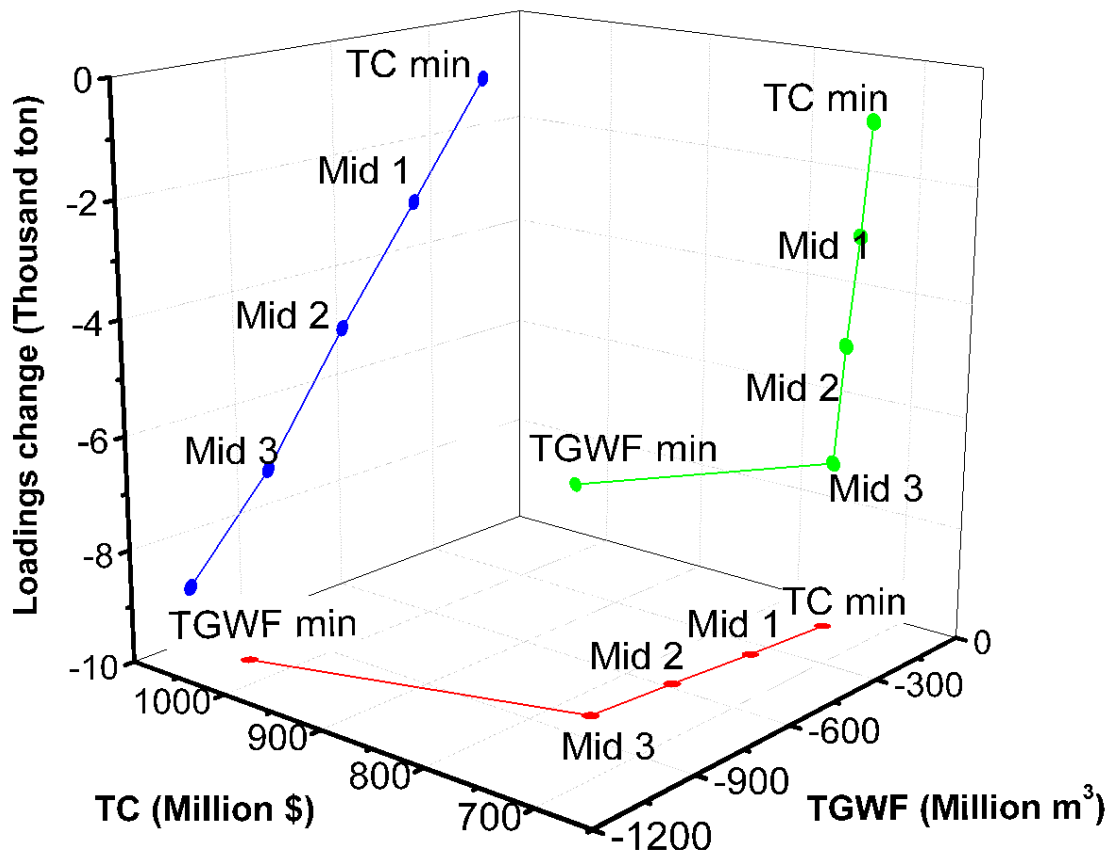


Figure 15 Tradeoff relations between *TC*, *TGWF*, and nitrate loading change.

