Multifunctional Landscapes: Site Characterization and Field-Scale Design to Incorporate Biomass Production into an Agricultural System

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ABSTRACT

Current and future demand for food, feed, fiber, and energy require novel approaches to land management, which demands that multifunctional landscapes are created to integrate various ecosystem functions into a sustainable land use. We developed an approach to design such landscapes at a field scale to minimize concerns of land use change, water quality, and greenhouse gas emissions associated with production of food and bioenergy. This study leverages concepts of nutrient recovery and phytoremediation to place bioenergy crops on the landscape to recover nutrients released to watersheds by commodity crops. Crop placement is determined by evaluating spatial variability of: 1) soils, 2) surface flow pathways, 3) shallow groundwater flow gradients, 4) subsurface nitrate concentrations, and 5) primary crop yield. A 0.8 ha bioenergy buffer was designed within a 6.5 ha field to intercept concentrated surface flow, capture and use nitrate leachate, and minimize use of productive areas. Denitrification-Decomposition (DNDC) simulations show that on average, a switchgrass (*Panicum Virgatum L.*) or willow (*Salix spp.*) buffer within this catchment according to this design could reduce annual leached NO_3 by 61 or 59% and N_2O emission by 5.5 or 10.8%, respectively, produce 8.7 or 9.7 Mg ha^{-1} of biomass respectively, and displace 6.7 Mg ha^{-1} of corn (*Zea mays L.*) grain. Therefore, placement of bioenergy crops has the potential to increase environmental sustainability when the pairing of location and crop type result in minimal disruption of current food production systems and provides additional environmental benefits.

Keywords: cellulosic biofuels, sustainability, GHG emissions, nitrate leachate, marginal lands, and nutrient recovery

1.0 Introduction

Meeting bioenergy production goals set by the Renewable Fuel Standards provisions of the 2007 U.S. Energy Independence and Security Act (EISA) requires finding economically viable, socially acceptable, and environmentally sustainable production strategies to grow bioenergy crops. Today, the major commercial feedstock for the U.S. ethanol industry is corn grain, with over 40% of the crop used for ethanol production [1, 2]. To minimize food, feed and energy competition, EISA mandates that a large percentage of fuel originate from lignocellulosic feedstock by 2022. Internationally, other energy policies such as the European Commission's Energy Policy have also led to the development of national renewable energy action plans, in which dedicated energy crops are a major component of the renewable energy portfolio [3, 4]. With one more competing use for finite land resources, and an increased focus on sustainable practices, there is traction to design new best practices that purposefully "engineer" sustainability into the production of bioenergy [5].

Several programs have been encouraging the establishment of a bioenergy supply chain. In 2007, the state of Tennessee funded the establishment of 2,064 ha of switchgrass as part of an integrated biofuel initiative of switchgrass-to-ethanol production chain [6, 7]. Farmers within an 80 km radius of a pre-commercial biorefinery were offered contracts to enroll. Enrolled farm sizes ranged from 6 to 121 ha. In 2008, the U.S. Farm Bill established the Biomass Crop Assistance Program (BCAP) to enroll land classified by the Farm Service Agency (FSA) as cropland and non-cropped agricultural land, to cover 75% of the establishment costs of lignocellulosic energy crops [8]. By 2012, there were 21,495 ha of land in 12 states enrolled into the BCAP to grow herbaceous and woody crops [8].

According to the updated U.S. “Billion-Ton” study, almost a billion tons of biomass could be available for cellulosic biofuel production by 2030 at a farm gate price of \$66 Mg⁻¹ [9, 10]. The projected biomass supply is assumed to be dominated by dedicated perennial grasses, short-rotation woody crops, corn stover, and woody residues from logging and forest-thinning operations. The updated U.S. “Billion-Ton” study assumes that at a price of \$66 Mg⁻¹ and under a high corn yield scenario, about 10.5 million ha of cropland and about 18.2 million ha of pasture would be converted to energy crop production. However, in the U.S. Corn Belt (Midwestern U.S.), the current state of farmer “buy-in” to switch from dedicated commodity to energy crops is limited because of various reasons, of which higher profit margins is the most relevant since profitability is the major motivator for adoption of new or old crops [10-12]. However, precision agricultural tools have demonstrated that intra-field variations in yields may result in areas of high and low return on investment [13], thereby opening up an opportunity such that areas of low return on investment can be converted to other cost effective crops.

