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Managing Multiple Mandates: A System of Systems Model to Analyze Strategies for Producing Cellulosic Ethanol and Reducing Riverine Nitrate Loads in the Upper Mississippi River Basin

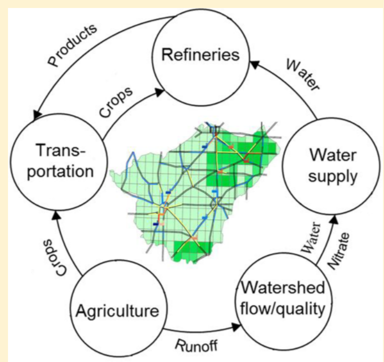
Mashor Housh,[†,‡] Mary A. Yaeger,[‡] Ximing Cai,[*,‡] Gregory F. McIsaac,[§] Madhu Khanna,[∥] Murugesu Sivapalan,[‡,⊥] Yanfeng Ouyang,[‡] Imad Al-Qadi,[‡] and Atul K. Jain[#]

[†]Department of Natural Resources and Environmental Management, University of Haifa, Haifa 3498838, Israel

[‡]Department of Civil and Environmental Engineering, [§]Department of Natural Resources and Environmental Sciences, [∥]Department of Agricultural and Consumer Economics/Energy Biosciences Institute, [⊥]Department of Geography and Geographic Information Science, [#]Department of Atmospheric Sciences, University of Illinois at Urbana−Champaign, Champaign, Illinois 61801, United States

Supporting Information

ABSTRACT: Implementing public policies often involves navigating an array of choices that have economic and environmental consequences that are difficult to quantify due to the complexity of multiple system interactions. Implementing the mandate for cellulosic biofuel production in the Renewable Fuel Standard (RFS) and reducing hypoxia in the northern Gulf of Mexico by reducing riverine nitrate-N loads represent two such cases that overlap in the Mississippi River Basin. To quantify the consequences of these interactions, a system of systems (SoS) model was developed that incorporates interdependencies among the various subsystems, including biofuel refineries, transportation, agriculture, water resources and crop/ethanol markets. The model allows examination of the impact of imposing riverine nitrate-N load limits on the biofuel production system as a whole, including land use change and infrastructure needs. The synergies of crop choice (first versus second generation biofuel crops), infrastructure development, and environmental impacts (streamflow and nitrate-N load) were analyzed to determine the complementarities and trade-offs between environmental protection and biofuel development objectives. For example, the results show that meeting the cellulosic biofuel target in the RFS using *Miscanthus x giganteus* reduces system profits by 8% and reduces nitrate-N loads by 12% compared to the scenario without a mandate. However, greater water consumption by *Miscanthus* is likely to reduce streamflow with potentially adverse environmental consequences that need to be considered in future decision making.



1. INTRODUCTION

Biofuels have been viewed as a promising strategy for mitigating dependence on foreign oil and reducing greenhouse gas emissions. To achieve these objectives, the Renewable Fuel Standard (RFS) requires that 136 billion liters of biofuel be produced annually by 2022, with the contribution from food-based crops limited to 56 billion liters.

Concerns about corn-based ethanol include its potential to raise food and feed prices[1] and to lead to expansion of nitrogen intensive corn acreage which could worsen nitrate-N leaching into surface water bodies and contribute to hypoxia in the Gulf of Mexico.[2,3] The RFS therefore stipulated that at least 60 billion liters of advanced biofuels be produced annually using cellulosic feedstocks like crop residues and dedicated energy crops (which are grown solely for the purpose of producing bioenergy).[4] Among energy crops, perennial grasses like *Miscanthus x giganteus* and switchgrass (*Panicum virgatum*) are particularly promising due to their high yields under rainfed conditions, low chemical input requirements, and ability to sequester carbon and other nutrients in their root systems. Additionally, *Miscanthus x giganteus* is not considered an invasive species in the Unitesd States.[5]

Field-scale experiments have observed that energy crops can lower nitrate-N leaching and runoff compared to corn/soybean production.[6,7] Thus, energy crops could potentially improve water quality by converting some corn/soybean production areas to perennial grasses. The lower nitrate-N runoff when land is converted from corn to *Miscanthus* is due to lower nitrogen fertilizer use, more extensive roots, longer growing season, and greater evapotranspiration (ET) such that fertilizer nitrogen and nitrate mineralized from soil organic matter are more likely to be taken up by a perennial grass than by corn or soybean.[6−8]

Perennial grasses also have higher annual ET than conventional crops due to their longer growing season.[6,9] Additionally,

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they have a denser canopy that intercepts more rainfall, further reducing soil moisture.[10,11] Due to its greater ET, large-scale planting of *Miscanthus* or similar perennial crops may cause water tables and surface water flows to decline, consequently altering flow regimes. Using a global dynamic vegetation model, Vanloocke et al.[12] found a decrease in the hillslope drainage to streams when a fraction of agricultural land was converted from conventional crops to *Miscanthus*; similar observations were obtained using watershed-scale hydrologic models for different perennial grasses.[13] While these dedicated energy crops can improve water quality, they may also reduce water flow to streams, thus decreasing water availability for other uses (e.g., municipal water supply, industrial cooling water, navigation, recreation, and aquatic life support). In the study region, low flows and water shortages typically occur in the months of August, September, and October, and have caused fish mortality and barge traffic delays in recent years. The impacts of converting land from existing uses to these energy crops are expected to be site-specific, depending on soil quality, topography, distance to water bodies and landscape characteristics.

