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Multifunctional Landscapes for Dedicated Bioenergy Crops Lead to Low-Carbon Market-Competitive Biofuels

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Abstract

Switchgrass is a promising feedstock for cellulosic biorefineries, due to its ability to maintain comparatively high biomass yields across a wide range of soil and climatic conditions. However, there is an incomplete understanding of the economic and environmental tradeoffs associated with cultivating switchgrass on low-productivity land for conversion to biofuels. This study surveys prior literature and demonstrates a new integrated assessment framework, including agroecological, ecosystem services valuation, technoeconomic, and life-cycle assessment models, to quantify and contextualize the economic and environmental impacts of switchgrass cultivation on marginal land with downstream conversion to biofuels. Monetizing and incorporating the value of ecosystem services, such as improved water quality benefits from nitrate and sediment reductions, climate change mitigation benefits from CO_2 emission reduction, and recreational and pollination benefits from increased biodiversity, the modeled multifunctional landscape reduces the ethanol production cost by 33.3-58.9 cents/L-gasoline-equivalent ($1.3-2.2/gge). Planting switchgrass in low productivity land improves soil health, resulting in the carbon footprint reduction credit of 12.8-20.2 gCO_{2e}/MJ. For an improved switchgrass-to-ethanol conversion pathway with the maximum benefits from ecosystem services, the minimum ethanol selling price and carbon footprint of ethanol, respectively, could reach to 31 cents/L-gasoline-equivalent (47% reduction relative to average gasoline price) and 3 gCO_{2e}/MJ (97% reduction relative to gasoline). This low carbon renewable ethanol leads to substantial State and/or Federal policy incentives (~$1/L-gasoline-equivalent) providing a large benefit to biorefinery operators, farmers, and the public as a whole.

Highlights

- Ecosystem services benefits reduced the delivered switchgrass cost by $29-104/bdt.
- Switchgrass grown on marginal land increased carbon sequestration by 0.1-0.36 MgC/ha.
- Ecosystem services benefits reduced ethanol selling price reduced by 20-55%.
- Carbon footprint of ethanol reduced by 44-81% with ecosystem services benefits.
- Biorefinery operators could make profit of 28 cents/L-gasoline-equivalent.

Keywords: Ecosystem services; Carbon credit, Switchgrass feedstock supply; Ionic liquid pretreatment; Techno-economic analysis; Lifecycle assessment

Word count: 9819

1. Introduction

A multifunctional landscape with an innovative bioenergy value-chain supports the bioeconomy, forestalls food-fuel conflicts, and provides ecosystem services that can mitigate climate change and contribute broadly to environmental sustainability [1,2]. Multifunctional landscapes refer to a diversified land use and complex land cover designed to provide a variety of environmental, social, and economic benefits [3]. Some examples of multifunctional landscapes include short rotation coppice willow production for bioenergy, switchgrass for ethanol, and eucalyptus for aviation fuel [4]. These landscapes produce biomass for biofuel production, as well as a number of other ecosystem services. Necessary conditions for the success of the bioeconomy are widespread adoption of bioenergy crops by farmers [5,6] and conversion of biomass to fuels and high-value products [7,8] by biorefineries at market-competitive costs. Economic returns to the farmers and biorefinery operators from biomass production largely determine the success of the value-chain [9]. However, the main focus has been on the production of biofuels or bioproducts and many of the ecosystem services provided by perennial bioenergy crops, such as nitrate and sediment reduction and increased soil carbon sequestration, have not been effectively monetized and internalized into the value chain. This raises the question how internalizing the ecosystem services value of bioenergy crops can impact the economics and carbon emissions of cellulosic biofuels. To answer this question, this study uses switchgrass as the exemplar feedstock and ethanol as a representative biofuel to integrate the value of a wide range of ecosystem services into a full biomass-to-biofuel model to better understand the impact on biorefinery economics and carbon emissions.

Switchgrass is a native North American high yielding bioenergy crop capable of generating multiple ecosystem services. Ecosystem services are those goods and services provided to people [10,11] by converting row crop land to switchgrass crops. This conversion generates several ecosystem services, including climate change mitigation, nutrient regulation, biodiversity conservation, and biomass production [12,13]. The ecosystem benefits offered by switchgrass are largely due to its higher levels of above and below ground biomass relative to conventional annual crops [13,14]. High yielding perennial bioenergy crops, such as switchgrass, accumulate more carbon in soil and lose less nitrogen when compared to annual crops like corn. The perennial crops can be rotated with corn and soybean where nutrients (C & N) can be used by annual crops to increase productivity[13,14]. Capturing and sequestering atmospheric carbon into soil supports climate change mitigation while improving soil health and productivity [4]. Strategic, large-scale cultivation of switchgrass (in the Mississippi River Basin) can retain nutrients (nitrates and phosphates) and sediments in soil and the resultant nutrient-loading reduction into water bodies increases the value of recreation such as fishing and swimming, decreases the water treatment costs, and reduces the size of the hypoxic area (for example in the Northern Gulf of Mexico) [15]. Prior studies highlight that converting annual marginal croplands to perennial native switchgrass restores the natural habitat impaired by row-cropping systems and the improved quality of habitat benefits arthropods, birds, and wildlife[4]. Increased biodiversity translates into multiple ecosystem services [16], for example increased pheasants and birds produce higher recreation value of the cropland itself and of the surrounding grasslands (hunting and birdwatching) [11]. Similarly, the nesting habitat, as well as foraging area provided by switchgrass for pollinators, supports pollinator population[17,18] and consequently increases fruit setting and crop yield in pollinator dependent crops. The abovementioned promising benefits of switchgrass enhance socioeconomic status of farmers, which increases the probability of adoption of switchgrass [19,20].

The ecosystem services benefits associated with biomass feedstock production and the biobased product utilization have not typically been included in prior techno-economic analyses (TEA) and life cycle assessments (LCA) of biomass-to-biofuel conversion pathways (Table 1). This study bridges these research gaps by (i) developing and demonstrating an integrated assessment framework for quantifying and evaluating the ecosystem services benefits of switchgrass using agroecosystem, technoeconomic and life-cycle assessment models; (ii) determining the impacts of ecosystem services on biofuel production cost and carbon footprint; and (iii) identifying the market competitive incentives to farmers to encourage switchgrass cultivation on low productive land (marginal land). This study considers one-pot, high-gravity ionic liquid-based biomass deconstruction and fermentation to ethanol as a model conversion process [21]. This study reports a stochastic minimum selling price and carbon footprint of ethanol with and without considering the value of ecosystem services.

2. Summary of prior studies and contributions of this study

A recent review [9] highlights the overarching needs of a rigorous analysis through a combination of agroecosystem, TEA, and LCA models to provide the overall environmental, social, and economic sustainability metrics for the biofuel systems. Achieving these goals requires quantification, monetization, and incorporation of ecosystem services to biomass-to-biofuels production system analysis. Several prior studies focused individually either on TEA and LCA (Table 1) or the agroecosystem of multifunctional landscape (Table 2) or only ecosystem services valuations [4,11,22]. Our primary contribution is the demonstration of an integrated assessment of a biofuel production system, including both upstream (feedstock production) and downstream (conversion to biofuel), using a set of agroecosystems, ecosystem service valuation, and TEA/LCA modeling framework.

Agroecosystem models are used to quantify environmental parameters under different scenarios (land use, management and climate), which are then converted to the environmental services. Recent review of the literature [23–26] shows multiple environmental indicators and their combination can be used to quantify the ecosystem services. However, earlier studies lack inclusion of different promising indicators for quantifying ecosystem services (Table 2). Here, this study used process-based models and existing literature to evaluate the ecosystem services using multiple environmental indicators, including the nutrient loss in water and soil, losses with air emission, recreational benefits and biodiversity.

Recent reviews and analysis on TEA and LCA of thermochemical conversion pathways [27–29] biochemical conversion pathways [30–33], and both of these pathways [34–36] provide a summary of the extensive research conducted in the first two decades of the 21st century. Some other reviews highlighted inconsistency in methodological approaches of environmental impacts analysis [23,24] and discrepancy in estimated production costs [25] of biofuel. However, none of these past studies have fully incorporated ecosystem services values for determining biofuels production costs and their carbon footprints. To address this knowledge gap, a recent study [37] has determined ethanol production cost and carbon footprint considering switchgrass biomass feedstock growing in the heterogeneous landscape around the biorefinery. However, this study only incorporated the soil organic carbon (SOC) sequestration benefits and determined biorefinery process costs by normalizing capital and operating costs reported in prior TEA studies. Not developing a detailed process model for the downstream conversion process results in a speculative cost and carbon footprint of biofuel (limitations acknowledged by the authors themselves [24]) because the capital and operating costs, as well as process energy consumption, are not linearly dependent on the size of biorefinery. Another study [38] uses a mixed integer linear programming model to optimize switchgrass feedstock supply cost considering marginal land; however, the downstream conversion process is not fully evaluated. Table 1 summarizes a few prior TEA and LCA studies on switchgrass-based ethanol production systems. Other TEA/LCA studies[39–42] also highlight the impacts of feedstock and conversion processes on the biofuel production cost and associated GHG emissions. All prior studies provided important information in this field; however, most of them are focused on optimizing production pathways without considering ecosystem services benefits.

While TEA and LCA studies of an integrated system combining ecosystem services and biofuel production pathways are limited (Table 1), there is significant interest in evaluating ecosystem services benefits (Table 2). The majority of the studies on ecosystem services quantification are associated with water quality and quantity [37–41], soil carbon change [42,43], and biodiversity [1,44]. The majority of studies on the valuation of ecosystem services are focused on potential payment for increasing ecosystem services, such as water quality improvement [45,46] and soil carbon sequestration attributed to replacing row crops with bioenergy crops. This study estimated the location specific value of the ecosystem services due to conversion of marginal land under corn-soybean rotation to switchgrass in the study [8]. The estimated ecosystem services values are used in TEA and LCA to assess their minimal and aggregated impacts. A comprehensive list of studies on quantification and the valuation of ecosystem services is provided in Table 2.

This study seeks to address these modeling and research gaps by developing an integrated modeling approach which combines biophysical models, ecosystem services valuation, TEA, and LCA models to perform rigorous cost and carbon footprint analyses. This study used the DayCENT and RUSLE process-based models to quantify the biomass production and soil erosion, as well as nitrate retention and carbon sequestration by converting corn-soy crop land to switchgrass. The ecosystem services generated by the multifunctional landscape is then quantified using the benefit transfer method. TEA and LCA tools are used to quantify the production cost and carbon footprint reductions considering ethanol as a representative biofuel. This study determines the threshold values of ecosystem services required to reach cost parity with gasoline and the net zero-carbon ethanol at the present state-of-the-art and for the optimal future case considering near theoretical limit of the switchgrass-to-ethanol conversion rate. This study also demonstrates the important ecosystem service indicators that significantly influence the production cost and carbon footprint of ethanol. The probability distribution of the production cost and carbon footprint of ethanol due to variabilities present in ecosystem service indicators are also presented in this study. This study further quantifies the minimum selling price of ethanol with California's low carbon fuel standard (LCFS) credits and Renewable Identification Numbers (RINs) under the Renewable Fuel Standard (RFS).