Current row crop production practices in the U.S. Corn Belt are a major contributor of nutrients to Gulf of Mexico hypoxic zones [14]. According to USEPA, agricultural systems contributed 75 % of nitrous oxide (N₂O) emissions in 2012 [15]. Also Fassbinder et al. reported up to 80 % of N₂O emissions from agricultural systems [16]. The N₂O emissions have a warming ability that is 310 times that of carbon dioxide (CO₂) emissions [15]. Nitrogen inputs are one of the highest contributors to the energy cost of row crops [17], therefore, approaches that aim at recovering the lost nitrogen are economically and energetically advantageous while improving the environmental footprint of the agricultural enterprise. We propose that the industrial ecology concept of resource recovery be applied to the agricultural production system by designing bioenergy crop systems that passively reuse the lost nitrogen from row crops to enhance the

yields of the bioenergy crop without additional fertilizer input. This integration of bioenergy crops into current agricultural systems at field-, farm- and watershed-scales should increase the actual nitrogen use efficiency at the field and farm scale. We hypothesize this could be accomplished by exploiting different root system exploration and nutrient capture patterns throughout the different parts of the soil profile. Perennial bioenergy crops have distinctive traits that can be exploited to provide environmental services: deeper root systems, the ability to thrive on poorer soils, the ability to survive more extreme conditions of drought and flooding after establishment [18, 19], and for some like poplars (*Populus spp.*) and willows (*Salix spp.*), the demonstrated ability to capture shallow groundwater plumes and hydraulically contain them and remove entrained pollutants by phytoremediation [20-23]. Capitalizing on these traits will allow for the engineered placement of bioenergy crops in sub-productive or critical areas, thus providing a potential environmental benefit with minimal disturbance of overall corn production.

This study presents a design methodology that integrates bioenergy crops into a continuous corn field to optimize land use for food, bioenergy crops, and ecosystem services. This approach utilizes four relatively simple environmental components of soil analysis, terrain analysis, site groundwater elevation, concentration of nitrates ($\text{NO}_3 + \text{NO}_2\text{-N}$) in subsurface soil-water, as well as an economic component of corn yield at the intra-field scale to direct the placement of a bioenergy crop “remedial” strip. Suboptimal corn yields were defined as less than 3.8 Mg ha^{-1} . Changes in leached NO_3 and N_2O emissions were simulated by a Denitrification-Decomposition (DNDC) model [24, 25].

2.0 Materials and methods

2.1 Site description

The study site is a 6.5-ha field near Fairbury, Illinois (Figure S1; latitude: 40.742°N, longitude: 88.499°W) under continuous corn rotation. The site is bordered by another field under a corn-soybean rotation to the east and a riparian forest to the west. The riparian forest is adjacent to the Indian Creek (which drains into the Vermilion River, IL) such that parts of the field flood under prolonged high flow conditions. The field is not drained by tiles and boundary roads hydrologically isolate it from adjacent fields. The site has two soil series, Comfrey loam in the lower flood plain and Symerton silt loam in the upland till plain [26]. The Comfrey loam has slopes of 0 – 2% and experiences frequent, brief periods of flooding, while some parts of the Symerton silt loam are eroded with slopes of 5 – 10%. The mean annual rainfall recorded at the nearby Fairbury waste water treatment plant (accessed through the Global Historical Climatic Network: GHCN) is 887 mm over a 31-year period (1981 to 2011), while the 13-year (2000 to 2012) mean annual total evapotranspiration using data from the North American Land Data Assimilation System (NASA-NLDAS [27]) is 661 mm.

2.2 Agronomic soil analysis

A GeoProbe® drilling system was used to collect continuous soil cores using a macro-core sampler (outer diameter of 2.54 cm) lined with acetate sleeves and directly push-drilled to a soil depth of 1.5 m below ground surface. Continuous soil cores were extracted at 30 locations (Figure S1) based on a regular grid sampling pattern of about 43 m by 43 m. For each sampling location, soil cores were analyzed for matrix color, texture, structure, consistence, presence of

roots, physiography (floodplains or upland till plains), compaction, and probable drainage class at soil depth intervals of 22 cm to 30 cm.

Soil cores at 30 locations and resultant soil map (Figure 1a), confirmed the physiography as a floodplain in the northern part and upland till plain in the southern part of the site. The sample-generated soil map was similar to the one from the NRCS web soil survey [26]. However, there was a 65.5 % difference in areal classification of the eroded Symerton silt loam (294C2) between the two maps (Figure 1a has 0.8 ha while Figure 1b has 2.35 ha), with the predominant difference being associated with boundaries for the 2 to 5% and 5 to 10% slopes of the Symerton series. This map provided an accurate analysis of the spatial features of each soil to understand issues of water conductivity, erodibility and fertility, which are determinants of the vulnerability of sub-field areas to environmental impacts. It also confirms the dependence of yields on soil properties and suggests the probable causes behind variations in yield maps.

