Supporting Information: Threshold Dynamics in Soil Carbon Storage for Bioenergy Crops

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Summary of the On-line Supplement
- Number of pages: 18
- Number of figures: 7
- Number of tables: 6
- Number of equations: 19

S1. Study Site

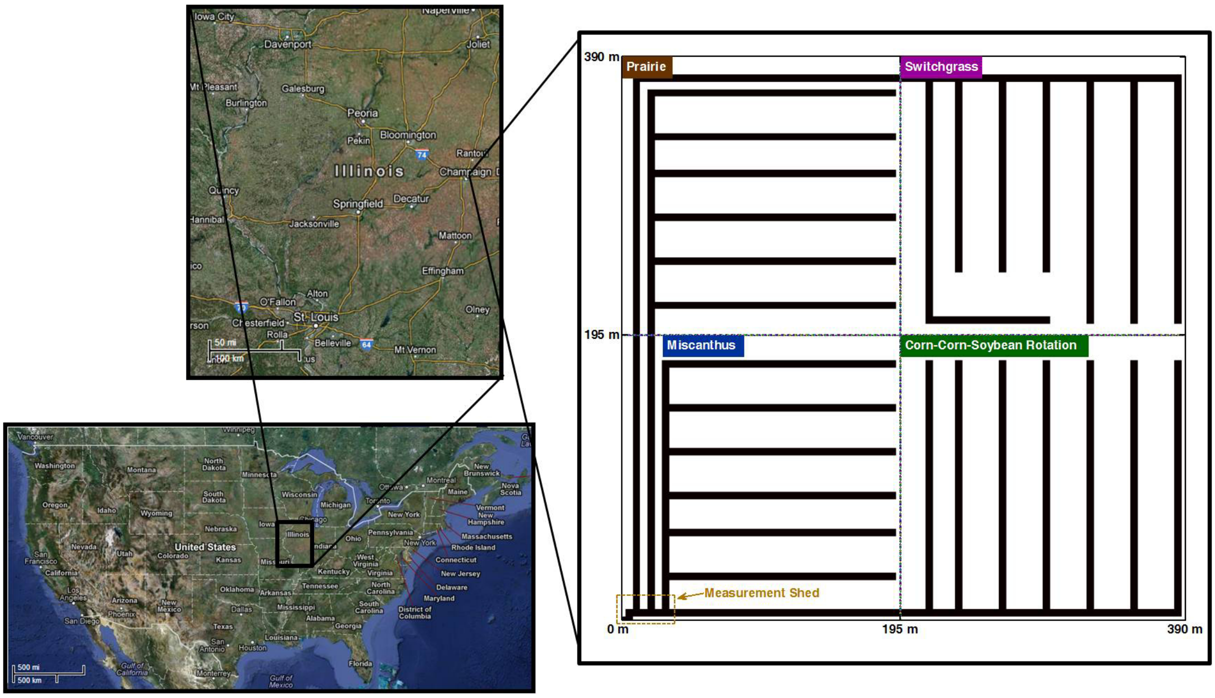

Figure S1. Location of the Energy Bioscience Institute (EBI) study site in Urbana, IL. The right panel shows the tile drainage, which is located at a depth of 1.22 m. The drainage in each plot is independent. Tile flow, and nitrate and ammonium loads are recorded at the southwest corner.

S2. Model

Table S1. PALMS phenological and physiological control parameters modified from default values for corn to values representative for switchgrass and miscanthus.

Parameter	Description	Default Value of Corn	Switchgrass	Miscanthus
Phonological control parameters				
$GDD_{maturity}$	Accumulated growing degree days (base 10 °C) needed for plant to reach vegetative and physiological maturity	2800	2850 [*VanLoocke et al.*, 2012]	3000 [*VanLoocke et al.*, 2010]
GDD_{silk}	Soil temperature summation Growing Degrees Days (base 0 °C) for emergence	1455	400 [*VanLoocke et al.*, 2012]	400 [*VanLoocke et al.*, 2010]
SLA	Specific leaf area ($m^2\ kg^{-1}$)	35	31 [*VanLoocke et al.*, 2012]	15 [*VanLoocke et al.*, 2010]
h_{grain}	Heat units needed to reach vegetative maturity	GDD_{silk}+100	GDD_{silk}+500 [*Dohleman.*, 2009]	GDD_{silk}+600 [*Dohleman.*, 2009]
z_{max}	Maximum crop height values (m)	2.5	2.0 [*Le et al.*, 2011]	3.5 [*Le et al.*, 2011]
LAI_{max}	Maximum LAI allowed	5	6.5 [*Heaton et al.*, 2008]	10.5 [*Heaton et al.*, 2008]
LAI_{cons}	Constant used in LAI senescence equation	1.2	1.0	0.75
a_{leafi}	Initial allocation of assimilated carbon to leaf	0.6	0.6 [*VanLoocke et al.*, 2012]	0.8 [*VanLoocke et al.*, 2010]
a_{stemi}	Initial allocation of assimilated carbon to stem	0.2	0.2 [*VanLoocke et al.*, 2012]	0.1 [*VanLoocke et al.*, 2010]
a_{rooti}	Initial allocation of assimilated carbon to root	0.2	0.15 [*VanLoocke et al.*, 2012]	0.1 [*VanLoocke et al.*, 2010]
a_{rootf}	Final allocation of assimilated carbon to root	0.2	0.05 [*VanLoocke et al.*, 2012]	0.1 [*VanLoocke et al.*, 2010]
$a_{rhizomei}$	Initial allocation of assimilated carbon to rhizome	-	0.05 [*VanLoocke et al.*, 2012]	- [*VanLoocke et al.*, 2010]
$a_{rhizomef}$	Final allocation of assimilated carbon to rhizome	-	0.025 [*VanLoocke et al.*, 2012]	- [*VanLoocke et al.*, 2010]
s_{sec}	Stem cross section diameter	0.025	0.016[a]	0.016 [*Heaton et al.*, 2008]
β	Rooting profile parameter in the asymptotic β model of *Gale and Grigal* [1987]	0.975	0.984 [*Monti and Zatta.*, 2009]	0.989 [*Neukirchen et al.*, 1999]
H	Harvest date	Auto	347[b] [*Smith et al.*, 2013]	365 [*VanLoocke et al.*, 2010]
Physiological control parameters				
V_{max}	Maximum Rubisco activity ($\mu mol\ m^{-2}\ s^{-1}$)	35	48 [*Le et al.*, 2011]	66 [*Le et al.*, 2011]
IQ	Intrinsic quantum efficiency	0.050	0.042	0.050
C_m	Coefficient for stomatal conductance relationship	4.0	8.0 [*Le et al.*, 2011]	5.7 [*Le et al.*, 2011]
C_b	Coefficient for stomatal conductance relationship	0.04	0.08 [*Collatz et al.*, 1992]	0.08 [*Collatz et al.*, 1992]

[a] Chosen based on miscanthus value.
[b] Value obtained from 2011 harvest practice at the study site.
* Parameters that are not shown in this table for switchgrass and miscanthus followed corn's default values.