Expansion of cellulosic biofuel production will require accompanying decisions about infrastructure design in the form of refinery locations and road networks. Biomass is bulky to transport, so refineries are likely to be built close to production sources, with roads being the primary mode of transportation, thus raising concerns about traffic congestion.[14,15] Furthermore, these infrastructure needs will be affected by the spatial pattern of energy crop production. Profit-maximizing landowners are expected to convert their land to energy crops if it yields a return that is at least as large as that from existing uses of the land. Under the RFS, these returns would depend on the implicit price of ethanol that is needed to achieve the targeted level of production.[16]

The purpose of this paper is two-fold. The first is to examine the effects of a targeted level of production of biofuels on streamflow and water quality in a watershed and on the location and system-wide costs of biofuel production, including costs due to land use change and accompanying infrastructure needs. The second is to examine how stringent water quality constraints in the watershed could alter the optimal allocation of land between food and energy crops, the spatial pattern of crop production and location of required infrastructure expansion. The latter includes the size and location of corn and cellulosic refineries, and the transportation infrastructure that connects agricultural fields to refineries and biofuel demand sites. Refinery location, land allocation, and the transportation infrastructure requirements are jointly determined and therefore will be affected by the inclusion of water quality concerns in biofuel production decisions. The costs of land use change and refinery infrastructure will also influence the mix of biofuel feedstocks and location of their production, and in turn affect the cost of meeting water quality constraints.

2. DESCRIPTION OF THE SYSTEM OF SYSTEMS MODEL FOR BIOFUEL DEVELOPMENT

This study applies an integrated framework that incorporates the multidirectional dependencies between the infrastructure systems and the environment and relies on a system of systems (SoS) modeling approach to model feedstock production, multiple infrastructure systems, and environmental impacts from these systems.[17] "System of systems" is a term used in fields such as systems engineering[18,19] to describe complex systems composed of large-scale concurrent and distributed systems that are themselves comprised of complex systems. The SoS modeling approach emphasizes the interdependencies between the various systems that are connected physically or functionally, while at the same time capturing the essential behaviors of individual systems.[20,21]

The SoS modeling approach used in this study includes interactions and feedbacks among multiple and interdependent natural, infrastructure, and economic systems that include the hydrological system, the conventional and energy crop growth system, the transportation infrastructure, and the biofuel production system (Figure 1). The land use decision, including

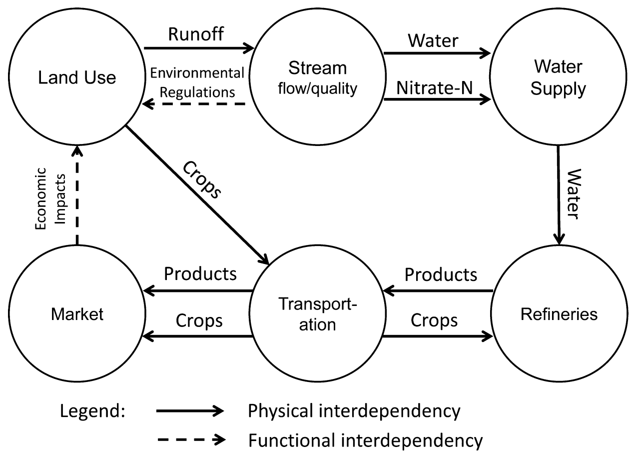

Figure 1. Model scheme showing subsystem interdependencies.

how much land is to be used for cellulosic biofuel feedstocks, is a key process in the model. The impacts of this decision are represented by two branches in the modeling scheme: (1) water and nitrate-N fluxes resulting from land use decisions affects water quality and water supply to downstream users, including refineries; and (2) agricultural products are transported through the transportation network to markets and to biofuel refineries. Refineries use the delivered raw materials (corn grain, the conventional biofuel feedstock, or *Miscanthus* and corn stover (residue in the form of leaves and stems of the corn plant) for cellulosic biofuels) and draw from the available streamflow to produce ethanol and coproducts, which are then transported back through the transportation system to markets. Thus, these two branches influence both refinery and transportation infrastructure decisions. Key relationships of the SoS modeling approach include the economic return on land use decisions and the feedback of environmental regulations on land use. Together, these two relationships form a feedback loop connecting the infrastructure systems, the market, and the environmental system.[22]

2.1. Model Formulation. The individual subsystems and their connectedness (Figure 1) are formulated within an economic equilibrium optimization model with the objective of maximizing the annual net profits of agricultural and biofuel producers in the watershed, given crop and biofuel prices and subject to constraints on land availability as well as constraints on environmental outcomes in the watershed.

2.1.1. Objective Function. The overall objective of the system is to maximize the profit from corn, soybeans, and biofuel production, which is calculated by the difference between the sum of revenues from selling corn grain and soybeans to demand nodes and the revenue from selling the

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refinery products and the total costs, including costs of transportation of biomass from producers to refineries; the cost of transporting ethanol, coproducts, corn, and soybeans from producers to demand nodes; and the annualized capital and operating costs of refineries for corn ethanol and cellulosic ethanol production. This is shown in eq S30 of the Supporting Information. For details on the mathematical model used in the analysis, the reader is referred to the Supporting Information which shows the set of equations used in each of the subsystems.

2.1.2. Decision Variables. The model determines (a) the allocation of land among various crops; (b) the location, type (corn vs cellulosic), and capacity of refineries; (c) the mix of biofuel types; (d) the amount of various commodities to be transported from producers to refineries to demand centers and the routes to be used; and (e) the resultant streamflow and nitrate-N loadings. The model is formulated as a mixed integer linear programming (MILP) model with the decision variables defined as continuous variables except for the decision to build a refinery in any candidate location, which is defined as a binary variable that takes value 1 if the refinery will be built in the candidate location as shown in eq S7−S13.

2.1.3. Constraints. Each subsystem is represented in the mathematical model as a set of constraints (eq S1−S29) which represents the physical relationships (e.g., mass balance) and the operational and regulatory conditions in which the subsystems should be maintained (e.g., maximum nitrate-N loading). The following paragraphs describe each of the five subsystems of the model: agriculture, transportation, refinery, environmental, and market subsystems.