Table 1. Summary of prior studies on techno-economic analysis and lifecycle assessment of Switchgrass-based bioethanol production systems and contributions of this study

Description	Prior studies											This study
	[43]	[44]	[45]	[46]	[38]	[47]	[48]	[49]	[37]	[50]	[51]	
Switchgrass feedstock cost ($/tonne)	-	130	-	100	188	64 to 68	30	-	113 to 124$^{\beta}$	-	76.6	128.2$^{\beta}$
Biorefinery size (tonne/day)	2000	2000	-	-	1839 to 3679$^{\phi}$	1152 to 3437$^{\phi}$	250	738	766	2000	2000	2000
Biorefinery operating hours (h) per year	8410	8406	-	-	7920$^{\phi}$	7920$^{\phi}$	8400	8400	7920$^{\phi}$	-	8406	7920
Pretreatment method	AFEX, DA	DA, AFEX	-	DA	-	-	Hot water	DA	DA	DA	Multiple$^{\omega}$	IL
Biofuel yield (L/tonne-biomass)	318-439	274-275	330	400	313	250 to 417	264	243	376	330	185 to 282	302
Analysis year	2015	2012	2014	2005	2013	2012	2019	2015	2016	2005	2011	2020
CAPEX ($MM)	-	-				190 to 400		-	-	-	325 to 385	423
MSP ($/L)	-	1.3-1.4		0.54	0.59	0.44 to 0.72	0.84	-	0.72 to 0.75	-	0.61 to 1.1	-0.02 to 1.7
Sensitivity analysis		√					√	√	√		√	√
Uncertainty analysis		√										√
Biomass farming on marginal land					√				√			√
Impact of ecosystem services												√
Quantified LCFS credits									√			√
GWP (gCO2e/MJ)	8-17	12-33	33					-9 to 80	22	-11		-38.8
Impact of N_2O emission	√							√	√			√
Impact of dLUCs	√		√					√	√			√

WSG = Whole sweet sorghum (grain, juice, and bagasse); SWG = Switchgrass;

$^{\phi}$Assumed 330 days of operation/year

$^{\beta}$Excluding social cost of carbon

$^{\omega}$Ammonia fiber explosion (AFEX), dilute acid (DA), Lime, liquid hot water, soaking in aqueous ammonia, SO_2

3. Materials and Method

3.1 Study Area and Modeling Overview

The modeled biorefinery with the nameplate capacity of 199.6 million liters of ethanol per year (2000 bone-dry-metric ton of switchgrass feedstock per day) is considered to be located in Dwight, Illinois, 80 miles away from Chicago, IL (Figure 1). This location is selected considering availability of the marginal land producing the required amount of biomass feedstock, access to road networks (for minimizing transportation cost and associated carbon footprint), vicinity to water resources, and vicinity to cities (for reducing ethanol transport distance). There is also a proposed ethanol facility (Illinois Valley Ethanol, LLC) with a nameplate capacity of 446.7 million liters per year (118 million gallons per year or about 4482 bone-dry-metric ton of switchgrass feedstock per day). In 2021, the United States (U.S.) produced about 56.78 billion liters (15 billion gallons) of ethanol [52], which requires more than

294 ethanol facilities of the same size considered for modeling in this study. The production volume of ethanol is sufficient to fully meet the 10 vol% blending with the U.S. convention gasoline demand (134.83 billion gallons were consumed in 2021 [52]).

The modeled biorefinery sourced the required switchgrass feedstock from the fuel-shed area (buffer zone) of 112.6 km (70 miles) around the site identified in this study (Figure 1). To fully evaluate the impacts of ecosystem services benefits of growing switchgrass in marginal land around the biorefinery, an integrated assessment framework was developed that couples agro-ecological models, ecosystem services valuation, feedstock production and supply, and biorefinery process model (Figure 2). The following sections provide the detailed description of the methods used in each section of the integrated assessment framework presented in Figure 2.

Table 2. Summary of prior studies on ecosystem services analysis and quantification

Region of Study (cite)	Analysis Year	Soil carbon sequestration	N_2O emission	Sediment reduction	Nitrate reduction	Nutrient reduction	Flow regime	Water-based Recreation	Biodiversity				References
									Pollinators	Pest Control	Bird Watching	Hunting	
Ecosystem Service analysis based on environmental indicators													
Big Creek Watershed, IL	2005			√	√	√	√						[23]
Nansihu Lake basin, China	2020			√	√	√	√						[53]
Mexico city, Mexico	2015			√	√	√	√		√		√		[54]
San Pedro River, Arizona	2013	√					√						[25]
Beaver River watershed, Rhode Island	2013				√	√	√						[24]
Broye catchment, Switzerland	2018	√	√	√	√	√	√						[55]
Global	2008	√					√						[26]
Dwight, Illinois	2020	√	√	√	√	√	√	√	√		√	√	This study
Studies on Ecosystem services valuation													
Chesapeake Bay	2018				\$13.29 kg^{-1}								[56]
Chesapeake Bay	2019				\$13.0-14.04/kg								[57]
US Northern Plains	2001	\$12-500/MgC											[58]
Illinois	2019	\$61.07/ha		\$4.35/Mg	\$38.37/kg			\$3.45-8.21/ha	NA		\$42.36/ha	\$9.97/ha	[11]
Dwight, Illinois	2020	\$15-123/$MgCO_{2e}$		\$3-5/Mg	\$13-30/kg			\$6-8/ha	\$24-85/ha	\$46/ha	\$11/ha	\$10/ha	This study

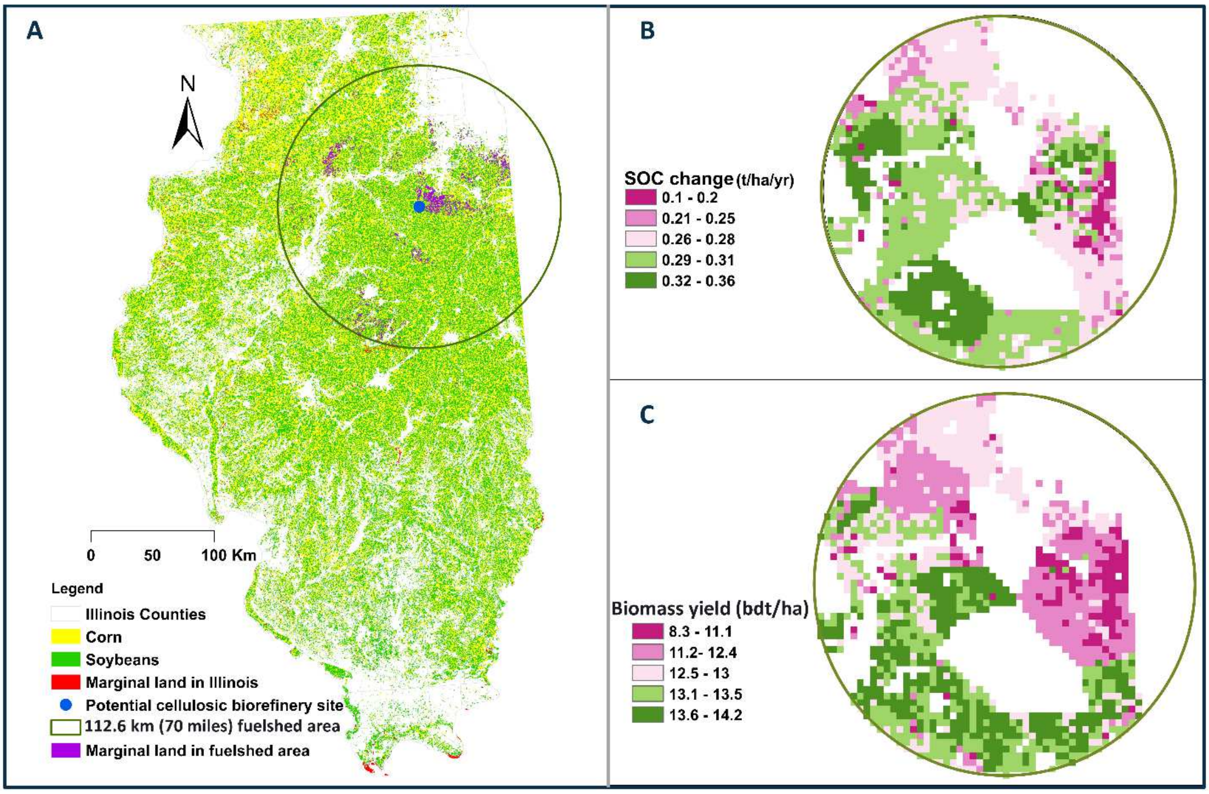


Figure 1. An overview of study area (A), soil organic carbon sequestration potential (B), and Switchgrass yield (C). ‘bdt’ represents bone-dry metric ton.

3.2 Biophysical modeling

This study identified marginal land within the fuel-shed area (Figure 1-A) based on soil and environmental properties. The soil carbon emission and biomass production were calculated using a process-based agroecosystem model (DAYCENT), and the erosion and nitrate losses were determined using the revised universal soil loss equation and methods reported in prior studies [59,60]. DAYCENT is a process-based agroecosystem model that simulates in daily time-step, the exchanges of soil nutrients (carbon, nitrogen, and sulfur) between the atmosphere and terrestrial ecosystems, as well as other soil water and temperature processes [61]. DAYCENT has been widely used to simulate the impact of land management and climate on biogeochemical cycles and predict soil carbon changes, GHG emissions, and plant productivity [62–64].

3.2.1 Identification of marginal and adjacent lands

The definition of marginal land is not consistent across the literature [65]. This study used the USDA's Soil Survey Geographic Database and identified land capability classes 5–8 as marginal lands. This approach uses soil properties and biophysical environmental properties to classify U.S. lands into eight distinct categories. As the number increases from 1 to 8, the land's suitability for vegetation growth decreases [65]. The acreage of marginal land under row crop (corn and soybean) cultivation was identified using cropland data layer map [66]. These areas were considered eligible for conversion from row crops to switchgrass.

3.2.2 Agroecosystem modeling to simulate biomass yield and emissions

The study area was divided into 4-km grid cells and the simulation was conducted at the centroid of the grid. A 4-km grid was selected considering the heterogeneity of soil, weather, computational efficiency, and modeling uncertainty. Grid scale simulation is commonly used to represent the processes at large spatial scale due to ease of computing [67]. Note that the DAYCENT model is designed to explicitly run at a point scale, which does not include any horizontal connection among the grids. To initialize the model prior to simulating switchgrass, the steady state soil organic carbon levels and the plant productivity under native vegetation over a 4000-year spin-up period were estimated. Region specific grass type based on earlier study [68] was used to simulate the equilibrium soil organic matter pools by using different grasses based on the region. For the historical simulation after the spin-up period, land use and management history were compiled from multiple data sources [68,69]. Historical management from the beginning of the agricultural revolution to modern agriculture was simulated with crop rotation and a management scheme compiled at the Major Land Resource Area level from different historical data sources [69]. Modern day agriculture management representation was based on analysis of multi-year National Land Cover Database analysis. The historical database was used to represent the average annual nitrogen fertilizer rates for each of the agricultural crops [70]. Switchgrass was cultivated in 2008 to study the impact of decade-long cultivation of the bioenergy crop. The assumption for large scale cultivation of switchgrass includes use of heat unit based agricultural management, same cultivar across the location, rainfed condition, common fertilizer application rate of 70 kg N per ha. The detailed methodology on large scale implementation of DAYCENT model can be found in Gautam et. al 2020 [64].

3.2.3 Sediment loss calculation using RUSLE

The potential soil loss was determined using the Revised Universal Soil Loss equation (RUSLE) considering soil properties, local climatic condition, land use and management practices implemented in the study area. The mathematical representation of the RUSLE [71] is given in Eq. 1 below.

$$A = R * K * LS * C * P \qquad \text{Eq. 1}$$

where, A is the spatial and temporal average soil loss in ton ha^{-1} yr^{-1}, R is the rainfall erosivity factor, K is the soil erodibility factor, LS is the topographic factor representing slope and steepness, C is the cover management and P is the conversion practice factor.

The rainfall erosivity factor was based on an Illinois R factor map from the U.S. Department of agriculture [72]. The soil erodibility factors were based on universal soil loss equation [73]. The LS factor represents the effect of slope length and steepness, erosion (rill and inter rill) by water, and is the ratio of expected soil loss from a field slope relative to the original USLE plot [74]. The management and supporting practice factors were based on a multi-location switchgrass and corn soybean study [60].

3.3 Valuation of Ecosystem Services

Ecosystem services are categorized as primary and secondary ecosystem services based on their trading markets, impacts, quantification methods, and associated uncertainties. The ecosystem services indicators, including nitrate, sediment, and carbon are categorized as a primary ecosystem services because these indicators have a market for trading, could have a large cost and environmental impacts, are quantified using biophysical models, and have a lower uncertainty in their quantification. Other ecosystem services indicators considered in this study, including water-based recreation, wildlife viewing, pheasant hunting, and pollination services, are categorized as secondary ecosystem services because these indicators do not have a well-established market for trading, are quantified using literature data, and have a higher uncertainty in their quantification. Nonetheless, the benefit transfer method was used for the valuation of ecosystem services generated by bioenergy crops. The benefit transfer method is used to predict the change in consumer welfare for a policy site using results from preexisting primary research at similar study site(s) [75]. As the benefit transfer method relies on earlier studies to predict the economic value, the method has some challenges. Some errors may be introduced during the transfer process because of the differences in environmental and economic factors of study site and policy site. In addition to that, the differences in the measures of welfare-change at study site and policy site can also introduce error [76,77]. This method has been widely used to estimate the values of ecosystem services under various scenarios [78–80]. In order to minimize the errors in the estimated value for our study area in Dwight, Illinois, we used the economic information from the studies conducted at the same or similar geographic areas, which valuated the ecosystem services of land use conversion from corn and soybean to switchgrass.