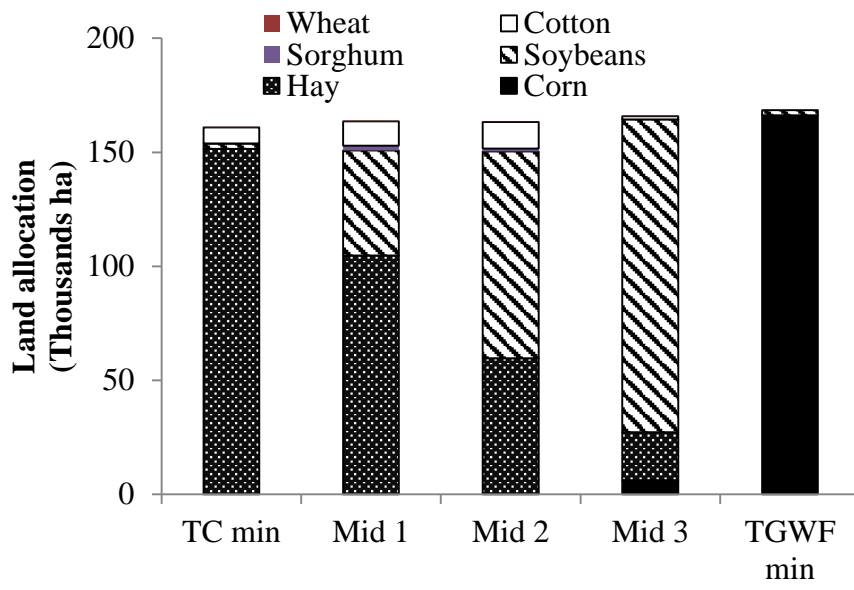


Figure 16 Land hectare allocation from crop types in each case

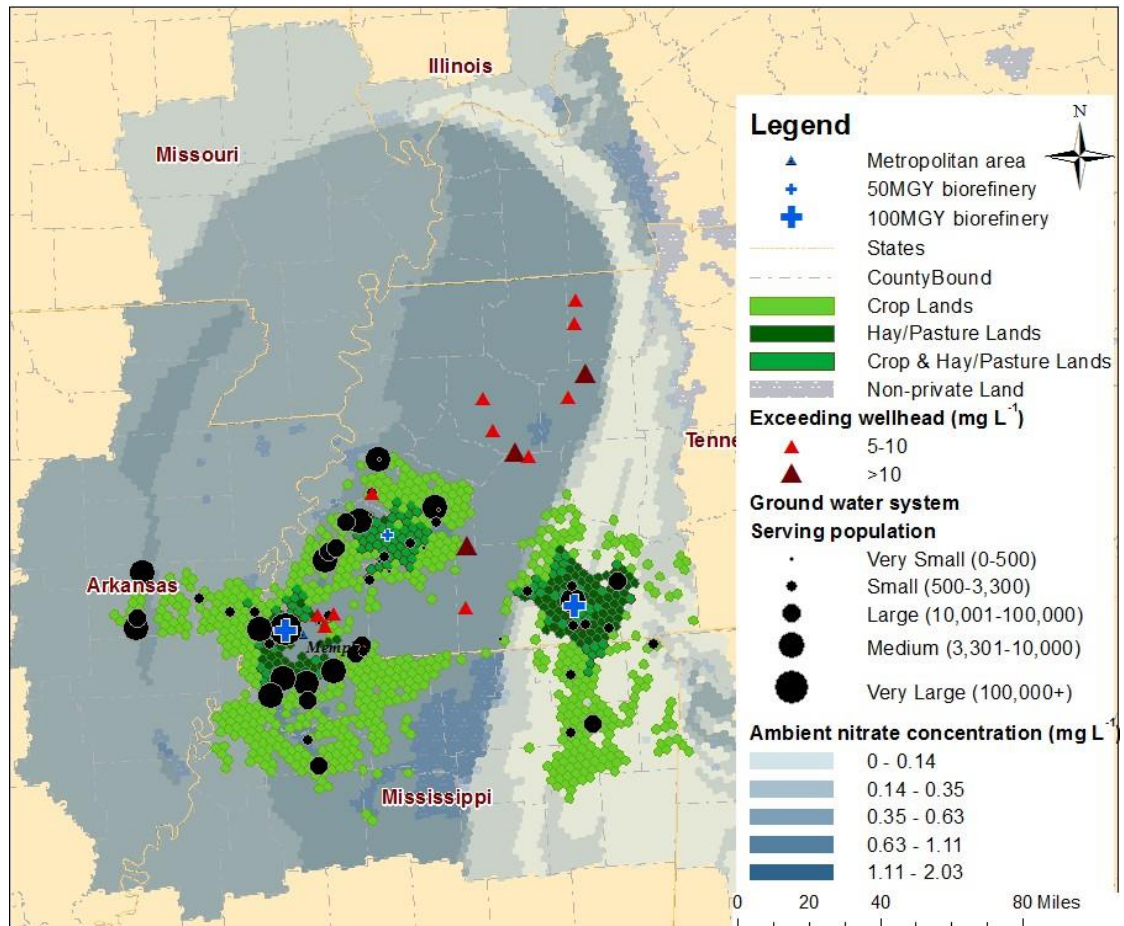


Figure 17 Placement of switchgrass supply chain for solution Mid3

CHAPTER IV CONCLUSIONS

This study examined the tradeoff relationship between the multi-objectives in designing the supply chain of switchgrass feedstock for bioenergy production in Tennessee. The first paper identified an efficient Pareto frontier surface that balances the objectives of minimization of industrial cost, GHG emissions, and soil erosion in the feedstock supply chain for a potential conversion facility. A multi-objective optimization model utilizing an improved augmented epsilon constraint method and the compromise solution method was applied to high-resolution spatial data in determining the optimal placement of the feedstock supply chains. The second paper focuses on the relation between economic cost and abated greywater footprint when supplying switchgrass for a cellulosic biofuel industry in west Tennessee, and the multiple conversion site selection for biorefineries using mixed integer linear program.