2.1.4. Agricultural Subsystem. The independent decision variables in this subsystem are the allocation of land between two conventional crops, corn, and soybeans, and an energy crop, *Miscanthus*, and the amount of corn stover harvested for cellulosic biofuel production. The land allocation decisions are subject to a constraint on the availability of cropland (eq S1) and constraints that limit the deviation in corn/soybean mix to less than 20% from the observed historical mix (eq S4). The production of *Miscanthus* is limited to a maximum of 60% of the land parcel area (eq S5). The harvestable corn stover is also subject to an upper limit (eq S2) of 30% of the stover produced per hectare to avoid negative environmental impacts.[23]

The SoS modeling approach is applied to the Sangamon Watershed, a 15 000 km^2 agricultural watershed in central Illinois (Figure 2). Spatial heterogeneity is incorporated on a 10 × 10 km grid, so that land allocation decisions can be made for each grid unit in the watershed. The crop supply from each grid unit is defined based on a predetermined crop yield per unit area for the various crops (eq S3). Cost per Mg of crop production differs across grid units due to differences in crop yields. The total cost of crop production in a grid is defined based on a predetermined cost per unit area for the various crops (eq S6).

Crop yield and cost per unit of production for each land use activity are shown in Figure S1. Historical county-level crop yield (1997−2010 from the USDA's NASS) and cost data for soybeans and corn were downscaled onto a 10 × 10 km land parcel grid.[24] The production costs and yields for soybeans and corn are based on conventional tillage rotation, which is currently the main practice in the Sangamon watershed. Corn stover yields were estimated on the basis of a 1:1 grain to stover mass ratio,[25] and assuming 30% of the corn stover is collected. According to a previous study,[26] no adverse environmental

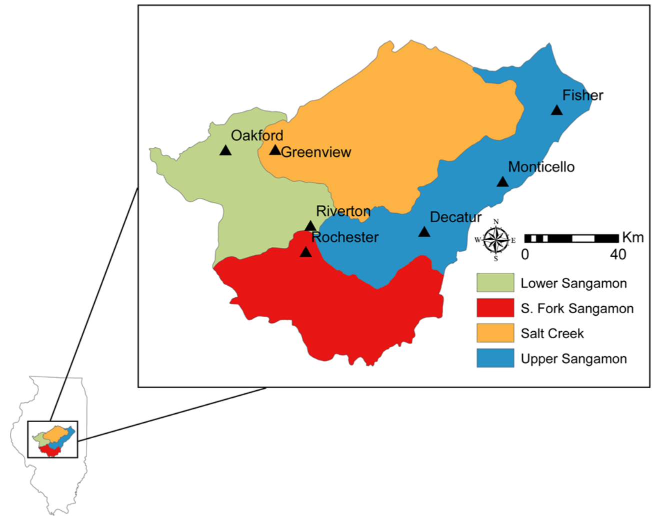

Figure 2. Location of the Sangamon River watershed and its major sub-basins in the state of Illinois. The HUC-8 cataloging codes are Upper Sangamon (07130006), South Fork Sangamon (07130007), Lower Sangamon (07130008), and Salt Creek (07130009).

effects are expected from this low stover collection rate because it is not likely to significantly impact the fertilization practices in the study area. *Miscanthus* yields are simulated using an extended version of the Integrated Science Assessment crop growth Model (ISAM) which consists of biophysical, physiological, and biogeochemical systems that affect crop growth.[27] Delivered *Miscanthus* yields are obtained assuming 20% harvesting loss, 7% storage loss, and 2% transportation loss.[28] Costs for *Miscanthus* planting and harvest were derived as described in Jain et al.[28] and differed across grids. A lifespan of 15 years is assumed, where there is no yield in the first year when *Miscanthus* is established, 50% of maximum yield in the second year, and then full yield in the remaining years of the life-span of the crop.

2.1.5. Refinery Subsystem. This subsystem accounts for the capital and the operating cost of refineries; the decision variables are the location, size, and number of corn-based and cellulosic-based refineries. The refinery capacity is subject to constraints on (1) minimum and maximum production levels (eq S7); (2) raw material conversion efficiency (eqs S8 and S9); (3) refinery water consumption (eq S11). The refinery cost includes both capital and operational costs in terms of fixed and variable annual costs (eq S13). The specific data used in the above constraints is provided in the Supporting Information. The model seeks the optimal size and location of refineries by weighing the benefits of economies of scale with larger refinery sizes against the costs of transporting feedstock and products.

2.1.6. Transportation Subsystem. The decision variables in this subsystem are the amount of feedstock to be transported from producers to refineries and the amount of products to be transported from producers to each of the demand nodes (eqs S14 and S15). The model also decides on the routes to use given the existing road network infrastructure (eqs S14 and S15), and its traffic bearing capacity (measured in terms of passenger car equivalents per hour per lane, pcphpl). The shipment routing is subject to constraints on congestion levels (eq S17), and the costs of transportation (eq S18). The transportation costs take into account the number of trips needed for each of the transported commodities, based on

Table 1. Optimal Configurations of Land Use, Ethanol Production, and Number and Type of Refineries and Resulting Profit, Nitrate Load, and Stream Flow during the Low-Flow Period (Aug−Oct) Determined by the SoS Integrated Model

	land use (km^2)		ethanol production (billion liters)			no. of refineries				average flow in low flow period (million cubic meters)		
scenario	*Miscanthus*	corn/soybeans	cellulosic	corn	total	cellulosic	corn	profit (b $)	nitrate-n load (1000s ton)	Monticello	Riverton	outlet
no-mandate	0	11000	0.000	1.363	1.363	0	6	1.757	25.6	21.8	96.1	224.7
mandate	1910	9120	1.590	1.136	2.725	5	5	1.616	22.5	18.9	91.2	213.4
NR16	2000	9030	1.590	1.136	2.725	5	5	1.604	21.5	20.7	94.2	211.4
NR20	2520	8510	1.893	0.833	2.725	5	4	1.578	20.4	20.9	94.5	208.4
NR25	3110	7920	2.256	0.757	3.013	6	3	1.523	19.2	20.6	92.6	202.8
NR30	3790	7240	2.650	0.693	3.343	7	3	1.465	17.9	20.7	93.1	200.9

truck capacity and the different commodities' densities (e.g., *Miscanthus* is less dense than corn grain, thus it has a higher transportation cost per unit mass). The specific data used in the above constraints is provided in the Supporting Information.