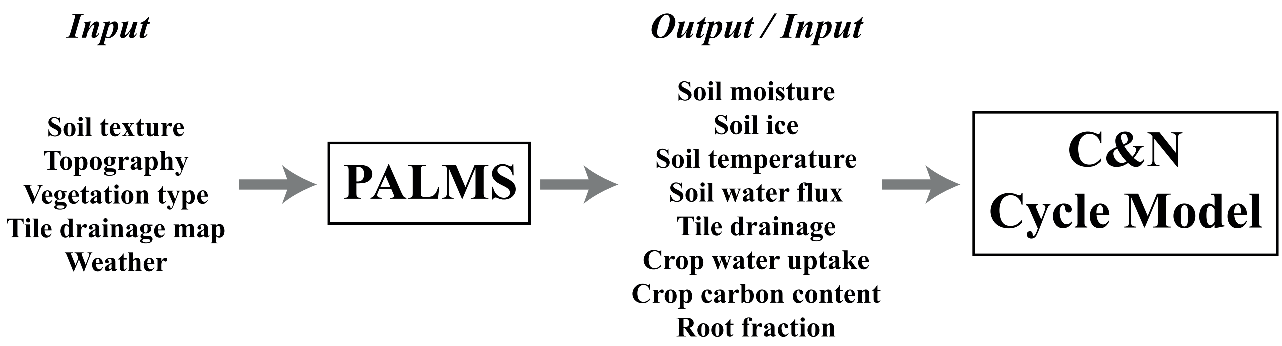

Figure S2. Schematic diagram showing the connection between PALMS and the soil carbon (C) and nitrogen (N) cycle model. Geometric, ecological, and climatic conditions of the study site were used to simulate eco-hydrological components with PALMS. Then, the eco-hydrological results from PALMS were used to drive the soil carbon and nitrogen model.

Physiological and phenological parameters of switchgrass and miscanthus used in PALMS are presented in Table S1. Figure S2 shows how we coupled PALMS with the soil carbon and nitrogen model. The schematic representation of the soil carbon and nitrogen model is presented in Figure S3. Table S2 to S5 show the parameters for the crops considered in this study used in the soil carbon and nitrogen model while Table S6 describes shared biogeochemical parameters used in the soil carbon and nitrogen model. Figure S4 shows the seasonal dynamics of switchgrass and miscanthus C/N ratios in the leaves, stems, and roots and rhizomes. The C/N ratios were constructed using previous studies [*Heaton et al.*, 2009; *Garten et al.*, 2010; *Strullu et al.*, 2011] and PALMS outputs. The generated stochastic weather variables to drive PALMS are presented in Figure S5.

In this paper, we made additional changes to the model presented in the previous study [*Quijano et al.*, 2013] for (1) litterfall, (2) crop nitrogen uptake, (3) nitrogen leaching through tile drainage, (4) fertilizer application, and (5) denitrification.

We developed a formulation for litterfall to account for the flux of carbon to the soil system from aboveground ($I(t)$) $[ML^{-2}T^{-1}]$ based on leaf phenology, and leaf carbon dynamics. Specifically, after a period of time during which leaves are physiologically active (leaf life span, S), the leaves die and fall off. In order to consider aboveground biomass inputs into the soil at harvest, we also employed a nondimensional factor, ξ, that represents the harvest litter drop fraction of the aboveground carbon biomass:

$$I(t) = \Delta\, {}^{l}C(t-S) + {}^{a}C(t)\xi\delta(t-H) \tag{S1}$$

where

$$\Delta\, {}^{l}C(t) = {}^{l}C(t) - {}^{l}C(t-1) \tag{S2}$$

where ${}^{a}C(t)$ is aboveground carbon biomass, which consists of leaf carbon biomass (${}^{l}C(t)$), grain carbon biomass (${}^{g}C(t)$), and stem carbon biomass (${}^{s}C(t)$) $[ML^{-2}T^{-1}]$, i.e. ${}^{a}C(t) = {}^{l}C(t) + {}^{g}C(t) + {}^{s}C(t)$. δ and H are the Dirac delta function and harvest day, respectively.

We modified the nitrogen uptake modeling approach that was originally suggested by *Porporato et al.* [2003] by developing formulations for the nitrogen fixation and plant nitrogen remobilization. The total nitrogen uptake at any time t, $U^{\pm}(t)$, is given as a sum of passive nitrogen uptake (${}^{p}U_i^{\pm}(t)$), active nitrogen uptake (${}^{a}U_i^{\pm}(t)$), nitrogen fixation (${}^{f}U_i^{\pm}(t)$) and plant nitrogen remobilization (${}^{r}U_i^{\pm}(t)$) in each i^{th} soil layer. That is:

$$U^{\pm}(t) = \sum_{i=1}^{X} {}^{p}U_i^{\pm}(t) + {}^{a}U_i^{\pm}(t) + {}^{f}U_i^{\pm}(t) + {}^{r}U_i^{\pm}(t) \tag{S3}$$

where the superscript $+$, and $-$ represent ammnonium-nitrogen, and nitrate-nitrogen, respectively. X is the number of soil layer. The passive nitrogen uptake is related to the nitrogen that is taken up by the plants as water is absorbed through the roots to meet the transpiration demand. In this study, we simulate this uptake as proportional to the plant water uptake, $W_i(t)$, $[LT^{-1}]$ and to the soil nitrogen concentration, $N_i^{\pm}(t)$ $[ML^{-3}]$. We consider that this formulation is appropriate since it has been shown that the passive uptake is significantly affected by the transpiration rate, even when the active uptake dominates [*Hopmans and Bristow*, 2002]:

$${}^{p}U_i^{\pm}(t) = \eta^{\pm} \frac{W_i(t)}{\theta_i(t) n_i Z_i} N_i^{\pm}(t) \tag{S4}$$

where θ_i, n_i, and Z_i are relative soil moisture, porosity, and soil thickness $[L]$ in the i^{th} layer, respectively. The term, $\theta_i(t)n_iZ_i$, defines the volume of water per unit area in the i^{th} layer. The nondimensional factors, $\eta^{\pm}$, refer to the respective fractions of dissolved mineral ammonium and nitrate. The factors used in this study are the same as those implemented in *D'Odorico et al.* [2003] ($\eta^{+} = 0.05$, $\eta^{-} = 1.0$).