2.3 *Terrain analysis*

The site point elevation data was collected using real time kinematic (RTK) GPS surveying system which gives centimeter-level accuracy [28]. The base GPS receiver was set at an arbitrary point at the northeastern corner of the field while the rover GPS receiver was mounted to an all-terrain vehicle (ATV) and set to record data continuously at an average horizontal interval of about 8 m. A total of 889 point elevations were collected, of which 185 were collected along the field boundary. The survey datum was considered to be a local datum because no national geodetic survey (NGS) benchmarks were cross referenced. The point elevation data was used to generate a regular 1 m by 1 m horizontal resolution digital elevation model (DEM) using the ANUDEM 5.3 algorithm[29] implemented in ArcGIS 10.1 software [30].

The terrain analysis focused on delineating the major surface flow paths as indicators of intrafield areas with high accumulation and transport of surface runoff and water erosion. Since the revised universal soil loss equation (RUSLE2) or the water erosion prediction project (WEPP) models [31, 32], are dependent on pre-defined hillslope profile and drainage network (terrain analysis), therefore, for same land use and land cover, soils, and climate, terrain analysis is an apt alternative to RUSLE2 or WEPP. The longest flow paths were generated from the DEM by the deterministic eight nodes (D8) algorithm which accumulates flow distances across the grid cells based on the largest flow path length of all upslope contributing areas [33].

2.4 *Hydrogeological investigations*

To generate a shallow groundwater numerical flow model, seven groundwater monitoring wells (Figure S1; MW1, MW2, MW3, MW4, MW5, MW6S, and MW6D) were installed along the boundary of the field and at one central location. During well drilling, soil and sediment samples were collected using continuous split spoons. At all well locations, except MW2, the soil profile comprises a topsoil and a glacial till, below which is a significant sand unit. The wells were screened in the sand. Monitoring well MW2, which is located at a topographically higher location, was screened in a thinner sand unit that was later found to be perched (higher than the main sand aquifer and hydraulically separated from the sand aquifer). Wells 6S and 6D are located in close proximity in the center of the field. One is screened at a shallow depth of 1.2 m to 3.0 m (MW6S) while the second at a greater depth of about 4 m to 6 m (MW6D).

Modeling of subsurface hydrology using MODFLOW[34] has been used to design efficient plantings that target specific water budgets and plumes [35]. A one-layer numerical groundwater MODFLOW model was constructed using Indian Creek as a specified head boundary condition

(west side of the field) and general head boundaries along other field boundaries. The domain of the MODFLOW model is the sand unit that is screened by most of the monitoring wells (MW1, MW3, MW4, MW5, MW6S, and MW6D) and a farm well, located near the northeast corner of the field. The top and bottom of this unit were both encountered in some of the monitoring well locations; in others, the bottom contact elevations were estimated based on nearby data. In addition to the numerical MODFLOW model, the modeling environment included the drilling data, water level data, interpolated water level surface, aerial photography, and U.S. Geological Survey topographic maps.

2.5 Soil-water nitrate

Thirty macro rhizons (Rhizosphere Research Products, Wageningen, Netherlands) were installed at a depth of 1.2 m to sample repeatedly the seepage of the soil water in the unsaturated zone from the same soil volume. The rhizons were installed using a Geoprobe® 2.54 cm rod beside the 30 locations where continuous soil cores were extracted (Figure S1). PVC liners (sleeves) were tightly fit into the drilled holes to minimize influence of preferential flow at the sampling depth. The rhizons filter the extracted soil water over a porous membrane with an outer diameter of 4.5 mm and a pore size of 0.15 µm. There were four soil-water sampling events after wet weather conditions of greater than 13 mm precipitation within a 5 day window (7/1/2011, 7/8/2011, 7/15/2011, and 8/12/2011). This condition lead to collection of a soil-water sample at more than 60% of the sampling locations. For each sampling event, a soil water sample was extracted by applying a vacuum on the in-situ macro rhizons using a tubing connector, a three-way luer lock, and two 60 mL syringes. The syringes act as both the vacuum pump and container for the soil water samples. After a collection time of 24 hours, the samples were immediately transported in a cooler with ice packs to the laboratory. For nitrate-nitrite ($\text{NO}_3+\text{NO}_2\text{-N}$)

analysis, the samples were preserved using sulfuric acid (H_2SO_4) and analyzed within the required shelf life by a contracted certified laboratory (Servi-tech Labs at Hastings, Nebraska) using U.S. Environmental Protection Agency (EPA) standard method (EPA 353.2).