2.1.7. Environmental Subsystem. The model quantifies the contribution of each land cover (corn, soybeans, and *Miscanthus*) to water yield and nitrate-N load for each subwatershed (eqs S21−S25) as well as the streamflow and the nitrate-N load in the stream reaches (eqs S26−S27). Environmental policies are addressed by imposing minimum streamflow constraints (eq S28) and maximum nitrate-N load constraints (eq S29) on stream reaches at the subwatershed level.

The Soil and Water Assessment Tool (SWAT) version 2005 is used to examine the hydrological responses of different land covers in the watershed. For the inclusion of *Miscanthus* as a bioenergy crop, the SWAT model was modified following Ng et al.[7] In the SWAT model, the Sangamon Watershed was delineated into 104 subwatersheds, ranging in area from 20 km^2 to nearly 100 km^2. As in Ng et al.,[8] only the major land use management practices (e.g., fertilization, tillage, tile drains) in each subwatershed were implemented. The model was run for 12 years (1992−2003), thus incorporating a range of dry and wet years, and was calibrated from 1992 to 1997 against historical observations of daily streamflow at four USGS gauges within the watershed, monthly nitrate-N load at the outlet of Salt Creek, and the annual crop yield from the entire watershed (Figure 2). The Nash Sutcliffe Efficiency (NSE) obtained in the calibration and the validation of the SWAT model indicated satisfactory model performance. For detailed results on the SWAT calibration and for more information on the parameters selected in the calibration, the reader is referred to Yaeger et al.[29]

Following the calibration and validation, the SWAT model was used to estimate monthly water yield and nitrate-N load from each grid unit under each of the different land covers. The estimated nitrate-N load and water yield in May (the month with the maximum contribution of nitrate-N) are shown in Figure S2. Nitrate-N loading and water yield are estimated for each month to reflect the intra-annual hydrological seasonality within the watershed.

2.2. Policy Scenarios. The state of Illinois is considered one of the major biofuel producers in the United States. Kang et al.[14] estimated the IL share of production to be about 20% of the total US mandate; therefore, a plausible biofuel target for the Sangamon watershed is 2% of the US mandate, obtained by prorating the mandate based on the agricultural area in the watershed relative to that in Illinois. In what follows, the implications of meeting the biofuel target of 2% of the RFS in the Sangamon watershed is analyzed. However, the framework developed here can be used to analyze the effects of higher and lower levels of biofuel production. Three basic scenarios are analyzed, and their results are presented for the year 2022: (1) No biofuel target scenario (no-mandate scenario) in which no target is imposed on either corn-based ethanol or cellulosic ethanol. In this scenario, biofuels are produced according to their profitability given an exogenously specified ethanol price of $0.64 per liter (average price in 2012−2013). The no-mandate scenario is used as a benchmark to evaluate the impacts of the biofuel target on the various subsystems, such as land use, refinery locations and sizing, transportation, and the environment. (2) Biofuel target scenario with no water quality constraint (Mandate Scenario), in which a minimum total ethanol production of 2.725 billion liters of both corn and cellulosic ethanol, with a minimum from cellulosic sources of 1.590 billion liters, is required. (3) Biofuel target scenario with riverine nitrate-N load reduction targets of 16, 20, 25, and 30%, abbreviated as NR16, NR20, NR25, and NR30, respectively.

3. RESULTS

3.1. Impacts of Biofuel Targets on Biofuel Development. Under the no-mandate scenario, it is most profitable to produce 1.363 billion liters of ethanol from corn grain (Table 1) with no cellulosic production. Under the mandate scenario, producing the minimum required amount of both total and cellulosic ethanol is most profitable. For example, of the mandated 2.725 billion liters of ethanol, 42% is from corn grain, and 58% is from cellulosic feedstocks (*Miscanthus* and corn stover). The area planted with *Miscanthus* is 17% of the watershed. Five cellulosic refineries are added to the system; these refineries use both *Miscanthus* and corn stover for producing ethanol. Under the mandate scenario, 15% of the cellulosic ethanol is produced from corn stover.

The total net profit under the mandate scenario is 8% lower than that under the no-mandate scenario (Table 1). This reduction in the total profit implies that the price of cellulosic ethanol will need to increase from $0.64 per liter (the ethanol price assumed in the model) to $0.80 per liter to provide incentives for refineries to meet the mandate requirement in the watershed. Thus, cellulosic ethanol will need to be sold at a premium of $0.16 per liter relative to corn ethanol in order to induce its production. This premium could be interpreted as the minimum difference in the value of a renewable identification number (RIN) between cellulosic and corn-based ethanol required for cellulosic ethanol to be profitable.