Porporato et al. [2003] define three cases where active nitrogen uptake occurs. These cases are defined based on the plant nitrogen demand and soil nitrogen availability. Here, we consider an additional uptake mechanism that involves the fixation of nitrogen. *Gopalakrishnan et al.* [2012] simulate the nitrogen fixation in switchgrass and miscanthus by considering a nitrogen fixation index defined as the ratio of total plant nitrogen uptake and plant nitrogen from soil. Here, we implement the same concept, and use a parameter, ω, that is defined as $\omega =$ plant nitrogen fixation/plant nitrogen uptake from soil. For developing the model, we hypothesize that if crop has a nitrogen fixation ability, the nitrogen demand from active nitrogen uptake will decrease:

$$ {}^{a}U_i^{\pm}(t) = \begin{cases} 0, & \text{if } M_i^{\pm}(t) - {}^{p}U_i^{\pm}(t) < 0, \\ (k_i(t)N_i^{\pm}(t))\gamma_{1,i}(t), & \text{if } k_i(t)N_i^{\pm}(t) \le M_i^{\pm}(t) - {}^{p}U_i^{\pm}(t), \\ (M_i^{\pm}(t) - {}^{p}U_i^{\pm}(t))\gamma_{2,i}(t), & \text{if } k_i(t)N_i^{\pm}(t) > M_i^{\pm}(t) - {}^{p}U_i^{\pm}(t). \end{cases} \tag{S5} $$

$$ {}^{f}U_i^{\pm}(t) = \begin{cases} 0, & \text{if } M_i^{\pm}(t) - {}^{p}U_i^{\pm}(t) \le 0, \\ ({}^{p}U_i^{\pm}(t) + {}^{a}U_i^{\pm}(t))\omega, & \text{if } M_i^{\pm}(t) - {}^{p}U_i^{\pm}(t) > 0. \end{cases} \tag{S6} $$

where the nondimensional parameters $\gamma_{1,i}$ and $\gamma_{2,i}$, $0 \le \gamma_{1,i}, \gamma_{2,i} \le 1$, are used to make the nitrogen fixation proportional to the nitrogen uptake from the soil and $M_i^{\pm}(t)$ is a variable computed as the plant nitrogen demand minus plant nitrogen remobilization (see equation S11). By changing the inequality signs to equality signs in equation S5, the values of $\gamma_{1,i}$, and $\gamma_{2,i}$ can be obtained:

$$ \begin{aligned} \gamma_{1,i}(t) &= \frac{M_i^{\pm}(t) - (1+\omega){}^{p}U_i^{\pm}(t)}{(1+\omega)k_i(t)N_i^{\pm}(t)} \\ \gamma_{2,i}(t) &= \frac{M_i^{\pm}(t) - (1+\omega){}^{p}U_i^{\pm}(t)}{(1+\omega)(M_i^{\pm}(t) - {}^{p}U_i^{\pm}(t))} \end{aligned} \tag{S7} $$

where $k_i(t)N_i^{\pm}(t)$ denotes the diffusive flux related to the concentration differences between the root surface and the adjacent soil. $k_i(t)$ $[T^{-1}]$ is a parameter representing the diffusion process relevant to the soil moisture level, and formulated as:

$$ k_i(t) = \frac{\eta^{\pm}}{\theta_i(t) n_i Z_i} \zeta(\theta_i(t))^{\kappa} \tag{S8} $$

where ζ, and κ are a rescaled diffusion coefficient $[LT^{-1}]$, and a nondimensional turtuosity factor, respectively. Both parameters are chosen based on *D'Odorico et al.* [2003].

Switchgrass and miscanthus experience nitrogen translocation during winter, whereby nitrogen moves from the aboveground to belowground plant components. During annual regrowths, the crops remobilize the nitrogen back into their shoots for growth [*Heaton et al.*, 2008, 2009; *Yang et al.*, 2009; *Strullu et al.*, 2011]. We implement a nitrogen remobilization pool (${}^{r}N^{\pm}$) to develop the formulation for the plant nitrogen remobilization. The nitrogen remobilization pool is updated at the first day of each growing season (V) and determined as a remobilization ratio (υ) multiplied by the nitrogen uptake allocated to the aboveground biomass during the previous growing season:

$$ {}^{r}N^{\pm} = \upsilon \delta(t - V) \sum_{t \in yr-1} {}^{a}U^{\pm}(t) \tag{S9} $$

where ${}^{a}U^{\pm}(t)$ represents the nitrogen uptake allocated to the aboveground biomass at any time t. The nitrogen remobilization occurs in two cases based on the plant nitrogen demand and the nitrogen remobilization pool. Here, we assume that during nitrogen remobilization, the crops do not uptake nitrogen from external sources (soil nitrogen and nitrogen fixation) since previous studies have observed the inhibition of the nitrogen uptake by the crops during this period [*Thornton and Millard*, 1997; *Louhalia et al.*, 1999; *Strullu et al.*, 2011]:

$$ {}^{r}U_i^{\pm}(t) = \begin{cases} D_i^{\pm}(t), & \text{if } {}^{r}N^{\pm} \ge \sum_{i=1}^{X} D_i^{\pm}(t), \\ {}^{r}N^{\pm} R_i, & \text{if } {}^{r}N^{\pm} < \sum_{i=1}^{X} D_i^{\pm}(t). \end{cases} \tag{S10} $$

$$ M_i^{\pm}(t) = \begin{cases} 0, & \text{if } {}^{r}N^{\pm} \ge \sum_{i=1}^{X} D_i^{\pm}(t), \\ D_i^{\pm}(t) - {}^{r}U_i^{\pm}(t), & \text{if } {}^{r}N^{\pm} < \sum_{i=1}^{X} D_i^{\pm}(t). \end{cases} \tag{S11} $$

$$\frac{d^rN^{\pm}}{dt} = -\sum_{i=1}^{X} {}^rU_i^{\pm}(t) \tag{S12}$$

where R_i is a root fraction [-] in the i^{th} layer. $D_i^{\pm}(t)$ is the plant nitrogen demand in the i^{th} layer $[ML^{-3}T^{-1}]$ that is modeled based on crop carbon dynamics and C/N ratios:

$$D_i^{\pm}(t) = \left(\frac{\Delta^l C(t)}{{}^l\mathrm{C/N}(t)Z_i} + \frac{\Delta^s C(t)}{{}^s\mathrm{C/N}(t)Z_i} + \frac{\Delta^g C(t)}{{}^g\mathrm{C/N}(t)Z_i} + \frac{\Delta^b C(t)}{{}^b\mathrm{C/N}(t)Z_i}\right) R_i \varphi^{\pm} \tag{S13}$$

where

$$\Delta^g C(t) = {}^gC(t) - {}^gC(t-1) \tag{S14}$$

$$\Delta^s C(t) = {}^sC(t) - {}^sC(t-1) \tag{S15}$$

$$\Delta^b C(t) = {}^bC(t) - {}^bC(t-1) \tag{S16}$$

where $\Delta^l C(t)$, $\Delta^g C(t)$, $\Delta^s C(t)$, and $\Delta^b C(t)$ indicate the respective carbon changes in the leaf, stem, grain, and belowground vegetation pools. When these pools are divided by the given C/N ratios and multiplied by the root fraction, the total plant nitrogen demand in i^{th} layer is obtained. Due to lack of data, in this study we assume that the grain C/N ratio is the same as the stem C/N ratio. It is difficult to distinguish the amount of nitrate or ammonium demands from the total nitrogen demand. Therefore, nondimensional fractions, $\varphi^{\pm}$, are used based on the fact that the active uptake becomes dominant in the low soil nutrient concentration [*Hopmans and Bristow*, 2002].