A continuous spatial map of the $\text{NO}_3+\text{NO}_2\text{-N}$ concentrations at a depth of 1.2 m was generated in ArcGIS 10.1 software using deterministic interpolation by a radial basis function (RBF) [36]. The RBF interpolates data using a sum of localized linear equations known as basis functions. The basis function used for this analysis was the completely regularized spline [37]. This method was chosen as preliminary analysis using the leave-out-one cross-validation (LOOCV) method gave better performance (based on the mean relative error) than Ordinary Kriging (OK) and Empirical Bayesian Kriging (EBK). The LOOCV method generates a prediction model using all data except a single data point. Then model validation is carried out by comparing the observed and predicted values at this point. The process is repeated a predefined number of times, where each time a different data point is excluded.

2.6 Crop yield map

Corn was planted in late April for the most recent five years by the same farmer using conventional plow tilling and a fall nitrogen application of 170 to 228 kg N ha^{-1} as anhydrous ammonia. A geo-referenced corn yield map of the 2011 corn harvest was generated by the John Deere ApexTM Farm Management Software based on the volumetric grain flow data generated by the GreenStarTM yield monitoring system (John Deere Company, Moline, IL). The raw yield data were pre-processed in ArcGIS 10.1 software to remove erroneous extreme values. Extreme values ($> 25 \text{ Mg ha}^{-1}$) may be recorded when the combine operator is turning at the end of the

row or due to start and end pass delays or due to loss of differential global positioning system (DGPS) signal [38, 39]. Therefore, values above 25 Mg ha⁻¹ were reclassified as “No data”.

2.7 Biogeochemical modeling

N₂O emissions and NO₃ leachate under corn and bioenergy crop buffer scenarios (willows or switchgrass) were modeled using the DNDC biogeochemical process model [40, 41]. The model consists of six interacting sub-models that simulate soil climate (soil temperature, moisture, and redox potential profiles), crop growth (water and N uptake, root respiration and plant growth), decomposition (CO₂ production and NH₄ volatilization), nitrification (conversion of NH₄⁺ to NO₃⁻), denitrification (production of NO, N₂O, and N₂), and fermentation (production of CH₄, oxidation and transport processes). Model processes are run on a daily time step and data inputs include daily climatic data (e.g., rainfall and temperature), soil data (e.g., texture, bulk density, initial soil organic carbon and pH), land use (crops and crop rotation) and land management (e.g., planting and harvesting dates, tillage and fertilizer). The model tracks microbial oxidation of NH₄ under aerobic conditions (nitrification) and sequential reduction of NO₃ under anaerobic conditions (denitrification) as the main sources of N₂O [42]. It assumes nitrification rates are controlled by soil temperature, moisture, pH and NH₄ concentrations. Denitrification rates are controlled by soil moisture and redox potential. More details on process equations and interactions are given by Li et al. [24, 40], Giltrap et al. [43], and Vogeler et al [44]. DNDC performance has been validated at multiple sites for simulation of N₂O [45, 46], leaching of NO₃ [47, 48], and simulation of soil organic carbon at field and regional scales [41, 49]. Borzecka-Walker et al. [50] used DNDC to simulate carbon and nitrogen balances under willow for several regions in Poland.