These two scenarios also result in different infrastructure decisions and environmental impacts (Figure 3). The mandate scenario leads to conversion of land from conventional crops to

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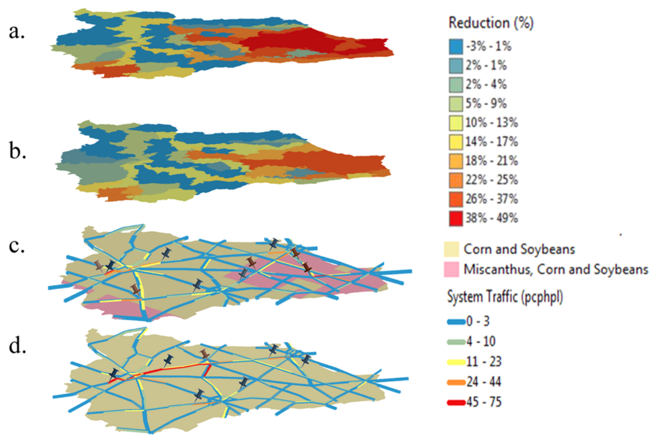

Figure 3. (a) annual nitrate-N load reduction with mandate Scenario as compared to the No-mandate scenario; (b) annual water flow reduction with Mandate scenario as compared to the no-mandate scenario; and refinery locations, traffic intensity and land allocation in 2022 in the (c) Mandate scenario and (d) the no-mandate scenario. Note: pinpoints represent selected refinery locations; pcphpl is defined as passenger cars per hour per lane.

Miscanthus in the Upper Sangamon sub-basin (Figure 3c) and the optimal development path would locate cellulosic refineries in the vicinity of the *Miscanthus* supply. Figure 3c, 3d shows differences in the optimal traffic routing and the resulting traffic congestion patterns in the no-mandate scenario and the mandate scenario.

Different development scenarios also have an effect on annual streamflows and nitrate-N loads, both in the regions where *Miscanthus* is planted and downstream of these regions (Figure 3a, 3b). The yearly nitrate-N load reduction compared to the No-mandate scenario approaches 49% in some of the subwatersheds that are converted to *Miscanthus*, and the streamflow also declines by up to 30% within these same subwatersheds. Furthermore, these impacts propagate and dissipate downstream of where *Miscanthus* conversion occurs; for example, the watershed outlet (Figure 2) exhibits only a 7% reduction in annual streamflow and a 12% reduction in annual nitrate-N load. In addition to reducing annual streamflow, the impacts from *Miscanthus* conversion also affect critical flows within the year. This is summarized in Table 1, which presents the annual reduction in nitrate-N load and corresponding streamflow reduction during the critical three-month low flow period of August, September, and October (ASO) at different locations in the watershed. In the Upper Sangamon, the region where most of the *Miscanthus* has been planted, the reduction in the average ASO flow at the Monticello gage is about 13%.

3.2. Impacts of Water Quality Targets on Biofuel Development. The results of the previous section show that meeting the targeted level of cellulosic biofuel production is likely to cause significant impacts on water quality and quantity as a result of converting land from corn/soybean to *Miscanthus*. Well-informed government policies and regulations might avoid or mitigate the streamflow reduction due to *Miscanthus* or optimize the benefits it provides by reducing the riverine nitrate-N load. Such environmental constraints will likely impose costs (reduce profits) on the system. As an example of such environmental constraints, different levels of nitrate-N load reduction are considered. To partially meet a 45% reduction target, suggested by the U.S. EPA Science Advisory Board to mitigate the hypoxia problem in the Gulf of Mexico,[30] annual nitrate-N load reduction constraints are imposed at the watershed outlet such that the outgoing nitrate-N load from the entire watershed area is reduced by various percentages (scenarios NR16-NR30).

As shown previously, the mandate scenario reduces the yearly nitrate-N load from the watershed outlet by 3081 Mg N yr^{-1}, which corresponds to a 12% reduction compared to the No-mandate scenario (Figure 3). Thus, *Miscanthus* may

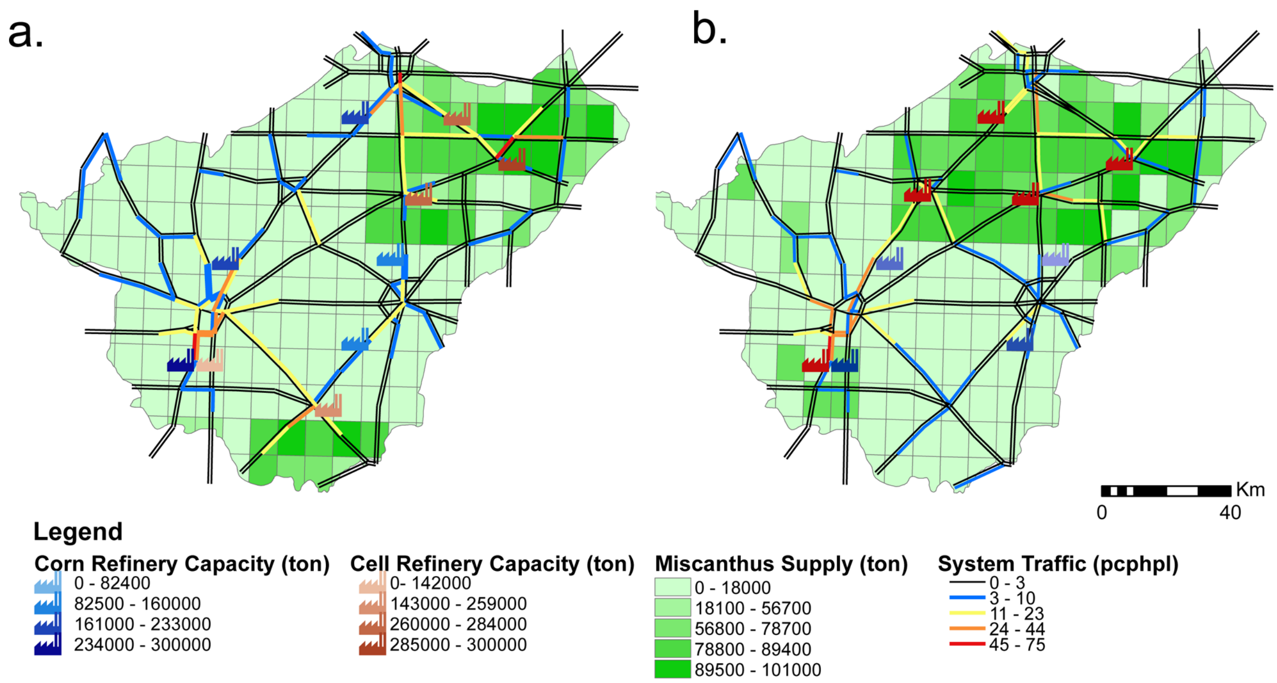

Figure 4. Optimal locations and capacities of ethanol refineries, *Miscanthus* production, and resulting traffic intensity under (a) mandate scenario, (i.e., without environmental constraints) and (b) NR20 scenario, with 20% nitrate-N reduction constraint.