The value of ecosystem services (V_{ES}) attributed to the land use change from row crops (corn and soybean) to bioenergy crop (switchgrass) was determined using the change in quantity of the ecosystem services indicator and value per unit change in ecosystem services (Eq. 2).

$$V_{ES} = \sum_{j=1}^{n} \Big((Q_{ESI_{sg}} - Q_{ESI_{rc}})_j * v_j \Big)_i \qquad Eq. 2$$

where Q_{ESI} is the quantity of ecosystem services indicator, *sg* is switchgrass crop, *rc* is row crops, *j* is the ecosystem services that range from 1 to n, and *i* is the land area used for analysis, v_j is the value per unit change in ecosystem services *j*.

In order to estimate the ecosystem services value of climate change mitigation V_{cm}, the following equation (Eq. 3) was used.

$$V_{cm} = \left[\frac{44}{12 * 10}\sum_{t=1}^{10}\left(Q_{SOC_{sg}} - Q_{SOC_{rc}}\right)_t\right] * v_{cc} \; Eq.3$$

where, the change in the quantity of soil carbon sequestration $(Q_{SOC_{sg}} - Q_{SOC_{rc}})$ is converted to climate regulating service, that is equivalent to a carbon credit (metric ton equivalent of CO_2) by using the molecular weight of carbon dioxide and atomic weight of carbon. The number of carbon credits generated per ha is then monetized by using the social cost of carbon (SCC). The SCC is estimated by Stiglitz, Stern, Hepburn [79] is \$40-80 $MTon^{-1}CO_2e$ for 2020 to \$50-100 $MTon^{-1}CO_2e$ for 2030. This study uses various price ranges to examine the impacts of carbon credits at a range of prices (Table 3 and Supporting Information (SI)-Table S11).

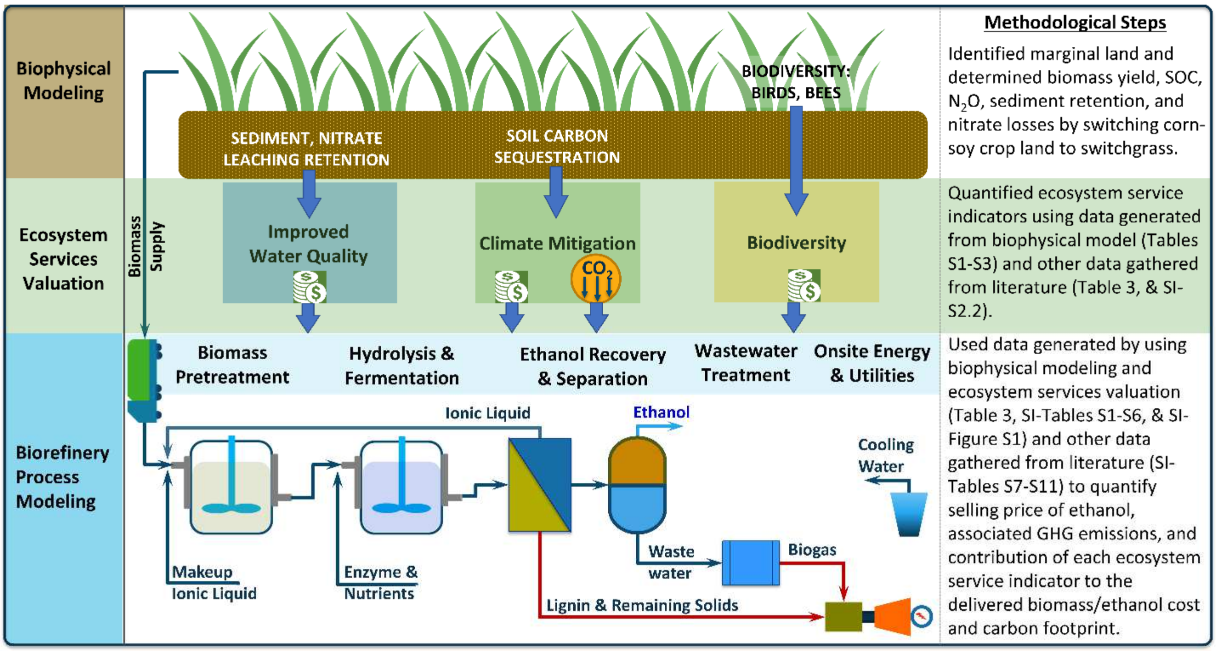
For the valuation of nutrient regulation (nitrate and sediment loss reduction), and biodiversity (wildlife hunting and bird watching, pollination services) conservation, the economic information and values from Mishra et al. [8] were used.. Following Mishra et al. [8], the information from Woodbury et al. [56] was used to calculate the value of nitrate loss reduction due to bioenergy crop as \$13.29 – 29.75 kg^{-1} nitrate. The study [37] estimated the value of N reduction on a potential nutrient credit trading system. This study estimated the value of sediment retention for 23 Illinois counties using the county level benefit per ton of sediment loss reduction through conservation practice from [80]. The study [65] calculated the values of sediment loss reduction using a number of benefits from such sediment reduction. This study used the increase in recreational value (fishing, swimming) due to conversion of row cropland into a conservation reserve program estimated by Baylis et al. [76] to estimate the water based recreational benefits downstream such as fishing, swimming and boating following [8]. In order to estimate the increase in the value of wildlife viewing and hunting we used the values estimated by Feather et al.[81]. Feather et al. [81] modeled the increase in number of trips taken for wildlife viewing and hunting to various landscape types and estimated the corresponding increase in consumer surplus attributed to those trips. The estimated increase in the value of wildlife viewing and hunting attributed to the conversion of row crop to conservation reserve area closely match with the benefits of the introduction of bioenergy crops in an intensively cropped landscape. The values presented in Table 2 are the values adjusted to 2019 U.S. Dollars.

The value of pollination services provided by switchgrass is estimated using the method following Winfree et al. [82] and Mishra et al. [22]. The method uses the pollination dependency ratio of crops for their yields, yields of crops, crops prices, and costs of production to estimate the value of crop loss without pollination services. As the value of pollination is realized at the sites with low abundance of pollinator populations, this study identified the areas with low pollinator population abundance (using the data from [81] and [83]). Then identified the areas under high pollination dependent crops within the pollinators foraging distance (3.2 km buffer zone [84,85]). The study region in Illinois has few pollinator dependent crops such as pumpkin, squash, cantaloupes, soybean, which have essential to moderate requirements for insect pollinators. Among them, only soybean crop acreage was higher than 100 ha. The estimated value of pollination provided by switchgrass crop for soybean crop is \$58.82/ha (\$23.60 – 85.17/ha), which is further discussed in SI-S2.

The certainty in generation of these ecosystem services depends on both the biophysical factors (the ecosystem service indicators) as well as the realization of the human utility or welfare due to the change in the quantity of the ecosystem service indicators. Changes in soil organic carbon, sediments, and nitrates and their ecosystem service values are determined using established models and are widely accepted in literature. Only a limited number of studies have quantified impacts of switchgrass on pollinators, bird watching and hunting. Therefore, we categorize these ecosystem services as secondary ecosystem service benefits of switchgrass crop.

3.4 Biorefinery process model

The biorefinery process model was developed by combining the switchgrass feedstock supply system with the downstream ethanol conversion process. The feedstock supply system was modeled to deliver 660,000 bone-dry-metric ton (bdt) of switchgrass feedstock per year (2000 bdt/day) at the pretreatment reactor throat. This study considered one-pot, high-gravity ionic liquid based biomass deconstruction and subsequent ethanol fermentation processes [21,86]. A conventional biorefinery process model was considered for analysis in this study where the carbohydrates fraction is routed to ethanol production and the lignin fraction is sent to the boiler to generate process heat and electricity. The overall biomass to ethanol conversion rate for the baseline scenario is 302 L/bdt, which is dependent on several parameters, including the total carbohydrates content in switchgrass, sugar yields during biomass deconstruction process, sugar to ethanol conversion rate, and ethanol recovery rate (Table 3). The detailed discussion of the different components/stages of the biomass supply chain [87,88], ionic liquid-based ethanol production process [21,89] are documented in prior studies. The following sections briefly discuss the modeling approach, data sources and assumptions made in this study.



Methodological Steps

Identified marginal land and determined biomass yield, SOC, N_2O, sediment retention, and nitrate losses by switching corn-soy crop land to switchgrass.

Quantified ecosystem service indicators using data generated from biophysical model (Tables S1-S3) and other data gathered from literature (Table 3, & SI-S2.2).

Used data generated by using biophysical modeling and ecosystem services valuation (Table 3, SI-Tables S1-S6, & SI-Figure S1) and other data gathered from literature (SI-Tables S7-S11) to quantify selling price of ethanol, associated GHG emissions, and contribution of each ecosystem service indicator to the delivered biomass/ethanol cost and carbon footprint.

Figure 2. An integrated modeling framework considered for determining the impacts of ecosystem services on the production cost and carbon footprint of ethanol. This integrates biophysical modeling, ecosystem services valuation, and biorefinery process models from field-to-ethanol production. Ethanol is considered as a representative biofuel. SOC = Soil carbon sequestration and SI = Supporting Information.

3.4.1 Switchgrass feedstock production and supply model

The switchgrass biomass feedstock production and supply model was developed considering prior switchgrass supply chain models [87,88] and other notable commercial-scale lignocellulosic biomass feedstock supply models developed by Oak Ridge National Laboratory (ORNL) [90] and Idaho National Laboratory (INL) [91]. Our model captures the variabilities associated with different input parameters (SI-Tables S7-S9) and provides the probabilistic cost and GHG emissions associated with each stage of the entire switchgrass production and supply chain. The different stages of the biomass supply chain considered in this study include switchgrass cultivation, harvesting (windrowing, baling, and stacking), transportation of bales from the field to the biorefinery, and outdoor storage outside the biorefinery. The results obtained from the biophysical modeling, including biomass yield and the SOC sequestration, were major inputs to the feedstock production and supply model.

As stated above, this study includes switchgrass cultivation cost and associated GHG emissions, which are often excluded for corn stover feedstock supply chain analysis [91] considering residue/waste or are entirely allocated to corn grain. Non-grain bioenergy crops, such as switchgrass, do not have such allocation privilege. The required switchgrass cultivation area was determined considering the biorefinery size of 2000 bdt/day, safety stock of 12.5% (assumed feedstock for 45 days [87]), dry matter losses of the entire supply chain, on average, of 11.6%

[92–95], moisture content, on average, of 20.4% [92,96–98], and switchgrass yield (Figure 1-C) in the study area, on average, of 12.7 bdt/ha. The modeled switchgrass production system includes land rent, establishment cost and materials (plant seed and fuel) as well as fertilizer, herbicides, and lime applications (SI-Table S1). The detailed methods and mathematical equations to determine capital and operating costs, as well as material and energy consumptions, are available in prior studies [90,91].

Switchgrass feedstock harvesting includes windrowing, baling, and stacking of bales at the field edge. This study considered large rectangular bales (2.43m x 1.17m x 0.97m [96,99,100]) with an average bulk density of 171.3 kg/m^3 [90,92,96,99]. The productivity, field efficiency, labor hour, and fuel consumption of windrower, baler, and stacker (SI-Table S2) are consistent with prior studies[90,91]. The detailed methods and mathematical equations to determine capital and operating resources are documented in prior studies [90,91].