Nitrogen leaching into the tile drain, $E^{\pm}(t)$, $[ML^{-2}T^{-1}]$ is estimated in a similar way to the soil nitrogen leaching equation within a layer where the tile drainage system is located (m):

$$E^{\pm}(t) = \nu^{\pm} \frac{Y(t)}{\theta_{i=m}(t) n_{i=m} Z_{i=m}} N_{i=m}^{\pm}(t) \tag{S17}$$

where tile flow $(Y(t))$ is in units of $[LT^{-1}]$. We assume that the magnitude of tile drainage ammonium leaching is two times higher than that of soil ammonium leaching: $\nu^{+} = 2\eta^{+}$; $\nu^{-} = \eta^{-}$.

Ammonium- and urea-nitrogen fertilizer applications $(F^{+}(t))$ are modeled as an instantaneous flux of nitrogen that is imposed to a depth of 0.1 m. We do not take into account the difference between the organic nitrogen (urea) and the inorganic nitrogen fertilizer since the transformation from urea to ammonium takes only a few days:

$$F^{+}(t) = J^{+}(1-\phi)\delta(t-G) \tag{S18}$$

where J^{+}, and ϕ are the fertilizer amount $[ML^{-2}T^{-1}]$, and volatilization fractions of urea and ammonium of the applied fertilizer, respectively. G is the day of fertilization. Similarly, the nitrate-nitrogen fertilizer application is obtained as:

$$F^{-}(t) = J^{-}\delta(t-G) \tag{S19}$$

N_2O flux from nitrification, and denitrification submodels are based on DayCent [*Parton et al.*, 1996, 2001; *Del Grosso et al.*, 2000]. It is hypothesized that N_2O flux from nitrification $(Q_i(t))$ $[ML^{-3}T^{-1}]$ is proportional to the nitrification rate (O_i), $Q_i(t) = \varpi O_i(t)$; $\varpi = 0.02$. The denitriciation model is developed as functions of soil nitrate, heterotrophic respiration, water-filled pore space, field capacity, and bulk density.

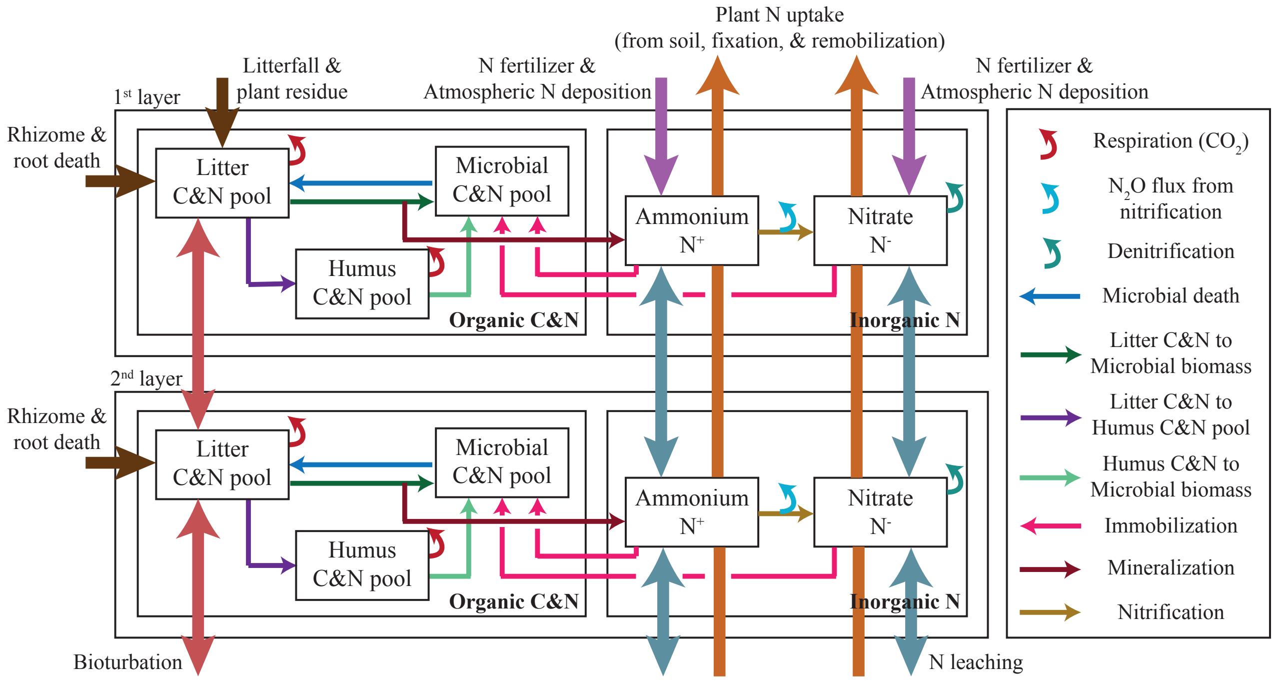

Figure S3. Schematic representation of soil carbon (C) and nitrogen (N) model for the first two layers of the multilayer model. Deeper layers follow layer 2 approach.

Table S2. Corn parameters in the soil carbon and nitrogen model. (M and S denote modeling parameter, and sampling value, respectively).