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generate a win-win situation for both human (i.e., profit) and environmental systems by improving profitability and water quality while at the same time meeting cellulosic ethanol production targets. The cost of using *Miscanthus* as an instrument for a range of reductions of agricultural nitrate-N pollution by constraining the maximum nitrate-N load leaving the watershed is quantified in Table 1, where the results under 16, 20, 25, and 30% nitrate-N load reduction constraints with a biofuel production target equal to 2% of the RFS are presented. Both the total ethanol production and the feedstock choices varied depending on the nitrate-N load constraint. Compared to the mandate scenario, three types of changes are identified: (1) Under the 16% nitrate-N reduction constraint, both the total and cellulosic ethanol production stay at the minimum target level, but *Miscanthus* begins to replace corn stover as a feedstock for cellulosic ethanol. For this case, an additional 85.6 km^2 are converted to *Miscanthus*, resulting in an additional 4% nitrate-N reduction. (2) Under the 20% nitrate-N reduction constraint, the total ethanol production remains at the target level, but the cellulosic ethanol production is above its minimum target and more land is converted to *Miscanthus*. Here, cellulosic ethanol production is 69% of the total, compared to 58% under the mandate scenario. (3) Under the 25 and 30% nitrate-N reduction constraints, total ethanol production increases beyond the specified target. When the 30% nitrate-N reduction target is imposed on the system, the total ethanol production increases from 2.725 billion to 3.343 billion liters, and the percentage of ethanol from cellulosic feedstocks increases to 79%.

The contribution of crop production to nitrate-N runoff depends on the soil quality, topography, specific crop management practices implemented, hydrological characteristics (e.g., upstream/downstream position and presence of tile drainage), and meteorological characteristics of the subwatersheds. As a result, the nitrate-N runoff differs not only across crops but also across locations for a given crop. Reduction in nitrate-N load therefore can be met at the lowest cost by converting corn/soybean land to *Miscanthus* and placing it strategically at locations where corn/soybean production leads to the highest levels of nitrate-N runoff. In this way, *Miscanthus* is planted in areas that are optimized to reduce the nitrate-N runoff most effectively. Figure S2 shows the spatial pattern of nitrate-N contribution estimated by the SWAT model. Figure S2f shows that the lowest nitrate-N runoff from corn is in the southern portion of the watershed; these locations would be less beneficial, in terms of nitrate-N reduction, when corn is replaced by *Miscanthus*.

Comparing the development under NR20 scenario (Figure 4b) to that under Mandate scenario (Figure 4a) shows that the land area converted to *Miscanthus* increases from 17 to 32% of the watershed, with the additional *Miscanthus* mainly planted in the Salt Creek tributary (the northern part of the watershed) under the NR20 scenario. In the southern part of the watershed, however, fewer land parcels are chosen for *Miscanthus* compared to Figure 4a. This is because nitrate-N yields from corn/soybeans were lowest in the south, and therefore, conversion to *Miscanthus* in the north produced greater reductions in nitrate-N load at lower cost. Refinery infrastructure choices are also affected; while five cellulosic refineries exist in both scenarios, the locations are altered to cope with changes in the raw material supply, and the capacity of the cellulosic refineries is increased to handle the *Miscanthus* added to the system under the NR20 scenario. The model chooses the optimal size and location of refineries and the optimal crop allocations simultaneously by balancing the transportation cost for both the feedstocks and the final products with the capital cost of constructing the refineries.

The number of corn ethanol refineries is reduced from five in the mandate scenario to four in the NR20 scenario. While the optimal locations of these four refineries are the same in both scenarios, their capacity is increased to accommodate the new optimal production levels. Lastly, the changes to the refinery infrastructure and the raw material production areas lead to different traffic patterns in the watershed (Figure 4). For example, under the mandate scenario, in the southern part of the watershed, the cellulosic refinery resulted in 11−23 pcphpl around the refinery, whereas in the NR20 scenario, the cellulosic refinery does not exist, reducing the traffic to 3−10 pcphpl. This additional traffic is added to rural areas where the refineries are to be built. An additional 23 pcphpl can have an impact on rural roads both in terms of increased maintenance and public resistance to congestion. Under this condition, the service level of the current transportation system is limited, especially in the southern part of the watershed. If no expansion of the current transportation system is allowed, this will lead to a cascade of impacts on all the individual subsystems, including refinery locations and capacities, transportation loads, and crop choices. The development plan when the southern part of the watershed has to maintain the same level of service without the possibility of expanding the transportation infrastructure in the area is presented in Figure S3.