The modeled transportation system includes a loader for loading switchgrass bales at the field edge and unloading them at the storage unit co-located with the biorefinery, as well as a 5-axle tractor-semitrailer (SI-Table S3). This truck can transport as much as 36 bales/trip [91] due to the Federal size limit. The biorefinery sourced switchgrass feedstock growing in the marginal land around the biorefinery with radial distance of as much as 112.6 km (70 miles) (Figure 1-A). The available marginal land or a land utilization factor (a ratio of switchgrass growing land and total area around the biorefinery) determined from the agro-ecosystem modeling was used to determine radial feedstock transport distance. The actual trucking distance was determined by multiplying the radial distance by the road winding factor (a ratio of total road length and radial biomass supply distance). The road winding factor in the study area was estimated to be in the range of 1.1 to 1.4 (an average value of 1.3).

Year-round biomass feedstock storage is required due to a short harvesting window of about 69 days [92,96,100]. This study considered an outdoor switchgrass feedstock storage unit, which was assumed to be co-located with the biorefinery. The modeled storage unit used tarp and gravel to protect bales from rain and moisture seepage from ground, respectively. The detailed methods to estimate the storage cost [91] and associated GHG emissions [101] are provided in the previous studies.

Table 3. Major input parameters used in techno-economic analysis and lifecycle assessment

Parameters	Units	Baseline	Optimistic	References
Ecosystem Service Indicators				
Switchgrass yield	bdt/ha	12.7	14.2	This study
SOC sequestration	$MgCO_{2e}$/ha	1.07	1.43	This study
Nitrate reduction	kg/ha	23.0	27.4	This study
Sediment reduction	kg/ha	1532.0	6990.0	This study
Value of Ecosystem Services				
Climate regulation (SOC)	$/MgCO_2e$	43	123	[79,102]
Nutrient regulation (Nitrate loss reduction)	$/kg	21.5	29.8	[37]
Nutrient regulation (Sediment loss reduction)	$/Mg	2.9	4.9	[65]
Recreational values (Water-based recreation)	$/ha	5.8	8.2	[66]
Recreational values (Biodiversity – Wildlife viewing)	$/ha	42.4	42.4	[67]
Recreational values (Biodiversity – Pheasant hunting)	$/ha	10.0	10.0	[67]
Recreational values (Biodiversity –Value of pollination services)	$/ha	58.8	85.2	This study

Contd.

Table 3. Contd.

Parameters	Units	Baseline	Optimistic	References
Biomass supply and composition				
Biorefinery size	t/day	2000	3000	Assumed
Feedstock cost at the biorefinery gate	\$/t	128.2	78.2	This study
Carbon footprint of feedstock supply chain excluding land use changes	kgCO_{2e}/t	117.2	69.8	This study
Cellulose	wt%	34.2	35.6	[103–112]*
Hemicellulose	wt%	21.5	29.1	
Lignin	wt%	19.6	10.4	
Pretreatment and hydrolysis				
Solid loading rate	wt%	30	30	[21,113]
Ionic liquid loading rate	wt%	10	5	[21,113,114]
Ionic liquid cost	\$/kg	2	0.5	[21,115]
Enzyme loading rate	mg/g-glucan	20	10	[21,113,114]
Cellulose to glucose	wt%	84	95	[21,113,114]
Xylan to xylose	wt%	80	90	[21,113,114]
Hydrolysis time	h	72	48	[21,113,114]
Enzyme price	\$/kg-protein	5	4	[115,116]
Bioconversion				
Bioconversion time	h	48	36	[21,116]
Glucose utilization	%	95	97	[21,116]
Xylose utilization	%	85	90	[21,116]
Recovery and separation				
Ethanol recovery	wt%	95	98	Assumed, [116]
Ionic liquid recovery	wt%	97	99	[117]

*Data gathered from several past studies [103–112] and average values were used for the baseline analysis.

3.4.2 Switchgrass-to-ethanol conversion process model

The process model for bioconversion is developed following the methods and assumptions reported in similar past studies developed as part of the Joint BioEnergy Institute projects [21,89] and by the National Renewable Energy Laboratory (NREL) [116,118]. The modeled switchgrass-to-ethanol conversion process comprises several unit operations, including biomass handling and preprocessing, one-pot high-gravity ionic liquid-based biomass deconstruction, bioconversion, ethanol recovery, wastewater treatment, onsite energy generation (process steam and electricity), and utility (except process steam and electricity) stages (Figure 2). The detailed discussion of these different unit operations and modeling methods are documented in prior studies [89,116] and some of them are modified/updated in this study. Briefly, the prior models considered corn stover feedstock, which was replaced with switchgrass in this study. Loaders and belt conveyors are used to transport switchgrass bales from the outdoor storage unit to the preprocessing unit at the biorefinery [119]. This study further added a size reduction operation (milling) to reduce bales into the required size of 3.81 cm (about 1.5 inches) [119] for the subsequent biomass deconstruction process (including pretreatment and enzymatic hydrolysis).

Biomass deconstruction process includes three main subsequent stages, including pretreatment, neutralization/pH adjustment, and enzymatic hydrolysis. Ionic liquid (cholinium lysinate) loading and the reactor operating conditions are adjusted based on the bench-scale experimental data (Table 3 and SI-Table S11). Process water is adjusted to maintain the solid loading in the pretreatment reactor— based on the whole slurry—of 30 wt% and in the enzymatic hydrolysis reactor of 25 wt%. Following the IL-pretreatment, the whole slurry is sent to the subsequent neutralization/pH adjustment reactor and then to the enzymatic hydrolysis reactor. Sugar yield and operating conditions for are consistent with prior experimental studies (Table 3 and SI-Table S11).

In the bioconversion reactor, simple sugars, such as glucose and xylose, produced during the biomass deconstruction process are metabolized by *Zymomonas mobilis* to ethanol. The modeling assumptions for the bioconversion process are consistent with prior studies [116,120]. Glucose and xylose utilizations were assumed to be 95% and 85%, respectively [116,120]. Following the bioconversion, the whole slurry is sent to the ethanol recovery and separation unit.

Ethanol is recovered using distillation and a subsequent molecular sieve adsorption [116]. This study assumes the overall ethanol recovery of 95% for the baseline scenario (Table 3). Along with ethanol, ionic liquid is recovered and recycled back to the pretreatment reactor. This study considers pervaporation-based ionic liquid recovery method with a baseline recovery rate of 95%, which is fully discussed in prior study [117]. Other modeling assumptions are consistent with prior studies [116,120].

The downstream processes and their modeling assumptions, including wastewater treatment, onsite energy generation (heat and power), and utility (process water, cooling/chilled water, and clean-in-place (CIP) system) are consistent with prior studies [116,120]. Table 3 and SI-Table S11 summarize the major operating data used to model the downstream conversion stages. The differences in biomass feedstock, deconstruction process processes alter the material flow and energy consumptions for the downstream processes. The biorefinery model developed in this study captures all these variations and accurately calculate the material and energy requirements and the resulting capital and operating costs. Table 3 summarizes modeling data inputs considered for the baseline and optimal future case scenarios. The results obtained from the valuation of ecosystem services are some of the key inputs to the biorefinery process model and focus area of this study. Full details of the biorefinery process modeling data inputs are documented in the SI-Table S11.

3.5 Technoeconomic Analysis and Life-cycle Assessment

To contextualize the value of ecosystem services in the broader biomass-to-biofuel framework, we used the biorefinery design described above to conduct a cash flow analysis. The different cost components for switchgrass-derived ethanol production (from the field to the biorefinery gate) include capital investment, ownership costs (depreciation, interest, taxes, insurance, and housing), and operating costs (repair and maintenance, fuel, lubrication, labor, and consumable materials) [90,91,116]. Benefits generated from ecosystem services were considered as operating revenues. The delivered cost of switchgrass feedstock and the minimum selling price of ethanol were determined by performing the discounted cash flow analysis considering service life of 30 years, internal rate of return of 10%, and income tax of 21% [118]. The biorefinery was assumed to be operated 7920 h/year (330 days/year and 24 h/day). The detailed cash flow analysis (Microsoft Excel sheet) is included in the additional data sources (see section ‘Data Sources’).

Material and energy consumptions data obtained from the field-to-ethanol production process model after a rigorous material and energy balanced analysis were served as major inputs to a life-cycle GHG emissions model developed in this study. The required resources were determined for each stage of the field-to-ethanol conversion process, including switchgrass production, supply, and handling, biomass deconstruction, bioconversion, recovery and separation, wastewater treatment, onsite energy generation, and utility. The GHG emissions footprints of process chemicals and energy were gathered from prior studies [89,121–123]. The excess electricity generated at the biorefinery was assumed to be displaced the same amount of the U.S. electricity mix.

The GHG emissions reduction benefits resulting from the SOC sequestration and the N_2O emissions resulting from the use of nitrogen fertilizer (Figure 1-B) were further included in this study. The net SOC sequestration and N_2O emissions were determined using the agro-ecosystem model. The CO_2 equivalent N_2O emission was determined considering 100-year global warming potential of 298. This study considered higher heating values of ethanol (SI-Table S10) and the functional unit of 1 MJ. Other assumptions and methods were consistent with prior studies [50,89,101]. These prior studies documented the detailed methods and GHG emissions impact vectors of different material and energy used in this study.

3.6 Sensitivity and uncertainty analyses

Variabilities associated with several input parameters are documented in SI-Table S11. The minimum and maximum values of each input parameter were used to perform single point sensitivity analysis. The single point sensitivity analysis was performed to identify the most important ecosystem service indicators and other biorefinery process parameters that largely alter the production cost and carbon footprint of ethanol. This study also performed two-point sensitivity analysis considering two most influential cost and carbon footprint drivers, including biomass-to-ethanol conversion rate and the cost or carbon reduction benefits generated from ecosystem services. This two-point sensitivity analysis determines the minimum required benefits from the ecosystem services to reach cost or carbon footprint parity with gasoline.

Uncertainties associated with the resulting baseline production cost and carbon footprint of ethanol were determined by modeling inputs with standard probability distribution functions, including uniform, triangular, normal, and lognormal (SI-Tables S11). The probability distribution functions were assumed primarily based on data availability and the nature of input parameters [87]. The probabilistic random inputs derived from the probability distribution function were used to determine uncertainties in the minimum selling price and carbon footprint of ethanol. The feedstock supply and ethanol production process models were integrated using Visual Basic (VB) Programming. The validated VB code written in this study generates random data inputs based on the defined probability distributions, feeds data to the process model developed in Microsoft Excel and SuperPro Designer, runs all the models, returns cost, material, energy, and ethanol production data to the analysis sheet, and finally performs the TEAs and LCAs. The uncertainty analysis was run for 10,000 trials.

4. Results and Discussion

4.1 Marginal land and benefits from integrated landscape

The total estimated marginal land in our study area (buffer radius of 112.6 km or 70 miles) is 127,400 ha (Figure 1-A). However, only 52% of this available marginal land is needed to meet the scale of the biorefinery of 2000 bdt/day considering the average switchgrass biomass yield of 12.7 bdt/ha (Figure 1-C). If all the 127,400 ha were converted, with the biomass yield in the range of 8.3 to 14.2 bdt/ha (Figure 1-C), the resulting switchgrass would sum to 1.0 to 1.8 million metric tons of annual production—sufficient to operate 1-2 biorefineries with a nameplate capacity of 2000 bdt/day. The results show that 56% of the total marginal land identified in our study area is available within 72.4 km (45 miles) of buffer radius. This indicates that the modeled biorefinery could source a major fraction of the required biomass feedstock from nearby fields, reducing biomass transportation cost and associated GHG emissions. The overall switchgrass production and supply cost at the biorefinery gate is estimated to be $121.2/bdt. For comparison, prior studies [87,100,124] reported switchgrass feedstock cost at the biorefinery gate in the range of $104.5/bdt to $128.7/bdt. These variations in switchgrass feedstock supply cost are mainly due to differences in switchgrass production cost and biomass yield.

Switching marginal cropland to bioenergy crops production in an integrated bioenergy landscape should generate more profits [9,125,126] compared to the profits from existing corn/soybean crops. The bioenergy crop production system is expected to provide substantial benefits to farmers, biorefinery operators, and the public as a whole. The estimated the ecosystem services benefits are in the range of $29.3/ha to $105.6/ha for climate change mitigation and $299/ha to 356.2/ha of nitrogen loss reduction, for example (Table 3 and Figure 3). Such benefits are more than the profits from corn and soybean planting in marginal land on an average of $37.4/ha (without considering government supports in various forms) and it could reduce the baseline switchgrass production and supply cost to $62.2/bdt (Figure 3). However, Figure 3 shows large variations in the expected ecosystem services benefits, which are due to the spatial variability in the quantity of ecosystem services indicators generated, as well as the large ranges of the value of the corresponding ecosystem services in the existing market and the value of societal costs assigned to the services (Table 3).