242 DNDC crop parameters for corn and willow were calibrated using historical field data at
 243 Fairbury, IL (Fairbury site) and Tully, NY [Tully site; 42.7970⁰, -76.1182⁰ [51] No willow data
 244 closer to the study site], respectively. Switchgrass crop parameters were based on validated data
 245 for a site in central Illinois [52], The Fairbury site was divided into three sub-fields to represent
 246 soil classifications of Comfrey loam, Symerton silt loam and eroded Symerton silt loam (Figure
 247 1). Fairbury site corn yields from 2008 to 2011 were used for calibration (No field data for 2012
 248 due to extreme drought). Site management activities include spring fertilizer application (30 kg
 249 N ha⁻¹ as anhydrous ammonia) and corn planting on April 28th, harvesting on October 15th, fall
 250 tillage (conventional ploughing up to 10 cm depth) on October 25th, and fall fertilizer application
 251 (170 - 228 kg N ha⁻¹ as anhydrous ammonia) on November 2nd. Willow yields at the Tully site
 252 were based on a four year rotation (1995 to 1999) with no fertilizer application (control
 253 treatment) to calibrate DNDC willow crop parameters. According to the U.S. web soil survey
 254 [53] the Tully site soils are predominantly well-drained Palmyra gravelly loam (pH=6.5; bulk
 255 density = 1.25 g cm⁻³; organic matter = 5%; clay content = 22%; and saturated hydraulic
 256 conductivity = 23 μm s⁻¹). Daily climatic data (temperature and precipitation) at Binghamton
 257 Broome County Airport, NY (GHCND station ID: USW00004725) were used for simulations at
 258 the Tully site. Willow biomass under treatments of sulfur coated urea (SCU) broadcast at the rate
 259 of 100 kg N ha⁻¹ and 300 kg N ha⁻¹, and composted poultry manure (equivalent to 1000 kg N ha⁻¹
 260 and total C = 379 g kg⁻¹) were used to validate the willow crop parameters under a broad range
 261 of nitrogen applications and sources at the Tully site. The willows under all treatments at the
 262 Tully site were coppiced in the first year. Because of limited and incomplete experimental data
 263 on NO₃ and N₂O for similar soils under corn and the two bioenergy crops, DNDC was not
 264 calibrated for NO₃ and N₂O. Therefore, simulations focus on expected relative changes rather

than actual values under the two bioenergy scenarios. Table 1 defines the literature based and calibrated willow crop parameters.

This DNDC study models three scenarios over a five-year period (2008 to 2012) to quantify relative changes in annual ecosystem services of NO₃ leachate and N₂O emissions: 1) business as usual with continuous corn (Corn), 2) replacement of corn in a contour strip with switchgrass (Corn/switchgrass) and 3) replacement of corn in a contour strip with short rotation willows (Corn/willow). DNDC is a site model that does not account for geospatial connections between sub-field areas, therefore the routing of NO₃ leachate from the upland corn field to the contour buffer was modeled by adopting a two-step approach. The first step independently simulated NO₃ and N₂O on soils upslope of the buffer, in the buffer, and below the buffer under corn production (Corn). The second step uses the fertigation module to apply the daily NO₃ from the upslope corn as the only source of fertilizer to the bioenergy crop (switchgrass or willow). The second step assumes 80% of the leachate is available to the buffer and is uniformly distributed across the buffer width. This assumption is based on the high shallow groundwater flow gradient in the upland till plains (Figure 2b).

The authors recognize the upslope NO₃ will vary across the buffer due to differences in micro-topography and soil heterogeneity. However, for modeling purposes the uniform distribution is assumed to represent average conditions. Reported values at the Fairbury site are area-weighted using areal extent of the three soil class series (Figure 1a). Model performance is evaluated using coefficient of determination ($0 \leq R^2 \leq 1$) and percent bias (Equation 1; $-100 \leq \text{PBIAS} \leq 100$). The optimal value is one for R^2 and zero for PBIAS. A positive or negative PBIAS is indicative of model under-prediction or over-prediction, respectively.

$$PBIAS = \left[\frac{\sum_{i=1}^n (Observed_i - Simulated_i) \times 100}{\sum_{i=1}^n Observed_i} \right] \quad [1]$$

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3.0 Results and discussion

3.1 *Field observations and data analysis*

Assessment of surface flow accumulation and transport using the longest flow paths (Figure 2a) offers two major observations. First, there are multiple points along the western field boundary where surface runoff and associated nutrients can flow to the riparian forest and Indian Creek. The second observation is that the dominant and longest flow paths (greater than 120 m) are concentrated in the southeastern part of the field where the Symerton series is found. Figure 2a shows most long flow paths for surface flow accumulation and transport do not directly discharge into the riparian forest (western part of the field), but rather flow from the upland till plains to the flood plain and thus are subject to concentrated flow. This results in greater erosive forces and suggests that planting bioenergy buffers to intercept and shorten flow path lengths could provide the best option for achieving concurrent biomass and environmental benefits.

Hydrogeological investigations show that monitoring well MW2 (Figure S1) is hydraulically separated from the sand targeted by other wells (MW1, MW3, MW4, MW5, MW6S, and MW6D). Well MW1 is influenced by drawdown from a neighboring farm well. Analysis of water level data for wells MW3, MW4, MW5, MW6S, and MW6D suggest a slight groundwater flow gradient paralleling the creek to the northeast, with values of 0.0006 to 0.001 m/m (Figure 2b). The gradient is somewhat steeper in the vicinity of MW1, but overall the rate is consistent with the average creek gradient, which based on USGS topographic maps is 0.00074 m/m. Shallow groundwater flow direction determined the probable path of nutrients, although we don't see the plume constantly going north.