3.3. Trade-offs among Water Quality Targets, Water Quantity, and Profits. The spatial shifts in *Miscanthus* planting altered streamflow regimes in different locations in the watershed. The trade-off between the nitrate-N reduction targets and the reductions in the ASO low flows is illustrated in Figure 5 at the five locations in the watershed shown previously in Figure 2. As the nitrate-N reduction target increased from 16 to 30%, more *Miscanthus* was planted in the Salt Creek tributary, which led to greater reductions in ASO flows in that area, for example, Greenview (Figure 5). On the other hand, as less *Miscanthus* was planted in other portions of the watershed,

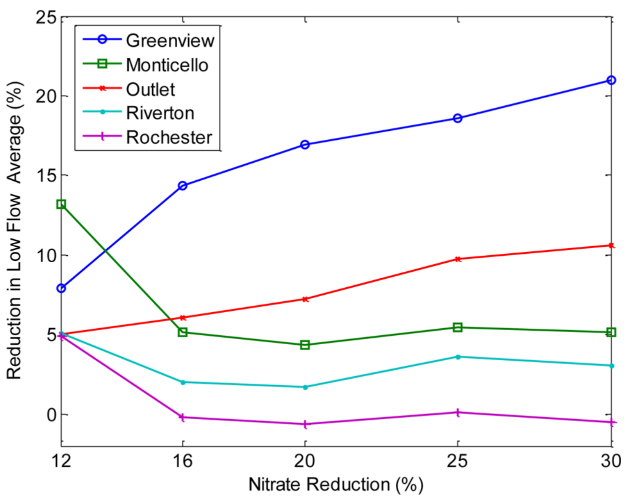

Figure 5. Estimated average streamflow reductions (relative to the no-mandate scenario) during August through October as a result of different nitrate-N reduction constraints imposed using the SoS model. Mandate scenario (0% nitrate-N constraint) resulted in a 12% nitrate-N reduction.

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the streamflow reductions declined at those locations (e.g., Monticello and Rochester). For the Sangamon Watershed as a whole, the area planted to *Miscanthus* increased as the nitrate-N reduction target increased, which led to increasing reductions of ASO flows at the outlet. The results above suggest that the trade-off between the water quality benefit and the water quantity effect can vary spatially. Thus, environmental regulations aimed at reducing nitrate-N should also take into consideration the impacts on streamflow at different locations in the watershed, because streamflow reduction during the low flow period would likely have negative impacts on aquatic and riparian ecosystems. Fish kills commonly occur in this region during the low-flow period, but additional factors such as temperature and pollution discharge are often involved. Additional research is needed to quantify the impacts of reducing low flows and extended periods of low flow that may result from extensive planting of perennial biofuel crops.

As the nitrate-N reduction target increases, the marginal cost (i.e., the profit loss) of nitrate-N reduction increases (Figure 6).

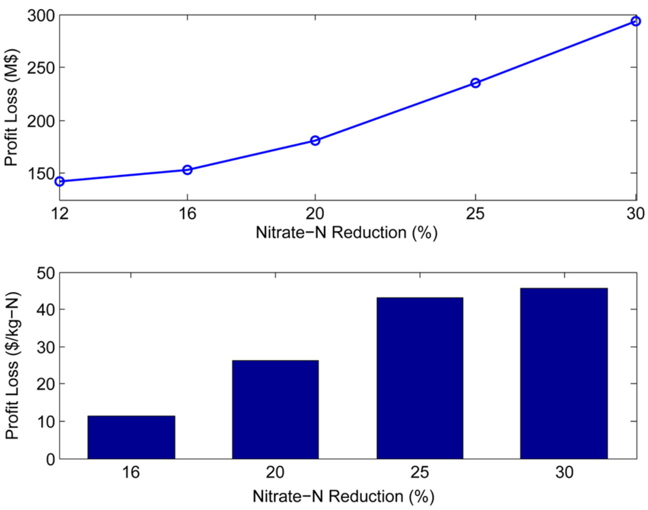

Figure 6. Estimated profit loss from no-mandate scenario (top panel) as a result of the biofuel target (12% nitrate-N reduction) and four levels of Nitrate-N reduction constraints; marginal cost of each nitrate-N load reduction constraint per kg nitrate-N reduced (bottom panel).

The mandate scenario reduces profit by \$141 million per year, an 8% reduction from the No-mandate scenario, while reducing nitrate-N loads by 3081 ton per year (12%). If all the cost of implementing the biofuel target is assigned to nitrate-N reduction, which was not the intent of the RFS, nitrate-N was reduced at a cost of \$45.5 per kg of N. Adding a nitrate-N reduction constraint of 16% reduces profit an additional \$11.8 million per year (a 1.7% reduction in profit from the Mandate scenario) and reduces nitrate-N loads by an additional 1000 ton, hence the per kg nitrate-N reduction cost is \$11.8 per kg of N. Increasing the nitrate-N reduction constraint from 25% to 30% costs \$45.6 per kg.

3.4. Sensitivity Analysis. The sensitivity of the model results to two critical parameters: (a) the biofuel production mandate assumed to be fulfilled within the watershed and (b) the maximum limit on land that can be converted to *Miscanthus* at each grid unit, is examined next. First, values for the mandate, ranging between 50 and 150% of the primary value, are considered; as shown in Figure S4, different levels of mandated biofuel production have different impacts on the system. Increasing the mandate level results in more *Miscanthus* planted in the watershed, accompanied by infrastructure development, and associated with changes in streamflow and nitrate-N load regimes in the watershed. As shown in Figure 4, the northeast portion of the watershed is found to be the preferable area for planting *Miscanthus* under the mandate scenario. As the level of the mandate increases, more *Miscanthus* is planted in that region. However, after the capacity of that region for growing *Miscanthus* is reached, *Miscanthus* planting moves to less favorable areas, and new infrastructure development and traffic patterns are introduced. The impacts of the different levels of mandated biofuels production on the annual streamflow and nitrate-N load at the Monticello gage is shown in Figure S4.

For all levels of biofuel mandate, the reduction in the streamflow is smaller than that in the nitrate-N load. When the mandate level is larger than 50% of the original value, the reduction in the flow and nitrate-N load demonstrates a concave relationship. Thus, the marginal reduction, both in streamflow and nitrate load, is decreasing with the mandate level. Noteworthy is that requiring more than 100% of the original mandated biofuel production from the watershed has little effect at the Monticello gage, indicating that the capacity of the Upper Sangamon to produce *Miscanthus* is nearly reached; thus, the streamflow and nitrate-N reduction at the Monticello gage are upper bounded.