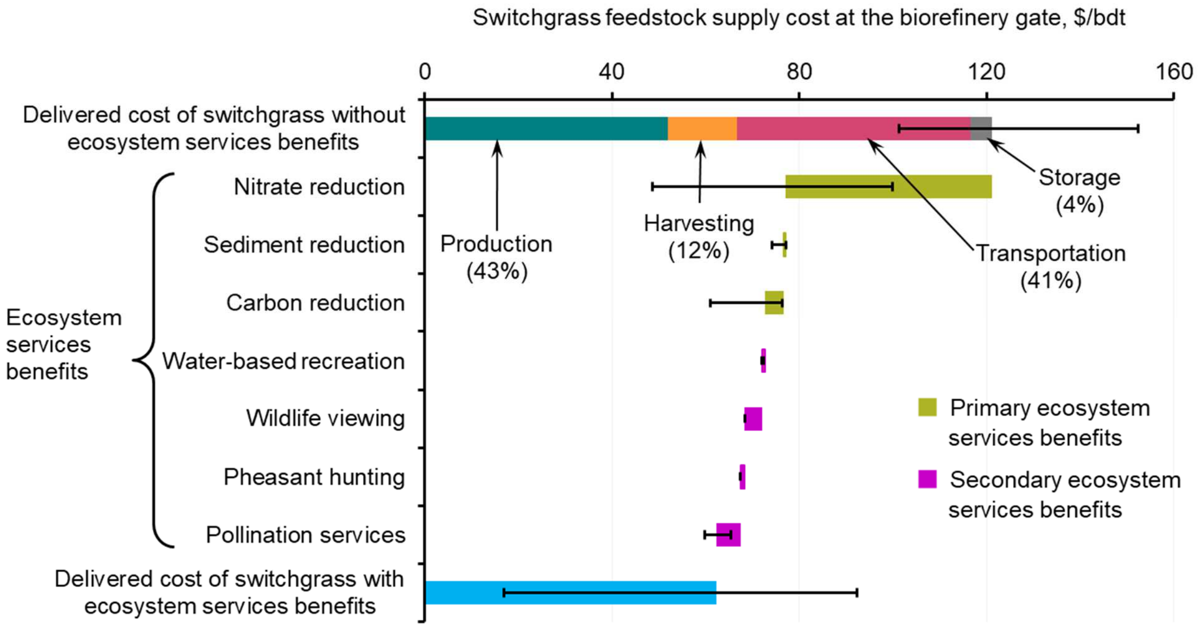


Figure 3. Switchgrass feedstock production and supply cost with and without ecosystem services benefits.

Ecosystem services valorization and market creation for ecosystem services requires a separate study and is beyond the scope of this work. This research lays groundwork for developing an understanding of the impacts of each of the ecosystem services benefits on the value proposition of the bioenergy crop. While a compensation for some of the ecosystem services generated, such as nitrate loss reduction and sediment retention, can offset the profit from producing corn/soybean on the same land, a substantial climate change mitigation benefit generated through soil carbon sequestration could add to the value proposition of the bioenergy crops. Switching row crop land to bioenergy crop (switchgrass) could result in the SOC sequestration in the range of 0.1 to 0.36 t C/ha/year(Figure 1-B). This large SOC sequestration is due to the deep-root system of switchgrass and variations across the study area are mainly due to variation in soil properties (initial soil SOC content) and climate [127]. The SOC sequestration from growing switchgrass in marginal land could reduce the carbon footprint of the switchgrass feedstock production supply chain by 26.7 to 112.6 $kgCO_2e/bdt$. The average soil carbon sequestration benefit of 84.3 $kgCO_2e/bdt$ (Figure 4) results in a low carbon footprint of switchgrass feedstock of 24.4 $kgCO_2e/bdt$, a 77.6% reduction relative to the baseline carbon footprint of the switchgrass feedstock supply chain of 108.6 $kgCO_2e/bdt$. Switchgrass production accounts for 60% of the baseline carbon footprint of the delivered switchgrass feedstock. Fertilizers used for switchgrass production and N_2O emissions from nitrogen fertilizer are primarily responsible for this large GHG emissions. For comparison, a previous study [100] also reported a large contribution (89%) from switchgrass production to the overall carbon footprint of the switchgrass production and supply chain; however, their biomass yield and trucking distance are 26% and 34% less than the values considered in this study (Table 3). The baseline switchgrass feedstock cost and carbon footprint, without ecosystem services benefits, could reach to $78.2/bdt and 69.8 $kgCO_2e/bdt$, respectively, for the optimal future case including high biomass yield, low nutrient application, and best management practices.

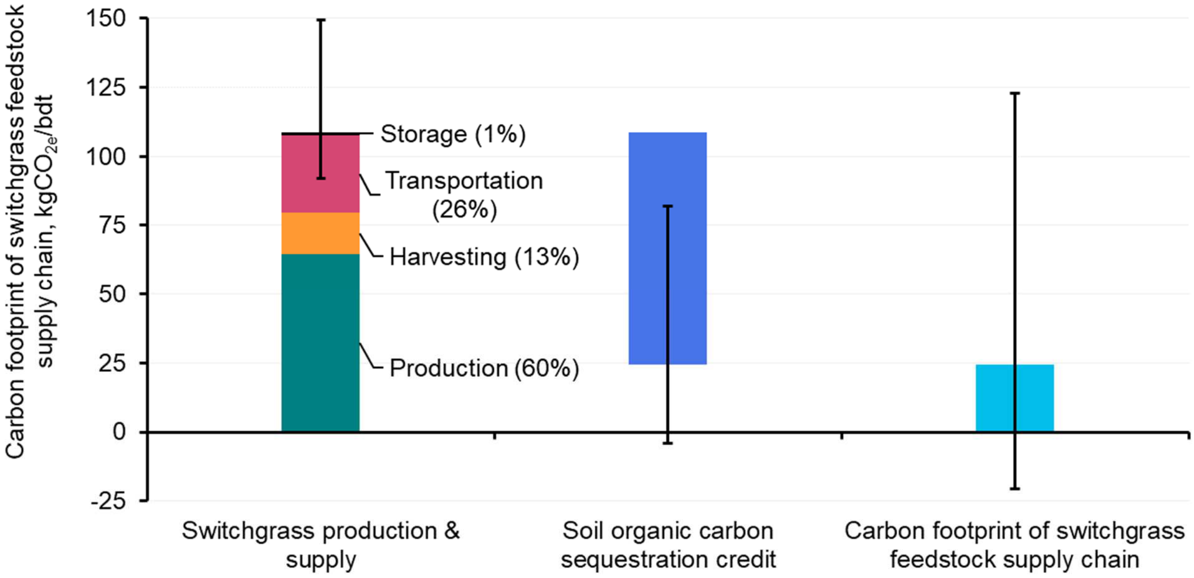


Figure 4. Carbon footprint of Switchgrass feedstock production and supply with and without ecosystem services benefits.

4.2 Ethanol Production Cost and Carbon Footprint

Figure 5 depicts the minimum selling price and carbon footprint of ethanol with and without considering ecosystem services benefits and policy incentives. Baseline data inputs (Table 3) results in the minimum selling price of $1.7/L-gasoline-equivalent. Key contributors to this selling price include the capital and operating costs associated with switchgrass feedstock supply (38%), pretreatment (17%), enzymatic hydrolysis (11%), ionic liquid and ethanol recovery (10%), and onsite energy generation (10%). While onsite energy generation and recovery stages are capital-intensive units, costs of ionic liquids and enzymes are mainly responsible for the higher cost contributions from pretreatment and enzymatic hydrolysis stages. The switchgrass-to-ethanol conversion rate is an important parameter that alters capital and operating costs of the facility by changing the amount of ethanol or material flow to the downstream processes, including recovery and separation, wastewater treatment, onsite energy generation and utility. For instance, in addition to the altering material flows to the downstream processes, a low biomass-to-ethanol conversion rate increases either the volume of biogas generated from the unutilized sugars (if the available sugars are not fully utilized in the fermentation reactor) or the solid fraction of biomass, including lignin, cellulose, and hemicellulose, (if cellulose and hemicellulose are not fully converted into sugars during the biomass deconstruction). Either of these cases increases the amount of onsite electricity; however, this is not desirable because electricity is cheap and it increases the overall capital and operation costs of the biorefinery by increasing the size of boiler, turbine, associated process equipment such as pump and compressor.

When the ecosystem service benefits are internalized at the average and maximum values, the baseline ethanol production cost is reduced by 20% and 35%, respectively, (Figure 5-a). These results highlight the importance of ecosystem services benefits to reduce the minimum selling price of ethanol. However, even the maximum ecosystem services benefit is not sufficient for achieving the targeted ethanol selling price of $0.79/L-gasoline equivalent ($3/gge).

For the baseline scenario, the targeted or market-competitive selling price of ethanol can be achieved by combining policy incentives with ecosystem services benefits. When the average monetary values of ecosystem services are added into the equation in combination with the LCFS credit (calculated excluding the SOC sequestration credit to avoid double counting), and with both LCFS and RIN credits, the minimum selling price of ethanol could be reduced, respectively, to $0.96/L-gasoline equivalent ($3.6/gge) and $0.49/L-gasoline equivalent ($1.84/gge). The maximum ecosystem services value along with both LCFS & RIN credits could further reduce the minimum selling price of ethanol to $0.23/L-gasoline equivalent ($0.88/gge) at the baseline switchgrass-to-ethanol conversion rate. This price is 60.7% less than the last 10-year average (2010-2019) gasoline selling price at the refinery gate of $0.59/L ($2.2/gal). These results show that the benefits from ecosystem services together with policy incentives provide substantial economic benefits to the biorefinery.

For the optimal future case considering near theoretical limit of switchgrass-to-ethanol conversion rate (Table 1), which admittedly is challenging to achieve, the selling price of ethanol could reach to \$0.68/L-gasoline equivalent (\$2.59/gge) without benefits from ecosystem services and excluding policy incentives. While process improvements are sufficient to meet the targeted selling price of ethanol, benefits from ecosystem services and further including LCFS and RIN credits reduce the optimal ethanol selling price by 54.5% and 200%, respectively. These credits all together provide the net profit of \$1.3/L-gasoline equivalent relative to the 10-year average gasoline selling price of \$0.59/L.

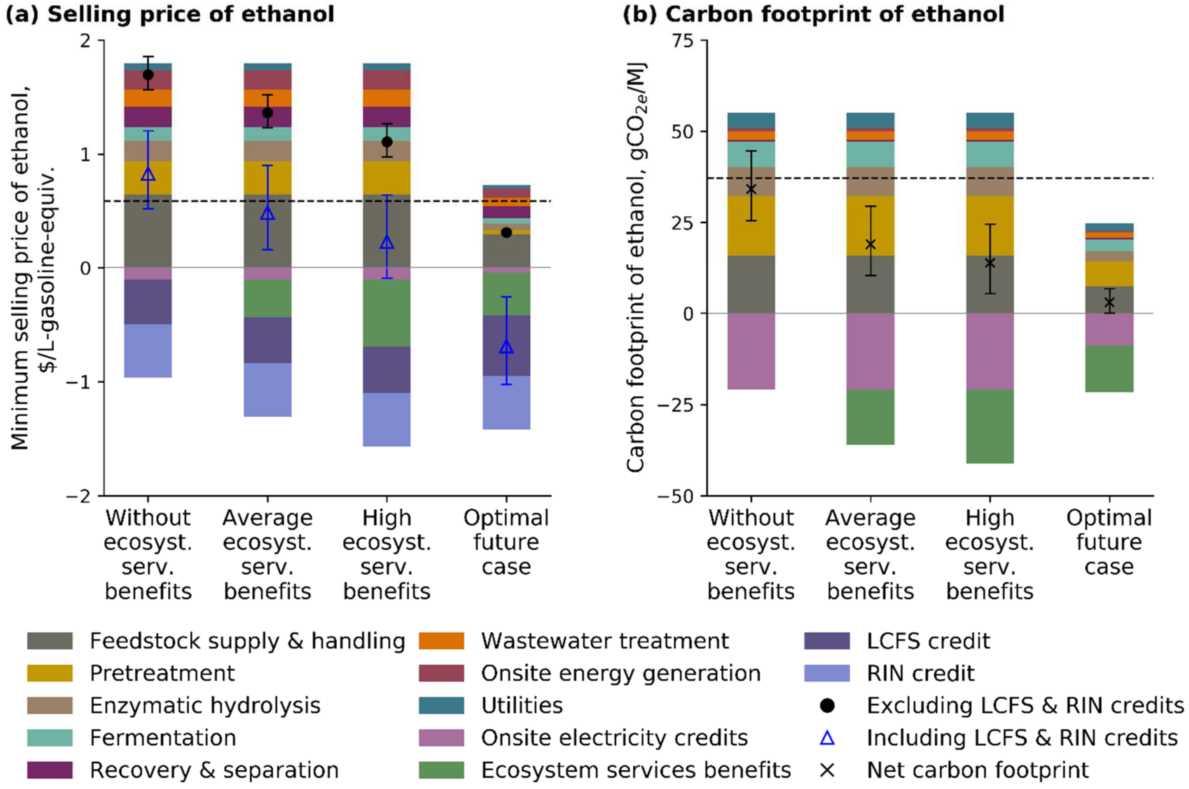


Figure 5. Minimum selling price and carbon footprint of ethanol with and without considering ecosystem services benefits. The dashed lines represent targeted cost of \$0.79/L-gasoline equivalent (\$3 gge) (a) and GHG emissions reduction of 60% relative to gasoline (b) of 37.2 gCO_{2e}/MJ[128].