316 The 07/01/2011 data show high (greater than 50 mg/L) concentrations in the southern part of the
317 field which is characterized by the Symerton series. Two weeks later (on 07/15/2011), data show
318 an overall increase in nitrate concentrations at 1.2 m depth, possibly due to percolation and
319 movement of high nitrate leachate from the northeast (similar to groundwater flow direction).
320 This observation is attributed to both variable vertical percolation due to soil profile
321 heterogeneity and lateral flow. Rainfall during this same time frame was about 12 mm.
322 Subsurface nitrate measurements one month later (on 08/12/2011) show the high concentration
323 zone had dissipated. Dissipation mechanisms may include percolation to the shallow
324 groundwater, lateral movement to Indian Creek, microbial processes or a combination of the
325 above. For reference, the $\text{NO}_3+\text{NO}_2\text{-N}$ levels in the deep (MW6D) and shallow (MW6S)
326 monitoring wells on 08/12/2011 were 36 and 24 mg/L, respectively. Rainfall during the month
327 was about 91 mm. It is also worth noting that most nitrate concentrations on 08/12/2011 were
328 greater than 30 mg/L with some greater than 50 mg/L. These values are 50 to 250% higher than
329 recommended average soil nitrate of 20 mg/L needed for plant growth [54] and 3 to 5 times
330 higher than the USEPA maximum allowable level of 10 mg/L for drinking water [55]. These
331 high concentrations were found at depths which are greater than most corn roots are expected to
332 reach. The data also show the highly dynamic nature of nutrient fate and transport.

333 Nitrate concentrations at 1.2 m on 07/01/2011 and 07/15/2011 (Figures 2d and 2f) suggest that
334 high (> 50 mg/L) concentrations of nitrates are removed from shallow soil by subsurface flow
335 which is predominantly moving parallel to flow in Indian Creek (Figure 2b). Therefore, to
336 capture the fugitive nutrients, bioenergy crops should have a rooting system deeper than corn and
337 their location in the field should be such that the roots intercept the nitrate before it is leached
338 deeper or transported northeastward to the creek.

339 Figure 2c shows the corn yield variation associated with the 2011 harvest. Higher yield areas (>
340 9 Mg ha⁻¹) were located in the flood plain on flat (0 to 2% slope) Comfrey loam (Figure 1).
341 Lower yielding areas (< 3.8 Mg ha⁻¹) were measured in the upland till plains on steeply sloping
342 (5 to 10%) Symerton silt loam. The low yielding areas coincide with those having high
343 subsurface nitrate concentrations. This reinforces the hypothesis that low crop yield areas for
344 shallow-rooted crops in this field are due to a combination of low soil fertility, low plant
345 available water, and high infiltration rates and therefore high leaching of N. This hypothesis was
346 supported by vertical hydraulic conductivity measurements of the Symerton topsoil (0.2 to 0.8
347 m) which were 0.28 cm day⁻¹ at MW6D compared to 0.01 cm day⁻¹ for Comfrey topsoil at MW4.

3.2 *Placement of bioenergy crops*

Based on the above field data analysis, a contour buffer strip (Figure 3) was designed to: (1) intercept concentrated surface flows; (2) capture and use the nitrate leachate before it percolates to the shallow groundwater or leaves the site by subsurface flow in a gradient parallel to the creek; and (3) utilize intra-field areas that are relatively less productive for corn. Based on the field monitoring (Figure 2), the practice of using edge of field buffers [56, 57] to capture nutrients in surface runoff would not capture, in this case, substantial nitrate lost through leaching because the Symerton silt loam that is susceptible to nitrate leaching is located in the upland till plain that is far up-gradient from the edge of the field. The designed contour strip occupies 0.8 ha with an average width of 30 m. According to Bentrup [58], more than 75% of reductions in shallow groundwater nitrate occur within 9 m to 30 m of the buffer width. Furthermore, a review of riparian and vegetated buffer strip widths by Fischer and Fischenich [59] recommends a 5 m to 30 m buffer width for water quality protection. Adjustments to this criterion for future use will be developed once performance data are generated.