There is also considerable uncertainty about the limit of 60% placed on the amount of land that can be converted to *Miscanthus* in each grid unit. The sensitivity of this parameter was analyzed within a range of 50−70%. The ranges of outcomes obtained and presented in Table S1 show that all values of the *Miscanthus* maximum limit lead to very similar nitrate-N and streamflow reduction, mix of biofuels, and infrastructure development. Similarly, the area planted with *Miscanthus* is relatively stable. However, with higher values of the parameter, *Miscanthus* is introduced on fewer land parcels, because there is greater concentration of production in areas with relatively high *Miscanthus* yield.

4. DISCUSSION

The interdependency between biofuel development and environmental targets was quantified through an SoS model combining agricultural land use, processing, and transportation infrastructure systems, and the environmental system. The analysis was conducted in the Sangamon River watershed in central Illinois, where, under the no-mandate scenario, high nitrate-N loads from intensive cultivation of corn and soybeans on tile drained soils have negative impacts on surface water quality. Implementing the advanced biofuels portion of the RFS mandate has the potential to reduce these nitrate-N loads by converting some land from corn/soybean rotation to *Miscanthus* production. Hence, replacing corn with a dedicated biofuel crop such as *Miscanthus* may be considered as a strategy for regional nitrate-N pollution mitigation. However, this would also result in stress on streamflow and associated ecosystem services (especially in the smaller order streams, which are more sensitive to flow variability) because drainage to streams is reduced due to the relatively high evapotranspiration under *Miscanthus*. It also imposes economic costs of changing land use from corn/soybeans to *Miscanthus* and developing the infrastructure to convert it to biofuel. It is thus important for decision makers to consider the trade-offs among water quality gains, streamflow reductions, and economic costs when

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increasing land area is converted to *Miscanthus*. Furthermore, the impacts of nitrate-N reduction targets on streamflow will vary with location in the watershed; in the study watershed, the low flows will be most adversely affected in the subwatersheds where *Miscanthus* cultivation is concentrated.

Compared to other practices, the cost of using *Miscanthus* to improve water quality is relatively high when the nitrate-N reduction target is high (~$45/kg-N at 30% nitrate-N reduction). A recent Iowa study corroborated this result and estimated that the cost of converting land from row crop production to perennial energy crops would be $47 per kg nitrate-N reduced.[31] Less costly practices, such as tile denitrification bioreactors ($2 per kg nitrate-N), constructed wetlands ($3 per kg nitrate-N), and winter cover crops ($13 per kg nitrate-N) are available for removing nitrate-N. However, *Miscanthus* production is motivated here by a biofuel mandate used to achieve some of the RFS mandate, and a modest additional expansion of *Miscanthus* can still be cost competitive with other means of reducing nitrate-N loads. Moreover, lower cost practices have a limited geographic range of suitability, and meeting a 45% nitrate-N load reduction target in Iowa and Illinois will likely require a combination of practices, including extensive use of winter cover crops, which reduce nitrate-N at a similar cost per kg nitrate-N as the 16% nitrate-N load reduction constraint presented in this study. On the basis of these results, policy makers considering *Miscanthus* as a biofuel feedstock and a tool for nitrate-N reduction need to decide on their willingness-to-pay for the reduction targets by balancing among water quality improvement, water quantity reductions, and economic profit loss.

Environmental policies, in the form of nitrate-N reduction targets, are demonstrated as a potential tool to enhance the environmental benefits of the biofuel mandates. Imposing such environmental constraints on the interdependent systems, however, reduces profit and changes the optimal biofuel development configuration and costs. The impacts of these constraints propagate to all systems related to the biofuel production. Optimal refinery locations and capacities, transportation loads, and land allocation will all be changed as a result of nitrate-N load constraints, and this cascade of impacts may be overlooked if the analysis were conducted only at the subsystem level. An SoS approach, as presented in this paper, can be an effective tool for exploring inter-relationships between infrastructure systems and the environment.

The analysis here assumed that binding nitrate-N reduction targets could be imposed on the watershed and would lead landowners to alter crop choices to achieve the targets. In practice, conservation policies have relied on financial payments to farmers to achieve water quality targets, through programs such as the Environmental Quality Incentive Program and the Conservation Reserve Program, for changing production practices and land use. Our research shows the loss in profits to farmers due to these nitrate-N reduction targets and the financial compensation they would need in order to induce farmers to shift land use from corn/soybeans to *Miscanthus*.

The framework developed here assumes that the effects of land use change on riverine nitrate loadings are known with certainty. In reality, nitrate loadings are dependent on soil, management, weather conditions and other factors that are uncertain. As a result, it is not feasible to achieve water quality goals with certainty; instead it may be more appropriate to specify probabilistic goals for water quality and examine the costs of achieving them with a given probability. We leave it to future research to develop relevant probability distributions of the impact of energy crop production on nitrate runoff and analyze its implications for the design of policies to achieve targeted levels of reduction in nitrate loadings. Additionally, we focused on economically significant costs in the Sangamon River watershed and have not considered economic impacts outside the watershed. Reduction of nitrate loadings in the watershed could lead to lower costs of water treatment downstream and higher profits to commercial fisheries due to increase in fish populations in the Gulf of Mexico. Estimating the extent to which these downstream benefits can offset the costs of abatement within the watershed is outside the scope of this study and we leave it to future research to determine the extent to which this is the case.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.est.5b02712.

Detailed mathematical formulation of the optimization model (PDF)

AUTHOR INFORMATION

Corresponding Author

*Phone: +1 (217) 333-4935. E-mail: xmcai@illinois.edu.

Notes

The authors declare no competing financial interest.

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