While the targeted production cost of ethanol cannot be attained without including the value of ecosystem services, the targeted carbon footprint of ethanol (60% reduction relative to gasoline) can be achieved without internalizing the ecosystem services benefits. Figure 5(b) shows the major contributors to the carbon footprint of ethanol and percentage reduction as follows: biomass pretreatment (30%), feedstock supply (29%), enzymatic hydrolysis (14%), and bioconversion (13%). While the increased onsite electricity production using biogenic energy sources, including biomass and the biomass-derived products, is not favorable from an economic point of view, this will reduce the overall carbon footprint of ethanol by displacing the same amount of the grid electricity. Results show that the GHG emissions generated from various production stages can be reduced by 38% including the onsite electricity credits. In addition to the electricity credit, we found that the SOC sequestration credits further reduced the baseline carbon footprint of ethanol by 15-20 gCO_{2e}/MJ resulting in the net carbon reduction of 79-85% relative to gasoline. For the optimal scenario, the carbon footprint of ethanol could be reduced to 3 gCO_{2e}/MJ (97% reduction relative to gasoline) with the maximum SOC sequestration credits. These results highlight that a low carbon fuel can be produced by growing switchgrass in marginal land, which not only improves the ecosystem health but also provides additional payments/credits to farmers and biorefinery operators.

4.3 Important parameters for ethanol production cost and carbon footprint

Benefits from nitrate reduction, SOC sequestration, pollination services, and wildlife viewing are key parameters for determining the net benefits from ecosystem services (Figure 6-a). Variations in these parameters directly alter credits from ecosystem services or the net operating cost of the biorefinery, thereby influencing the minimum selling price of ethanol. Other ecosystem services parameters, including water-based recreation and pheasant hunting, are expected to generate low revenues (Figure 6-a) and are less influential to the minimum selling price of ethanol. For instance, an increase in ecosystem services benefit of $19.87/ha decreases the minimum selling price of ethanol by 1 cent/L-gasoline-equivalent. These results highlight the importance of ecosystem services benefits for providing substantial revenues to biorefineries.

The most important biomass-to-ethanol conversion process parameters shown in Figure 6 (b) either alter capital and operating costs of the biorefinery or the amount of ethanol. Variations in some of the key input parameters, including switchgrass feedstock cost, ionic liquid cost, and enzyme cost, directly alter the operating cost of the biorefinery and consequently influence the selling price of ethanol. Among them, biomass feedstock cost is the largest contributor to the minimum selling price of ethanol (Figure 6-b). An increase in feedstock cost of $2/bdt increases the minimum selling price of ethanol by 1 cent/L-gasoline-equivalent. Ionic liquid is one of the expensive process chemicals; however, its impact on ethanol selling price is contingent on its loading and recovery rates. Ionic liquid loading and recovery rates not only determine the makeup ionic liquid but their variations alter capital and energy costs required for handling and recovery of ionic liquid. Cellulose and hemicellulose contents in switchgrass, cellulose to glucose conversion rates, and the utilization of glucose, xylose and extractives (only sugar fractions [118]) for ethanol production are the other important switchgrass-to-ethanol conversion process parameters. Variations in these parameters alter the selling price of ethanol by directly changing the amount of ethanol produced and, in part, altering capital and operating costs as well as revenue generated from onsite electricity. Solid loading rate alters the capital and operating costs of the downstream processes, including recovery and separation, wastewater treatment, onsite energy generation, and utility, thereby influencing the selling price of ethanol. Other parameters, including biorefinery size, enzyme loading rate, and enzyme cost alter either both the capital and operating costs or only the operating cost thereby affecting the production cost of ethanol.

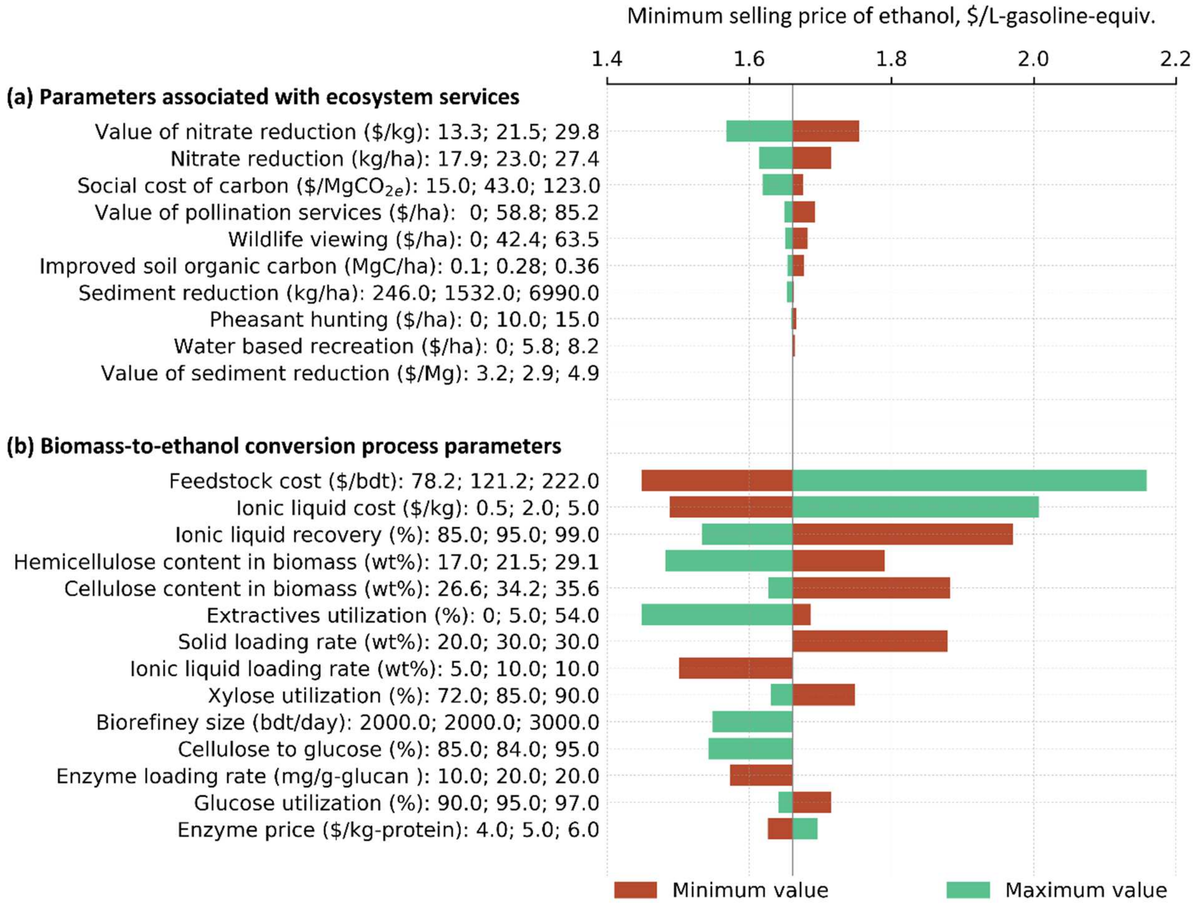


Figure 6. Important parameters determining the minimum selling price of ethanol.

The rationale for converting low productive croplands into bioenergy crops, in part, is the SOC sequestration because it largely alters the overall GHG emissions of ethanol (Figure 7-a) by providing direct carbon footprint credits. For instance, increasing the SOC sequestration by 0.1 MgC/ha decreases the overall carbon footprint of ethanol by 6.4 gCO$_{2e}$/MJ. Apart from the SOC sequestration, other biomass-to-ethanol conversion process parameters, including ionic liquid recovery and loading rates, carbon footprint of switchgrass feedstock supply, and solid loading rates have the largest impact on the carbon footprint of ethanol. Ionic liquid recovery and loading rates primarily alter the makeup ionic liquid, thereby influencing the carbon footprint of ethanol. Variabilities associated with biomass yield, fertilizer application, and trucking distance (determines diesel fuel required for transportation) are primarily responsible for variations in the GHG emissions from switchgrass feedstock supply chain, which directly alters the carbon footprint of ethanol. An increase in carbon footprint of switchgrass feedstock supply by 7

$kgCO_{2e}/bdt$ increases carbon footprint of ethanol by 1 gCO_{2e}/MJ. Solid loading rate is relatively more influential to GHG emissions relative to the selling price of ethanol. This is mainly because it alters system wide energy requirements, specifically for ethanol recovery, wastewater treatment, onsite energy generation, and utility. Additionally, changes in the energy requirement for the biorefinery's use alters the carbon footprint credits from excess electricity. Parameters that determine the biomass-to-ethanol conversion rate, including carbohydrate content in biomass, sugar yield, and sugar utilization, alter the carbon footprint of ethanol by directly altering the amount of ethanol produced. Similar to ionic liquid, changes in the enzyme and sulfuric acid loading rates alter the carbon footprint of ethanol by changing the required amounts of those chemicals. Retention time of reactors, including bioconversion and pretreatment reactors, alters their energy consumption and is also found to be influential to the carbon footprint of ethanol. Additional less influential parameters to the carbon footprint of ethanol are shown in Figure 7.