3.3 *Calibration of DNDC crop parameters*

The DNDC model over-predicts corn yields in years when the observed yields are less than 12 Mg ha⁻¹ (dry matter) and slightly under-predicts when the observed yields are over 12 Mg ha⁻¹ (Figure 4a). A similar trend is observed for willow stem biomass where on average the model over-predicts during the first two years after willow coppicing with relatively low observed biomass and under-predicts in the third year (Figures 4b to 4d). According to model diagnostics, the above observations are moderated by water and nitrogen stress. During years of observed low biomass, modeled nitrogen and water stress dynamics were not limiting factors and thus

simulated high yields and over-prediction. This difference may be attributed to heterogeneity of field soil conditions compared to assumed uniform soil conditions by the DNDC model. The willow yields under composted poultry manure treatment (Figure 4e) are consistently under-predicted. This observation is attributed to characterization of actual applied N and the C:N ratio of the manure. Overall, the model representation of crop growth and biomass partition of the two crops under site specific conditions and management is good because 90% of the variability of the observed biomass is explained by model simulation (Figure 4f; $R^2 = 0.9$). These results depict the value of model performance metrics comparing model simulations and site observed data to establish the reliability of the model in representing the physical processes. For example, the PBIAS of 3.9% (Figure 4f) shows that on average the model slightly under-predicts biomass yields (PBIAS < 10%). And therefore, this information contributes to the development of models whose margins of error are understood and accounted for.

3.4 Modeling results at the Fairbury site

Simulated switchgrass yields in the contour buffer (Table 2) at the Fairbury site are consistent with simulations by Gopalakrishnan et al.[52] for edge-of-field buffer in central Illinois (11.1 – 12.8 Mg ha⁻¹ yr⁻¹) and comparable to yields of fertilized switchgrass on dedicated fields in the Midwest USA [60]. Simulated willow yields at the Fairbury site are higher than yields at the Tully site with no fertilizer application (5.7 – 8.4 Mg ha⁻¹ yr⁻¹) and comparable to yields under the treatment of 100 kg N ha⁻¹ of sulfur coated urea (9.8 – 11 Mg ha⁻¹ yr⁻¹). Simulations that replace corn in the buffer with switchgrass reduce leached NO₃ for the entire site by an average of 61% and N₂O emissions by 5.5% (59% and 10.8%, respectively for willow). The simulated reduction in emissions is significant considering the buffer is 12.5 % of the field. Because the bioenergy buffer targets the major source of nitrate leaching, the DNDC simulated field

reductions in leached NO₃ are comparable to observed differences (61 – 93 %) between corn-corn-soybean-corn rotation and switchgrass plots in central Illinois [48, 60].

3.5 *Scaling-up: field to watershed assessments*

This study highlights the importance of accurate characterization of sub-field soil variability, terrain analysis and subsurface flow direction when designing buffers to provide ecosystem services and feedstock for cellulosic biofuels. The challenge of replicating this work at other sites or scaling it up to a watershed scale is the intensive field monitoring, and associated costs. However, use of readily available soil data may provide insight into site characterizations such as the spatial variability of areas susceptible to nutrient leaching and crop productivity. For the United States, the spatial variability of the above soil-based metrics can be derived from soil survey geographic (SSURGO) data, collected and archived by the Natural Resources Conservation Service (a branch of the U.S. Department of Agriculture). Use of SSURGO data for the site (refer to Fig. 2b) and a classification method by Keefer [61] showed that areas characterized by Symerton soil series are susceptible to nitrate leaching. Keefer [61] used data related to the depth to the uppermost aquifer (within 15 meters), soil hydraulic properties, thickness of soil horizons, and the soil organic matter content. Terrain analysis at a watershed scale is accomplished using digital elevation models while normalized difference vegetation index derived from satellite imagery, is an appropriate surrogate for yield data. The above data resampled at a 30-m horizontal resolution provide a practical method of identifying zones of low

crop productivity and zones susceptible to erosion or nutrient leaching at sub-field level for watershed-scale assessments.

4.0 Conclusion

This study highlights the importance of accurate characterization of subsurface flow direction and susceptibility of the soils to nitrate leaching when designing energy buffers to provide environmental services and biomass feedstock for cellulosic biofuels. In this study, we have provided a methodology for design, and modeled results showing the potential environmental benefits of the designed buffer. However, a critical element in the potential success of the use of buffers for bioenergy and environmental services is farmer adoption. Farmer adoption hinges on economic feasibility, on the presence of a market for the produced biomass, and on the acceptance of the practice within a cultural and practical context. Long-term monitoring data from actual implementations need to provide the performance and logistics information to develop reasonably accurate cost and lifecycle assessments of these integrated systems that will help farmers and other decision makers to implement the designs.