Parameter	Description	Value	Source and estimation
^{l}C/N	Leaf C/N ratio	22	1)*Smith et al.* [2013];(S)
^{s}C/N	Stem C/N ratio	56	Location: study site, Urbana, IL, USA
^{b}C/N	Belowground C/N ratio	27	Sampling: aboveground C/N ratio of 30.7 and 32.2 when harvested in 2009 and 2011, respectively. 2) *Johnson et al.* [2007] Location: Stevens County, MN, USA Soil type: loam Annual average precipitation: 631 mm Yearly mean temperature: 6.1 °C Sampling: leaf, stem, and belowground carbon: 416, 458, and 343 $g\ kg^{-1}$ plant material, respectively; leaf, stem, and belowground nitrogen: 13.6, 5.86, and 9.09 $g\ kg^{-1}$ plant material, respectively when harvested. Estimation: we multiplied plant nitrogen observed in *Johnson et al.* [2007] by 1.4 to obtain aboveground C/N ratio of 32 as observed in the study site.
S	Leaf life span (day)	115	1)*Smith et al.* [2013];(S) Location: study site, Urbana, IL, USA Sampling: natural litter inputs were measured during study period. Estimation: chosen based on natural liter input.
λ	Constant ratio of 'natural root & rhizome death' to 'natural litterfall'	0.21	1)*Lemus and Lal* [2005];(S) Location: Bear Creek, IA, USA Soil type: loamy sand Annual average precipitation: 865 mm Yearly mean temperature: 7.5 °C Sampling: mean aboveground litter carbon pool: 1,042 $kg\ ha^{-1}$; mean dead root carbon pool: 208 $kg\ ha^{-1}$, which were estimated by collecting monthly to a depth of 1.25 m during the growing season in 1996 and 1997. 2) From PALMS Root percentage to a depth of 1.25 m: 95.21% Estimation: we assumed that decomposition rate of aboveground litter carbon pool was similar enough to that of dead root carbon pool. Thus, $\lambda = [(208) \times (1 + 1 - 0.9521)]/(1042) = 0.21$
ω	Nitrogen fixation index (plant nitrogen from fixation / plant nitrogen from soil)	0	1)*Davis et al.* [2010];(M) Location: Urbana, IL, USA (adjacent to the study site) Soil type: loamy sand Annual average precipitation: 865 mm Estimation: a trivial amount of nitrogen fixation might exist. However, the over-fertilization dilutes its contribution to the total nitrogen balance.
φ^{+}	Fraction of ammonium demand from total nitrogen demand	0	Estimation: crop nitrogen demand dynamics has not yet been fully understood. Thus, we chose these values based on study
φ^{-}	Fraction of nitrate demand from total nitrogen demand	1.0	site observations, such as (1) total plant nitrogen uptake, (2) nitrogen loads at the tile drainage flow, (3) mineralization, and (4) nitrification. Note that zero ammonium demand does not mean that zero ammonium uptake by crop due to passive nitrogen uptake process.
ς	Fraction of total belowground carbon for direct harvest carbon losses	1.0	Estimation: we assumed that all of root and rhizome died at harvest
χ	Nitrification rate ($m^3\ d^{-1}\ gN^{-1}$)	0.00004	Estimation: nitrification rate dependent on fertilizer type and amount, soil type, and vegetation [*Stange and Neue*, 2009; *Tecimen and Sevegi*, 2010; *Subbarao et al.*, 2012]. Thus, we chose these values based on observed nitrification in the study site.
ζ	Rescaled diffusion coefficient for computing active vegetation nitrogen uptake ($m\ m^{-3}$)	0.06	Estimation: ζ should be decided in a way that the proportion of active nitrogen uptake to the total is within the 50-80% [*Porporato et al.*, 2003].

Table S3. Soybean parameters in the soil carbon and nitrogen model. (M and S denote modeling parameter, and sampling value, respectively).

Parameter	Description	Value	Source and estimation
^{l}C/N	Leaf C/N ratio	6	1)*Smith et al.* [2013];(S)
^{s}C/N	Stem C/N ratio	22	Location: study site, Urbana, IL, USA
^{b}C/N	Belowground C/N ratio	13	Sampling: aboveground C/N ratio of 9.0 when harvested in 2010. 2) *Johnson et al.* [2007] Location: Stevens County, MN, USA Soil type: loam Annual average precipitation: 631 mm Yearly mean temperature: 6.1 °C Sampling: leaf, stem, and belowground carbon: 439, 468, and 467 $g\ kg^{-1}$ plant material, respectively; leaf, stem, and belowground nitrogen: 15.8, 4.36, and 7.48 $g\ kg^{-1}$ plant material, respectively when harvested. Estimation: we multiplied plant nitrogen observed in *Johnson et al.* [2007] by 5.0 to obtain aboveground C/N ratio of 9 as observed in the study site.
S	Leaf life span (day)	65	1)*Smith et al.* [2013];(S) Location: study site, Urbana, IL, USA Sampling: natural litter inputs were measured during study period. Estimation: chosen based on natural liter input.
λ	Constant ratio of 'natural root & rhizome death' to 'natural litterfall'	0.35	1)*Lemus and Lal* [2005];(S) Location: Bear Creek, IA, USA Soil type: loamy sand Annual average precipitation: 865 mm Yearly mean temperature: 7.5 °C Sampling: mean above-ground litter carbon pool: 625 $kg\ ha^{-1}$; mean dead root carbon pool: 208 $kg\ ha^{-1}$, which were estimated by collecting monthly to a depth of 1.25 m during the growing season in 1996 and 1997. 2) From PALMS Root percentage to a depth of 1.25 m: 95.21% Estimation: we assumed that decomposition rate of aboveground litter carbon pool was similar enough to that of dead root carbon pool. Thus, $\lambda = [(208) \times (1 + 1 - 0.9521)]/(625) = 0.35$
ω	Nitrogen fixation index (plant nitrogen from fixation / plant nitrogen from soil)	0.3	1)*Salvagiotti et al.* [2008];(S) Mean value was derived from 108 studies that included a total of 637 data sets
φ^{+}	Fraction of ammonium demand from total nitrogen demand	0	Estimation: crop nitrogen demand dynamics has not yet been fully understood. Thus, we chose these values based on study
φ^{-}	Fraction of nitrate demand from total nitrogen demand	1.0	site observations, such as (1) total plant nitrogen uptake, (2) nitrogen loads at the tile drainage flow, (3) mineralization, and (4) nitrification. Note that zero ammonium demand does not mean that zero ammonium uptake by crop due to passive nitrogen uptake process.
ς	Fraction of total below-ground carbon for direct harvest carbon losses	1.0	Estimation: we assumed that all of root and rhizome died at harvest
χ	Nitrification rate ($m^3\ d^{-1}\ gN^{-1}$)	0.00004	Estimation: nitrification rate dependent on fertilizer type and amount, soil type, and vegetation [*Stange and Neue*, 2009; *Tecimen and Sevegi*, 2010; *Subbarao et al.*, 2012]. Thus, we chose these values based on observed nitrification in the study site.
ζ	Rescaled diffusion coefficient for computing active vegetation nitrogen uptake ($m\ m^{-3}$)	0.06	Estimation: ζ should be decided in a way that the proportion of active nitrogen uptake to the total is within the 50-80% [*Porporato et al.*, 2003].

Table S4. Switchgrass parameters in the soil carbon and nitrogen model. (M and S denote modeling parameter, and sampling value, respectively).