Multi-objective optimization model characterized with improved augmented epsilon constrains and compromise solution methods was applied to high-resolution spatial data to determine the optimal placement of the feedstock supply chains and associated economic and environmental performance.

Results of the first show that the type of agricultural land converted to switchgrass production is crucial to determining feedstock costs and environmental impacts of the feedstock supply chain. Converting crop lands to switchgrass incurred higher opportunity cost from land use change but stored more soil carbon and generated less soil erosion. The opportunity cost of converting hay and pasture lands to switchgrass was lower but likely released more soil GHG emissions and caused higher soil losses. A mix of crop, hay, and pasture lands could help to achieve the goal of integrating three objectives in the switchgrass supply chain.

Given the tradeoffs among minimization of feedstock costs, GHG emissions and soil erosion on the regional Pareto frontier surface, the imputed cost of abating GHG emissions

and soil erosion on was derived by the approach of marginal rate of substitution. The average imputed cost of abating GHG emissions and soil erosion on the Pareto frontier surface was \$2,378 and \$10, respectively. This finding suggests that soil erosion could be a more cost effective environmental criterion than GHG emissions in the development of a sustainable switchgrass supply chain in Tennessee. Also, the compromise solution location for the conversion facility generated 63% higher feedstock cost compared to the cost minimization location, but reduced soil erosion up to 70 times and GHG emissions by 27%. The derived imputed cost of abating GHG emissions and soil erosion in switchgrass supply chain in Tennessee could provide policy makers important information to expedite the development of a sustainable switchgrass biofuel industry.

Result from the second study found that in west Tennessee, where most of aquifers underwent groundwater quality deteriorating processes with pressures from both public water supply and agricultural use, the industrial bioenergy feedstock supply chain design was heavily influenced by the type of land converted for switchgrass production based on different objectives. Multiple sites selection on different capacity scales with allocation of surrounding feedstock land made it possible to accomplish the different goals. Findings that (1) The selections of hay/pasture lands with lowest opportunity determine the performance of total cost; (2) The economic crops of corn/soybeans affect significantly the GWF and nitrate loadings; (3) Higher nitrate concentration in Mississippi embayment aquifer system was prior to get converted for purpose of GWF minimization, were the basic logic behind this MILP model. Their tradeoff relation between feedstock costs and GWF therefore was also obtained by using the improved augmented ϵ -constraint method. GWF factor for switchgrass in the groundwater system was firstly obtained from this study. Both two methods of imputed average cost and compromise solution method that found Mid 3 case was the most preferred solution by balancing the two metrics. This optimal solution showed the relatively stable

imputed cost of decreasing GWF at \$0.94/m³ GWF, while increasing the total cost by 3.5%. However, the GWF was reduced by 6.5 times with additional 6.4 times less nitrate loading was discharged compared to the cost minimization case.

A limitation of this study is a screenshot case study based on the static database for mature switchgrass production. The potential impact from the climate variation and first few establishment years on crop yield was not considered in this study. Future studies could associate the uncertainty of weather, yield in supply chain design. More extensive work could incorporate several other policies, such as carbon tax, import tax on oil, export tax on corn to explore the economic, environmental effects of biofuels from policy.

This study provides important information for policy makers and researchers interested in the sustainable development of the cellulosic biofuel industry in the U.S. Many manage key factors from the interest of farmers were provided in this study concerning cropping types converted for specific environmental amenity purpose, the spatial distribution of feedstock area with land intensity, and the ambient cultivation environment response in determining the tradeoff relation between the feedstock costs and environmental performance of GHG emission, soil erosion, and grey water footprint. From the standpoint of decision maker, the balance between the economic and environmental externality metrics suggested a sustainable design of switchgrass supply chain. By implementing RFS2 plan and produce positive social externality in GHG reduction, soil quality improvement, and grey water footprint abatement, the final solution offers potential assurance of demand for high-cost biofuels and while it can contribute to energy security and economic benefits to US economy.

VITA

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