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Supporting information

The supporting information includes a site map with monitoring points (Figure S1)

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TABLES

Table 1. DNDC calibrated willow crop parameters

ID	Crop parameter	Value	Reference / comment	Calibrated values
1	Maximum grain production (kg dry matter/ha/year)	235	Controls the fraction of maximum below and above ground biomass	400
2	Grain fraction of total biomass	0.01	a low value for no grain	0.01
3	Leaf fraction of total biomass	0.10	Pacaldo et al.[63]	0.12
4	Stem fraction of total biomass	0.56	Pacaldo et al.[63]	0.62
5	Root fraction of total biomass	0.33	Pacaldo et al.[63]; Heller et al.[64] Zan et al.[65]	0.25
6	C/N ratio for grain	23	Assumed same as leaves	12
7	C/N ratio for leaf	23	Pacaldo et al.[63]; Chauvet[66]	12
8	C/N ratio for stem	98	Pacaldo et al.[63]	98
9	C/N ratio for root	81	Pacaldo et al.[63]	81
10	N fixation index (total plant N/plant N taken from soil)	1	For perennials according to DNDC	1.08
11	Water requirement (kg water per kg dry matter biomass)	210	Lindroth et al.[67]	210
12	Optimum temperature ($^{\circ}\text{C}$)	30	SWAT crop database [68]	25
13	TDD (accumulative degree days for maturity, degree C)	2484	Kopp et al.[69]. Used a base of 5°C	2500
14	Vascularity index (0-1)	0		0
15	This is a perennial plant	Yes		Yes

Table 2. Simulated average (and standard error) annual yields, leached NO₃, and N₂O emissions at the Fairbury site, IL for 2008 to 2012.

Scenario ^a	Yield	Leached NO ₃	N ₂ O flux
	Mg ha ⁻¹ yr ⁻¹	kgN ha ⁻¹ yr ⁻¹	kgN ha ⁻¹ yr ⁻¹
Corn	10.4 ± 1.7	31.9 ± 4.4	2.2 ± 0.3
Corn/switchgrass	8.7 ± 1.0	11.6 ± 1.6	2.0 ± 0.2
Corn/willow	9.7 ± 0.6	12.5 ± 1.6	1.9 ± 0.2
% reduction ^b	---	61.0 ± 6.2	5.5 ± 3.1
	---	59.3 ± 4.0	10.8 ± 2.6

^aCorn scenario is the continuous corn while corn/switchgrass and corn/willow scenarios replace only corn in the buffer with one of the energy crops. The yields under scenarios two and three are for the energy crops in the buffer. The NO₃ and N₂O are area weighted values for the entire field and thus include areas still under corn.

^bTop values are percent reductions when the buffer is under switchgrass and the bottom values under willow

FIGURES

Figure 1. (a) Soil classification based on 30 soil cores and topographic survey. (b) Classification based on the web soil survey data [33]. The soil series 294B is the Symerton silt loam with slopes of 2 to 5 %, 294C2 is Symerton silt loam with slopes of 5 to 10 %, and 3776A is Comfrey loam with slopes of 0 to 2 %. There is a 65.5 % difference in areal classification of the 294C2 soil series between the two maps [(a) has 0.8 ha (b) has 2.35 ha].

Figure 2. (a) Length and direction of surface flow paths, indicative of areas of dominant accumulation and transport of surface runoff and sediment. (b) Domain of site MODFLOW model and the associated head solution used to estimate the groundwater flow gradient. (c) 2011 variable corn yield (Mg ha^{-1}). (d) to (f) are spatially explicit maps of nitrate ($\text{NO}_3 + \text{NO}_2$) concentration (mg L^{-1}) at a depth of 1.2 meters 07/01/2011, 07/15/2011, and 08/12/2011. At this depth, the nitrate is believed to be inaccessible to most corn roots.

Figure 3. Location of the strip contour buffer for the growth of cellulosic bioenergy crops. The strip is designed to intercept concentrated surface flow (flow path lengths greater than 120 m), allow for capture and re-use of nitrate leachate, and minimally encroach on high yield field areas.

Figure 4. Observed and DNDC simulated biomass for corn and short rotation coppiced willows. and. (a) Continuous corn with conventional tillage and fall fertilizer application at Fairbury, IL. (b) Willows at Tully, NY with no fertilizer application. (c) to (e) Willows under different fertilizer application rates. (f) Overall DNDC performance using calibrated crop parameters for both corn and willow biomass at Fairbury and Tully sites.