Parameter	Description	Value	Source and estimation
^{l}C/N	Leaf C/N ratio	Fig.S4	1)*Heaton et al.* [2009];(S)
^{s}C/N	Stem C/N ratio	Fig.S4	Location: Urbana, IL, USA (adjacent to the study site) Sampling: nitrogen mass in leaf and stem during 2005 growing season 2) From PALMS; (M) Carbon mass in leaf and stem during 2005 growing season Estimation: carbon from PALMS divided by nitrogen from *Heaton et al.* [2009], then interpolated.
^{b}C/N	Belowground C/N ratio	Fig.S4	1) *Garten et al.* [2010]; (S) Location: University of Tennessee's Research and Education center, Tennessee, USA Soil type: silty loam Annual average precipitation: 1295 mm Yearly mean temperature: 14 °C
S	Leaf life span (day)	180	1)*Smith et al.* [2013];(S) Location: study site, Urbana, IL, USA Sampling: natural litter inputs were measured during study period. Estimation: chosen based on natural liter input.
λ	Constant ratio of 'natural root & rhizome death' to 'natural litterfall'	1.58	1)*Hartman et al.* [2012]; Based on the fact that switchgrass root biomass is four to five times greater than corns, the potential belowground litter input into soil is estimated as 220 $g\ C\ m^{-2}\ year^{-1}$ 2) From soil carbon and nitrogen model Mean natural aboveground litter input into soil over the next 100 years: 139 $g\ C\ m^{-2}\ year^{-1}$ Estimation: $\lambda = 220/139 = 1.58$
ω	Nitrogen fixation index (plant nitrogen from fixation / plant nitrogen from soil)	0	1)*Gopalakrishnan et al.* [2012];(M) Location: a farm field, Urbana, IL, USA (adjacent to the study site)
φ^{+}	Fraction of ammonium demand from total nitrogen demand	0.1	Estimation: crop nitrogen demand dynamics has not yet been fully understood. Thus, we chose these values based on study
φ^{-}	Fraction of nitrate demand from total nitrogen demand	0.9	site observations, such as (1) total plant nitrogen uptake, (2) nitrogen loads at the tile drainage flow, (3) mineralization, and (4) nitrification.
ς	Fraction of total below-ground carbon for direct harvest carbon losses	0.0	Estimation: we assumed that harvest practices do not affect root and rhizome biomass
χ	Nitrification rate ($m^3\ d^{-1}\ gN^{-1}$)	0.0002	Estimation: nitrification rate dependent on fertilizer type and amount, soil type, and vegetation [*Stange and Neue*, 2009; *Tecimen and Sevegi*, 2010; *Subbarao et al.*, 2012]. Thus, we chose these values based on observed nitrification in the study site.
ζ	Rescaled diffusion coefficient for computing active vegetation nitrogen uptake ($m\ m^{-3}$)	0.015	Estimation: ζ should be decided in a way that the proportion of active nitrogen uptake to the total is within the 50-80% [*Porporato et al.*, 2003].
υ	Nitrogen remobilization ratio	0.4	1)*Yang et al.* [2009] Location: A field of the Samuel Roberts Noble Foundation, Ardmore, OK, USA Soil type: clay loam Annual average precipitation: 975mm Yearly mean temperature: 16 °C

Table S5. Miscanthus parameters in the soil carbon and nitrogen model. (M and S denote modeling parameter, and sampling value, respectively).

Parameter	Description	Value	Source and estimation
$^{l}C/N$	Leaf C/N ratio	Fig.S4	1) *Heaton et al.* [2009];(S)
$^{s}C/N$	Stem C/N ratio	Fig.S4	Location: Urbana, IL, USA (adjacent to the study site) Sampling: nitrogen mass in leaf and stem during 2005 growing season 2) From PALMS; (M) Carbon mass in leaf and stem during 2005 growing season Estimation: carbon from PALMS divided by nitrogen from *Heaton et al.* [2009], then interpolated.
$^{b}C/N$	Belowground C/N ratio	Fig.S4	1) *Strullu et al.* [2011]; (S) Location: Picardie region of Northern France Soil type: silty loam Annual average precipitation: 625 mm Yearly mean temperature: 11 °C
S	Leaf life span (day)	195	1) *Smith et al.* [2013];(S) Location: study site, Urbana, IL, USA Sampling: natural litter inputs were measured during study period. Estimation: chosen based on natural liter input.
λ	Constant ratio of 'natural root & rhizome death' to 'natural litterfall'	0.4	1) *Amougou et al.* [2012]; Location: INRA experimental site, Northern France Soil type: silty loam Annual average precipitation: 1091mm Yearly mean temperature: 3 °C Natural aboveground litter contribution to soil carbon is 0.50 $Mg\ C\ ha^{-1}\ year^{-1}$ while natural above- and belowground litter contribution to soil carbon is 0.70 $Mg\ C\ ha^{-1}\ year^{-1}$ Estimation: we assumed that decomposition rate of aboveground litter was similar enough to that of belowground litter. Thus, $\lambda = (0.70 - 0.50)/0.50 = 0.40$
ω	Nitrogen fixation index (plant nitrogen from fixation / plant nitrogen from soil)	2[a]	1) *Gopalakrishnan et al.* [2012];(M) Location: a farm field, Urbana, IL, USA (adjacent to the study site)
φ^{+}	Fraction of ammonium demand from total nitrogen demand	0.45	Estimation: crop nitrogen demand dynamics has not yet been fully understood. Thus, we chose these values based on study
φ^{-}	Fraction of nitrate demand from total nitrogen demand	0.55	site observations, such as (1) total plant nitrogen uptake, (2) nitrogen loads at the tile drainage flow, (3) mineralization, and (4) nitrification.
ς	Fraction of total below-ground carbon for direct harvest carbon losses	0.0	Estimation: we assumed that harvest practices do not affect root and rhizome biomass
χ	Nitrification rate ($m^3\ d^{-1}\ gN^{-1}$)	0.00021	Estimation: nitrification rate dependent on fertilizer type and amount, soil type, and vegetation [*Stange and Neue*, 2009; *Tecimen and Sevegi*, 2010; *Subbarao et al.*, 2012]. Thus, we chose these values based on observed nitrification in the study site.
ζ	Rescaled diffusion coefficient for computing active vegetation nitrogen uptake ($m\ m^{-3}$)	0.035	Estimation: ζ should be decided in a way that the proportion of active nitrogen uptake to the total is within the 50-80% [*Porporato et al.*, 2003].
υ	Nitrogen remobilization ratio	0.5[a]	1) *Strullu et al.* [2011] Location: Picardie region of Northern France Soil type: silty loam Annual average precipitation: 625 mm Yearly mean temperature: 11 °C

[a] We assumed that miscanthus did not have nitrogen fixation and remobilization abilities from 2008 to 2010 due to its replantation.

Table S6. Biogeochemical parameters in the soil carbon and nitrogen model.