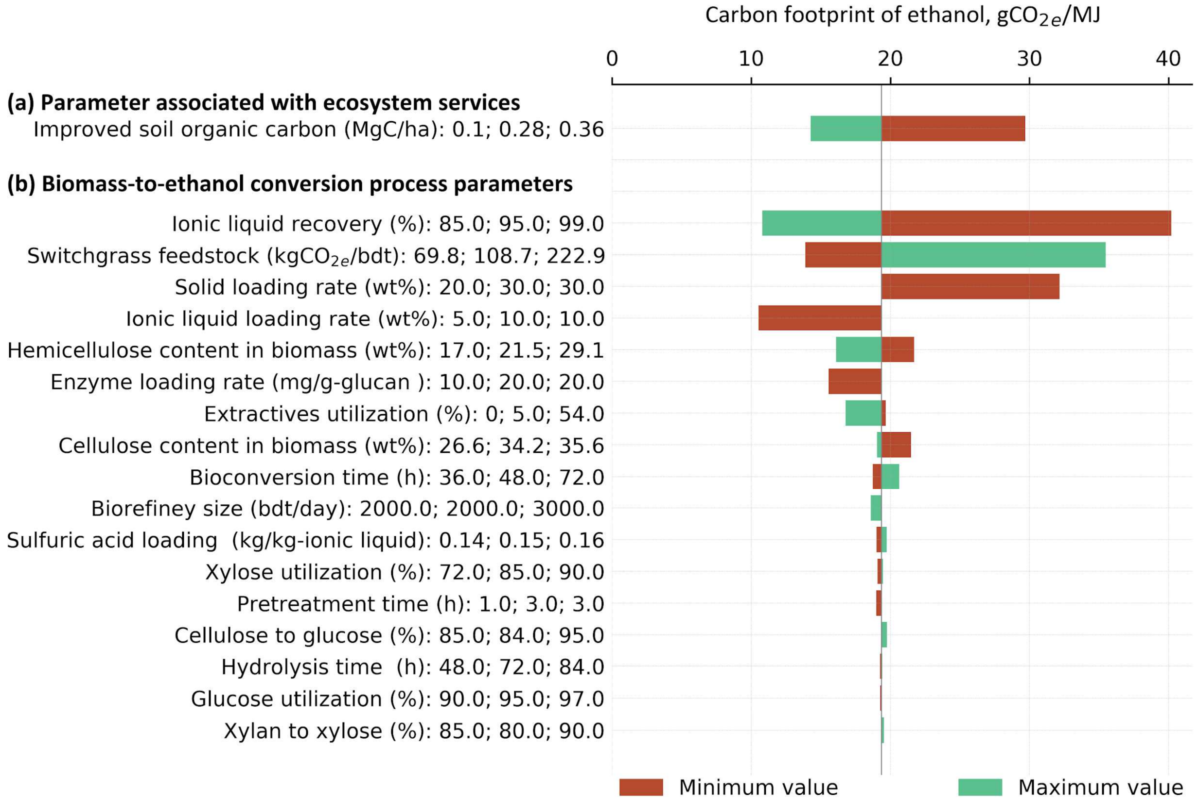
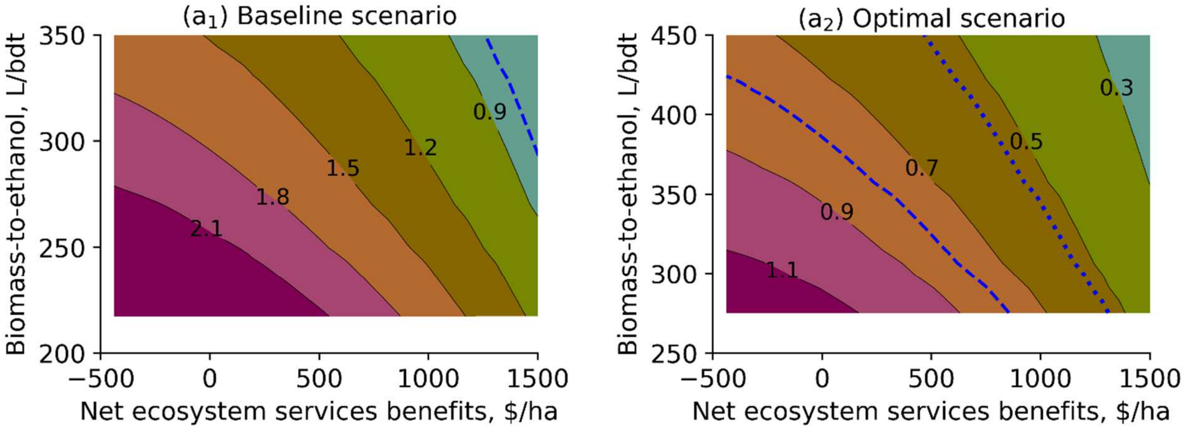


Figure 7. Important parameters determining the carbon footprint of ethanol.

4.4 Importance of Ecosystem Services Benefits for Cellulosic Biorefineries

The baseline and optimal scenario results show that internalizing the value of ecosystem services could improve the value proposition for bioenergy crops and ethanol production by reducing the selling price and carbon footprint of ethanol. Here, this study further demonstrates the net value of ecosystem services required for achieving the targeted cost and carbon footprint of ethanol at different biomass-to-ethanol conversion rates and without any policy incentives (Figure 8). For the baseline biomass-to-ethanol conversion rate of 302 L/bdt, the net value of ecosystem services of $1472/ha is required to achieve the targeted selling price of ethanol of $0.79/L-gasoline equivalent ($3/gge). This is a challenging target as the maximum benefit from ecosystem services estimated in this study is $1105.3/ha. However, the targeted ethanol selling price can be achieved for the optimal future case scenario even with the net loss in the ecosystem services benefits of $437/ha. This result suggests that the targeted ethanol selling price of $0.79/L-gasoline equivalent ($3/gge) can be achieved, either further enhancing ecosystem services benefits and/or converting a high productive cropland—very unlikely—into switchgrass field. Reaching cost-parity with the last 10-year (2012-2021) average gasoline price at the refinery gate of $0.54/L[129] requires the ecosystem services benefits of $587/ha for the optimal future case scenario.

(a) Minimum selling price of ethanol ($/L-gasoline-equiv.)



(b) Carbon footprint of ethanol (gCO$_{2e}$/MJ)

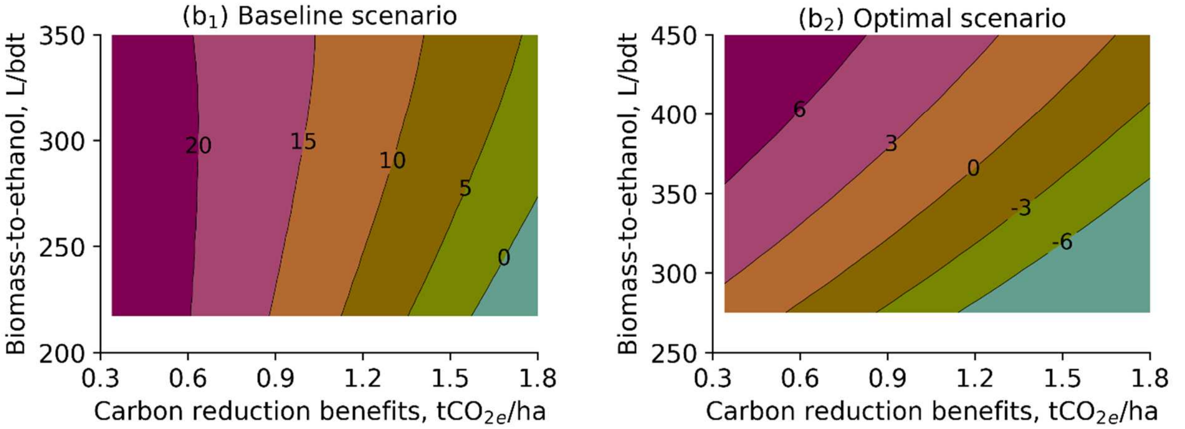


Figure 8. Impacts of ecosystem services benefits on the production cost and carbon footprint of ethanol. The dashed lines represent targeted cost of $0.79/L-gasoline equivalent ($3.gge) and the

dotted line represents last 10-year (2012-2021) average gasoline price at the refinery gate of \$0.54/L[129].

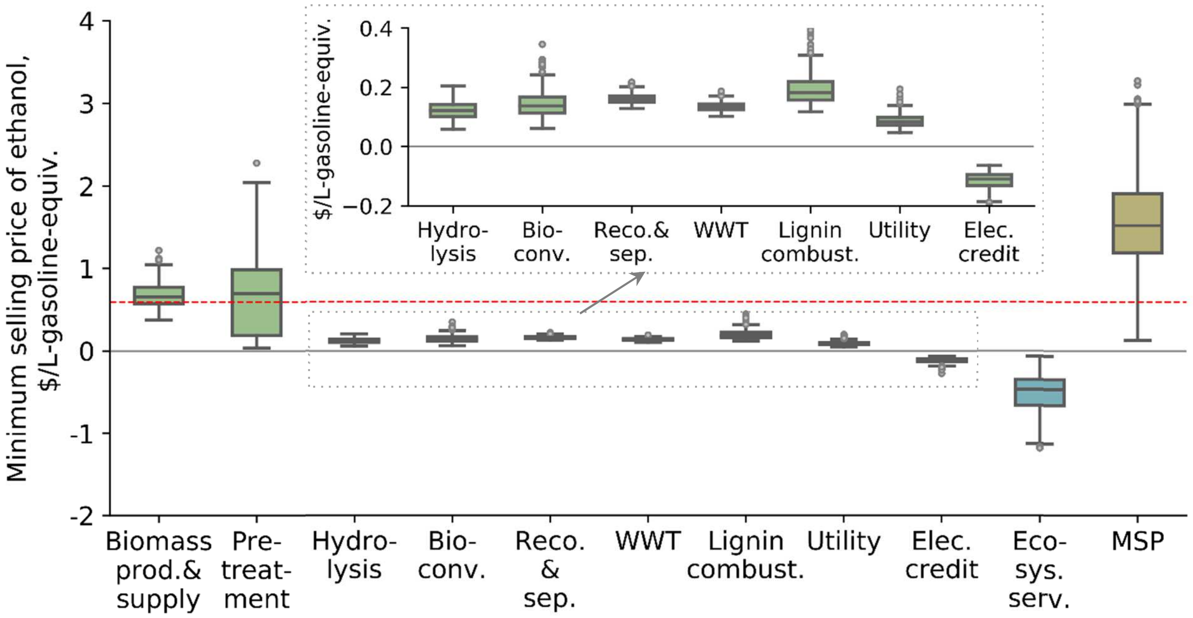
In contrast to selling price, the GHG emissions reduction mandate of cellulosic biofuel—60% reduction relative to petroleum—can be easily achieved for the baseline and optimal future scenarios. At the maximum SOC change estimated in this study at 1.43 tCO_2e/ha, the carbon footprint of ethanol could further be reduced by 92% and 98% relative to gasoline for the baseline and optimal future scenarios, respectively. More importantly, at the higher SOC changes and/or optimal process conditions, the carbon footprint of ethanol increases with increasing the biomass-to-ethanol conversion rate. This is mainly due to reduction in carbon footprint credits from excess electricity as an efficient biomass-to-ethanol conversion process reduces the biogenic fuel sources—mainly biogas generated from the unutilized sugars—to the boiler. For the baseline scenario (Figure 8-b1), producing the net zero-carbon ethanol requires the SOC reduction benefits of more than 1.8 tCO_{2e}/ha, which is unlikely as the required SOC sequestration is more than the maximum SOC sequestration estimated in this study of 1.43 tCO_{2e}/ha. For the optimal future case (Figure 8-b1), producing the net zero-carbon ethanol requires the SOC sequestration benefit of 1.55 tCO_{2e}/ha. Achieving the net zero-carbon ethanol at lower SOC sequestration requires to source renewable energy sources instead of natural gas considered in this study as a makeup energy source for the boiler.

4.5 Sources of Uncertainty and Future Improvement Opportunities

Uncertainties in the minimum selling price and carbon footprint of ethanol are presented in Figure 9, which are largely derived from the variabilities associated with key input parameters (Figures 6 and 7). Without other policy incentives, including LCFS and RIN credits, benefits from ecosystem services are important to reduce the minimum selling price of ethanol. Results show a 95% likelihood of obtaining cost credit from ecosystem service below -\$0.97/L-gasoline equivalent (-\$3.7/gge) while mean value is -\$0.47/L-gasoline equivalent (-\$1.8/gge) (Figure 9-a). This large uncertainty is due to variabilities associated with value and amount of nitrate reduction, increased SOC, social cost of carbon, and pollination services. Biomass-to-ethanol conversion stages, specifically feedstock supply and pretreatment, largely contribute to the uncertainty in the minimum selling price of ethanol. Results show a 95% likelihood of resulting cost from all the ethanol production stages below \$2.7/L-gasoline equivalent (\$10.2/gge) with a mean value of \$1.5/L-gasoline equivalent (\$5.8/gge). The major sources of uncertainty in feedstock supply costs are variabilities associated with biomass yield and trucking distance. Variations in the makeup ionic liquid determined by ionic liquid loading and recovery rates are the major sources of uncertainty in pretreatment cost. The uncertainties in the benefits from ecosystem services and the cost contributions from different ethanol production stages together result in a 6% likelihood of achieving targeted selling price of ethanol of \$0.79/L-gasoline equivalent (\$3/gge) for the baseline scenario excluding LCFS and RIN credits.

One of the biggest advantages of planting switchgrass on marginal lands is the SOC sequestration benefits. Results show a 95% likelihood of obtaining carbon footprint credits of as much as 32.9 gCO_2e/MJ from the direct carbon sequestration. The mean carbon footprint credit (-26.5 gCO_2e/MJ) from the SOC changes is close to the 95% certainty value, suggesting a higher probability of achieving a large carbon footprint credit from the SOC change. Ethanol production stages show a 95% likelihood of a resulting carbon footprint below 109.5 gCO_2e/MJ. This positively skewed probability distribution indicates a greater change of GHG emissions from the production stages above the mode value of 34.3 gCO_2e/MJ. Switchgrass feedstock supply, pretreatment, fermentation, onsite energy generation, and electricity credit are the major contributors to the uncertainty in GHG emissions from ethanol production stages. The major sources of this uncertainty include variabilities associated with fertilizer application, trucking distance, makeup ionic liquid (determined by ionic liquid loading and recovery rates), nutrient and electricity required for fermentation (mainly determined by solid loading rate), and electricity required for onsite energy generation. In contrast to the selling price of ethanol, results show a 34% likelihood of achieving the targeted carbon footprint of ethanol.

(a) Selling price of ethanol



(b) Carbon footprint of ethanol

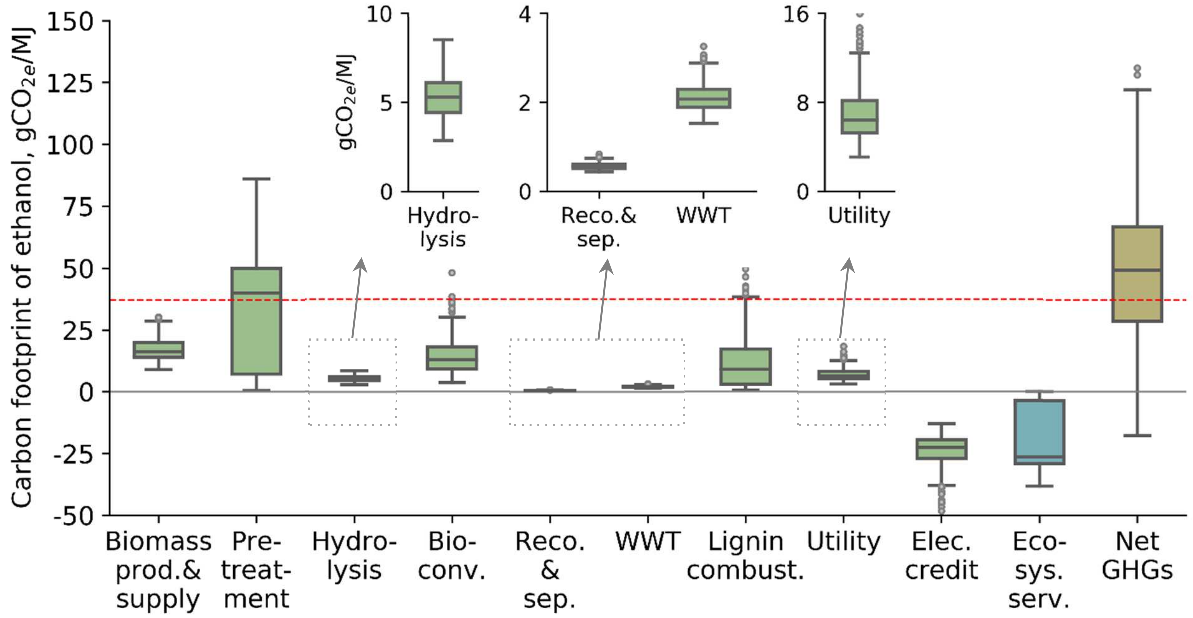


Figure 9. Uncertainties in the minimum selling price (a) and carbon footprint (b) of ethanol for the baseline scenario. In this figure: prod. = production; conv. = conversion; reco. = recovery; sep. = separation; WWT = wastewater treatment; combust. = combustion; elec. = electricity; sys. = system; serv. = services; MSP = minimum selling price; and GHGs = greenhouse gas emissions.

A 6% likelihood of achieving the targeted selling price without policy incentives, such as LCFS and RIN credits, or process optimization highlights the importance of future process improvements to achieve the targeted selling price of ethanol with a high certainty. The process optimization specifically related to reduction in the required process chemical and energy, as well as improvements in conversion efficiency or biomass-to-fuel conversion rate, reduce both the selling price and carbon footprint of ethanol. Future research could focus on optimizing fertilizer application rates, ionic liquid recovery and loading rates, enzyme loading, and biomass deconstruction and bioconversion efficiencies. Additionally, a high carbohydrate content switchgrass variety could be planted in a low productive land, which not only increases biomass-to-fuel conversion rate and the SOC sequestration but also reduces opportunity cost of land.

Future improvement opportunities also exist in incorporating the socioeconomic impacts of production of biomass and biofuels into the assessment framework presented in this study. Introduction of the bioenergy value chain in the rural U.S. can generate new economic opportunities creating jobs and supplying cleaner fuel. Such practices can result in benefits from improved soil health, carbon credits, nutrient trading credits, and provide new sources of income to farmers in the rural areas. Locating the biomass and biofuel production facilities by considering the geographic distribution of disadvantaged communities and historically underserved people can also support Justice 40 initiative's goal [130].

Moreover, this study only considers ethanol as a representative biofuel to quantify the impacts of ecosystem services benefits; however, the quantified impacts on per unit mass of delivered biomass feedstock and per unit volume or energy density of ethanol can be used to determine their impacts on the production cost and carbon footprint of biofuels derived from other pathways, including thermochemical and hybrid conversion pathways. This study establishes methods to quantify the impacts of ecosystem services benefits to the production cost and carbon footprint of biofuels, which can be implemented into future studies comparing multiple biofuels or other bioenergy crops.

4.6 Practical Implication of Ecosystem Services Benefits

The distribution of the profit resulting from the ecosystem services along with policy incentives among the farmers and biorefineries could encourage farmers to convert their low productive agricultural lands into switchgrass fields, which is essential for an uninterrupted operation of cellulosic biorefinery in future. This could be supported by future state- and national-level biofuel policies that are critical to maximizing ecosystem services benefits to the farmers, biorefinery operators, and the public as a whole.

The distribution of profits/benefits of the integrated bioenergy systems depends upon the contractual arrangements among the farmers, investors in the ecosystem service markets, and biorefinery operators. Under a vertically integrated bioenergy system, wherein biorefineries lease land from farmers, farmers receive the land rent at a mutually accepted rate, and the biorefineries receive the net profit from the production and conversion of biomass. Additionally, some of the ecosystem service payments such as carbon credits, nutrient trade permits, and in some cases benefits from hunting and bird watching will be accrued to the leaseholder division of the biorefinery company. If the farmers produce and sell or deliver biomass to the biorefinery, the profits from biomass and the payment for ecosystem services will go to the farmers. Such a contractual arrangement provides leeway for the farmers for reduction in the farm-gate price or the delivered cost of biomass while providing low-carbon biomass feedstock to the biorefinery. The reduction in biomass feedstock cost and associated GHG emissions, a key contributor to the ethanol production cost and carbon footprint, will then lead to the reduction in the minimum selling price of ethanol and its carbon footprint.

In addition to the cost of switchgrass production, the farmers or biorefineries also incur the harvest, collection, transportation, and storage costs. Based on the type of contract between farmers and biorefineries, any additional payments to farmers or biorefineries could incentivize the value chain and thus is the key for sustainable operation of cellulosic biorefinery. The increasing ecosystem services markets for carbon, water quality trading, as well as government programs to facilitate payment for carbon emission reduction and improvements in environmental quality can be combined to support planting bioenergy crops in an economically and environmentally sustainable way. In the case where biorefineries lease land from farmers, an incentive to the farmers could be a payment additional to the land rent. This is because the farmers will compare the land rent with their current profits from corn/soybean production. The sum of several cost items could be packaged into a financial incentive to farmers. The cost items include the net profit from current land uses (50/50 corn-soybean), land loan and interest (if farmers are paying loan for their lands), or opportunity cost of land due to alternative business, cost of custom services (custom operations and technical services), cost of unpaid labor (farmers work themselves and biomass production labor will reduce due to perennial bioenergy crop), and cost of seed (farmers could use their own corn/soybean seeds) [131].

A recent study [126] reported that most farmers (68 out of 135) are willing to cultivate switchgrass if there is a possibility of earning a profit of at least 50% higher than the current land use. Other studies [9,125] found that farmers are willing to switch to new crops when the profit from new crops exceeds the present profit by a factor of 2. The ecosystem services benefits generate substantial credits; however, it may not be sufficient for paying off the expected incentive to the farmers due to a large spatial variability in ecosystem service quantity and benefits (Table 1). Identification of locations that generate higher ecosystem services quantity and value from planting bioenergy crops and biofuel refineries could be one way to foster feedstock supply and bioeconomy.

Thoroughly evaluating the socio-economic benefits of switchgrass and educating farmers through an extension program are required to enhance switchgrass cultivation on marginal land. This study demonstrated how the evaluation and incorporation of ecosystem service co-benefits can reduce the costs of biofuel production and support towards decarbonizing transportation sector. The nitrate retention benefit specifically could be considered among the set of best practices to address downstream water quality issues including the hypoxia in the Gulf of Mexico. The results of the integrated assessment of the bioenergy value chain demonstrate its connection to a number of sustainable development goals such as clean water, clean energy, and climate action – decarbonization.

5. Conclusions

The overall success of the future cellulosic biofuel value chain requires an improved understanding of strategic integration of bioenergy crops into the current agricultural landscape to ensure supply of feedstock that profits both farmers and biorefineries. This study is the first to combine biophysical, ecosystem services valuation, technoeconomic analysis, and lifecycle assessment models to evaluate several ecosystem services of growing switchgrass on marginal land and their impacts on the ethanol production cost and greenhouse gas emissions. Additionally, this study quantifies the soil organic carbon sequestration potential of switchgrass growing on marginal land, associated N_2O emissions, and determines their impacts on the overall carbon footprint of ethanol. The results demonstrate that changing marginal lands to switchgrass production sequesters soil organic carbon in the range of 0.1-0.36 MgC/ha/year and generates ecosystem services benefits in the range of $29.3/ha to $105.6/ha for climate change mitigation and $299/ha to 356.2/ha of nitrogen loss reduction. Incorporating the monetary value of these ecosystem services result in reductions of ethanol production cost and carbon footprint in the range of 33.3 to 58.9 cents/L-gasoline-equivalent (126 to 223 ¢/gge) and 13 to 20 gCO_2e/MJ, respectively, depending on the switchgrass-to-ethanol conversion rates. These cost and carbon footprint reduction benefits could reduce the overall ethanol-selling price to 31.2 ¢/L-gasoline-equivalent ($1.2/gge) and carbon footprint of ethanol to 3 gCO_2e/MJ for the optimal future case considering near theoretical limits of switchgrass to ethanol conversion rate. The benefits from ecosystem services, along with California's Low Carbon Fuel Standard credits, result in the net profit—when compared to an average market price of gasoline—of 80.8 cents/L-gasoline-equivalent ($3.1/gge). This profit could increase to $1.3/L-gasoline-equivalent ($4.8/gge) including ecosystem services benefits, and LCFS and RIN credits. This large profit, in part, could be distributed to farmers as an incentive because sustainable supply of biomass feedstock is important for an uninterrupted operation of cellulosic biorefineries in future. Results highlighting those benefits from the soil carbon sequestration, pollination services, and nitrate reduction are key for the commercial success of bioenergy crops production and utilization schemes demonstrated in this study. Moreover, this can help to promote and advance the acceptance of this kind of benefit analysis to other industries. Achieving the future target demonstrated in this study and deploying the proposed integrated landscape for bioenergy crops production and utilization on a national scale require further research, development, and demonstration efforts. By coupling the fundamentals of multidisciplinary sciences and modeling, the framework developed and demonstrated in this study allows accounting for spatial variability in environmental characteristics as well as economic and environmental costs/benefits that could be applied for identifying optimal locations to foster bioenergy value chains in other U.S. states and beyond.

Data Sources

All the modeling and experimental data inputs, and workable process model/spreadsheets can be freely accessed via DRYAD using this link (doi:10.7941/D1K62R or https://datadryad.org/stash/share/_fygv2pi2Gdf3ALXLuQOv71CfGbpdlEFKG30HGpGrz8).

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