Parameter	Description	Value
^{h}C/N	C/N ratio of humus	22 [*D'Odorico et al.*, 2003]
^{d}C/N	C/N ratio of microbial biomass	11.5 [*D'Odorico et al.*, 2003]
τ	Respiration coefficient	0.60 [*D'Odorico et al.*, 2003]
ϱ	Minimum fraction of decomposed litter that undergoes hummification	0.15 [*Porporato et al.*, 2003]
ϑ^{+}	Ammonium immobilization coefficient ($m^3\ d^{-1}\ gN^{-1}$)	1 [*D'Odorico et al.*, 2003]
ϑ^{-}	Nitrate immobilization coefficient ($m^3\ d^{-1}\ gN^{-1}$)	1 [*D'Odorico et al.*, 2003]
η^{+}	Fraction of dissolved ammonium	0.05 [*D'Odorico et al.*, 2003]
η^{-}	Fraction of dissolved nitrate	1 [*D'Odorico et al.*, 2003]
κ	Tortuosity factor in active nitrogen uptake	3 [*D'Odorico et al.*, 2003]
ϖ	Fraction of nitrification lost as N_2O flux	0.02 [*Parton et al.*, 2001]
ϕ	Volatilization fraction of urea and ammonium of applied fertilizer	Urea: 0.205 Ammonium: 0.61 [*Jones et al.*, 2007]
B	Bioturbation diffusion coefficient at soil surface ($m^2\ h^{-1}$)	1×10^{-7} [*Cousins et al.*, 1999]

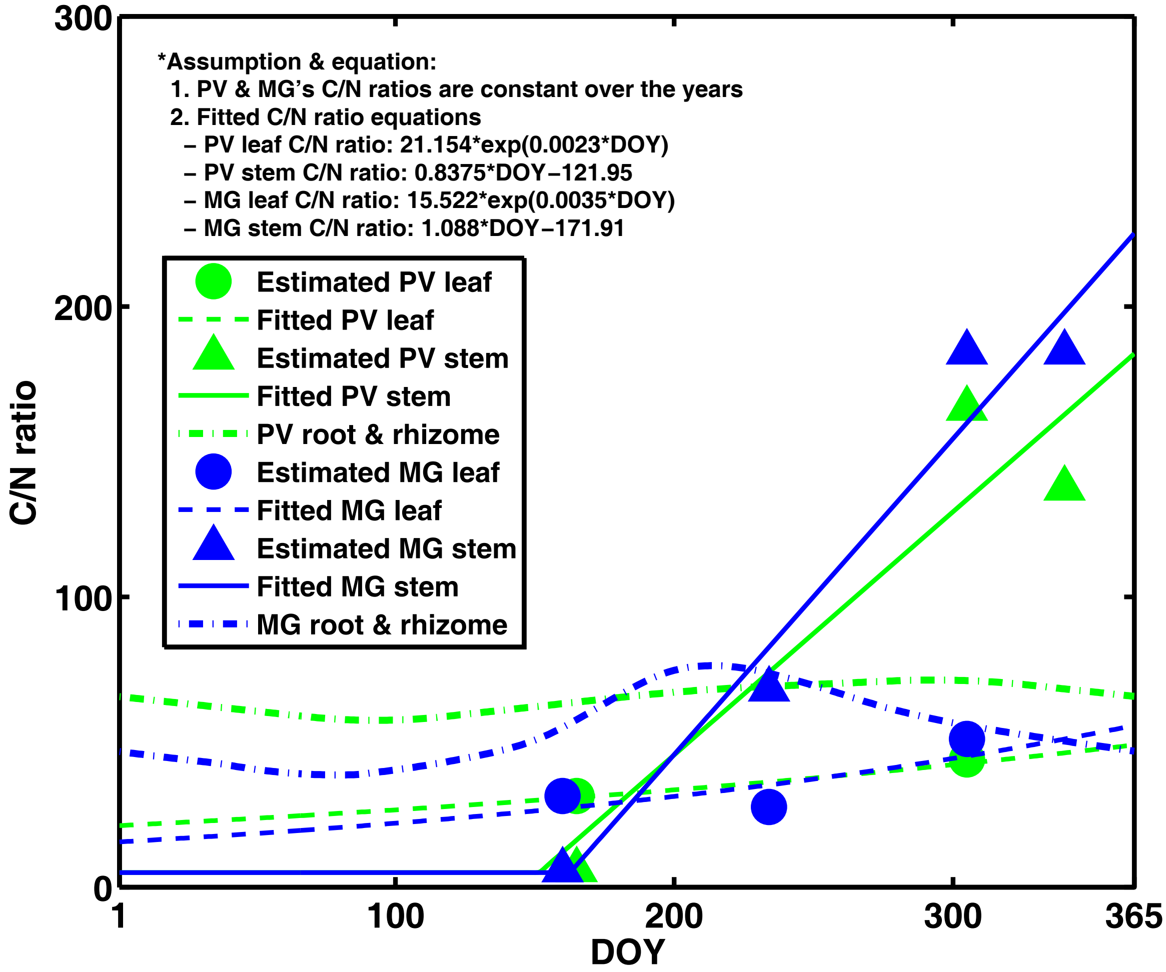

Figure S4. Annual C/N dynamics in the leaf, stem, and root and rhizome for switchgrass (PV) and miscanthus (MG). We used fitted lines based on estimated C/N ratios of leaves (circle) and stems (triangle). The estimated C/N ratios were calculated as 'carbon masses in leaves and stems in 2005 obtained from the PALMS simulation' divided by 'nitrogen masses in leaves and stems in 2005 from *Heaton et al.* [2009]'. The switchgrass and miscanthus roots and rhizomes C/N ratios were obtained from *Garten et al.* [2010], and *Strullu et al.* [2011], respetively. More details are discribed in Table S4 and S5.

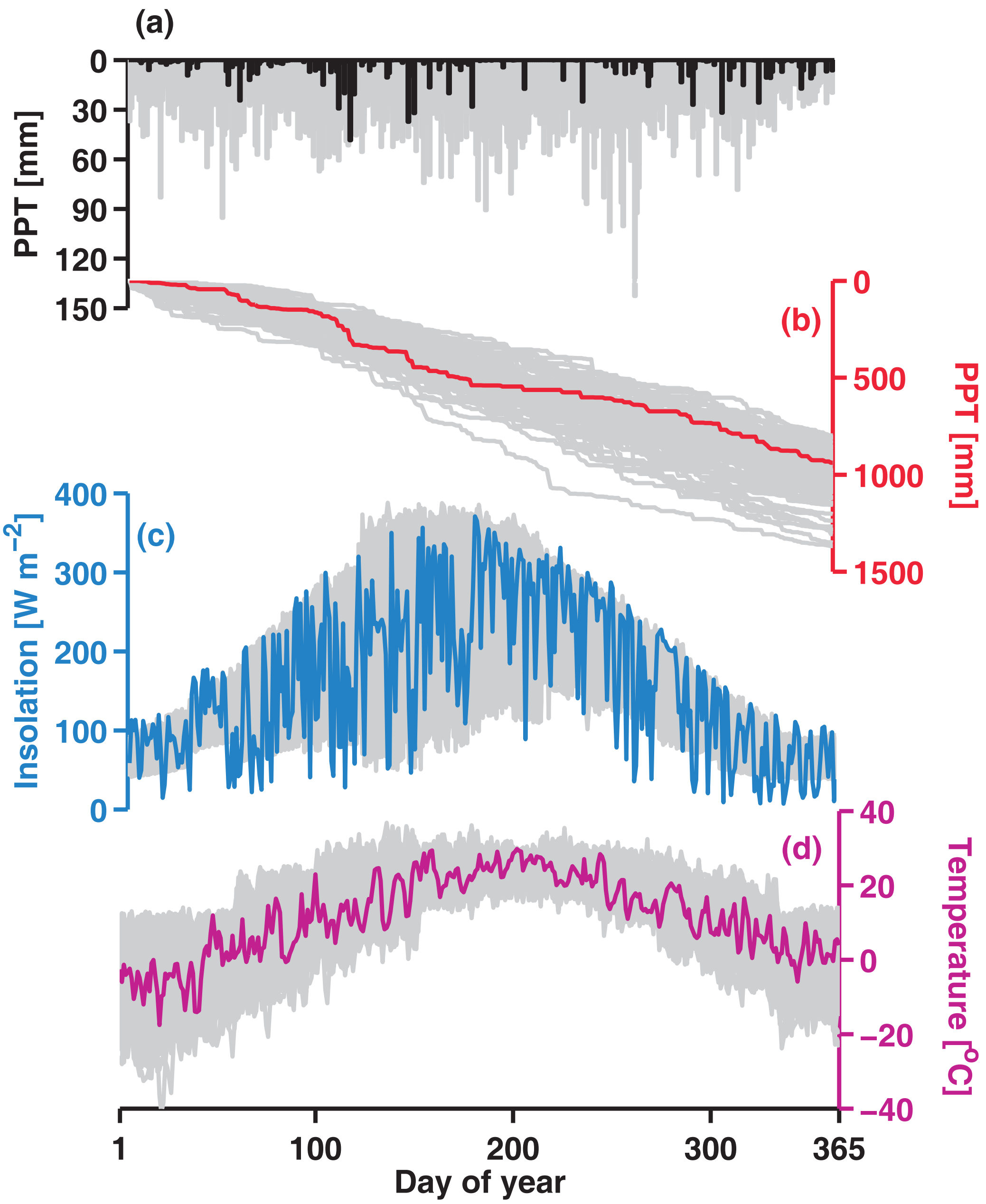

Figure S5. Observed meteorological forcing data in 2011 overlaid on the ensemble of stochastic weather variables generated using data from 2002 to 2011: (a) daily precipitation, (b) cumulative precipitation, (c) solar insolation, and (d) daily temperature.

S3. Results

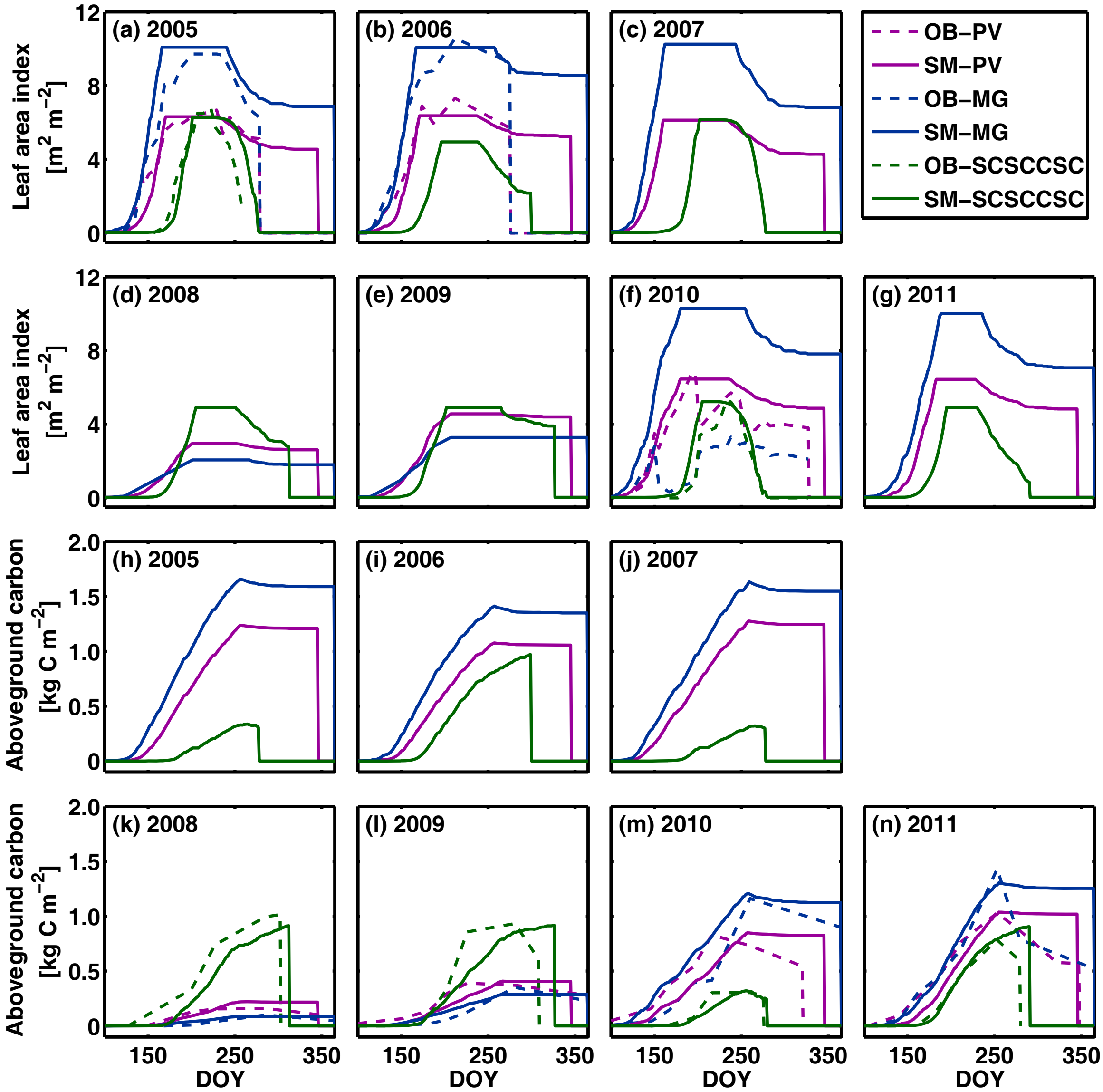

Figure S6. Simulated (SM) and observed (OB) (a–g) leaf area index (LAI), and (h–n) aboveground carbon throughout the growing season from 2005 to 2011. The observed LAI data of 2005 and 2006 were obtained at Bondville, IL, which is adjacent to the study site [*Heaton et al.*, 2008]. The information of 2010 was recorded at the study site [*Zeri et al.*, 2011]. All observed aboveground carbon was obtained from the study site [*Anderson-Teixeira et al.*, 2013]. SCSCCSC, PV, MG, and DOY represent soybean–corn–soybean–corn–corn–soybean–corn, switchgrass, miscanthus, and day of year respectively (corn–corn–soybean rotation from T0=2008 to T0+50; corn–soybean rotation from T0-100 to T0-1).

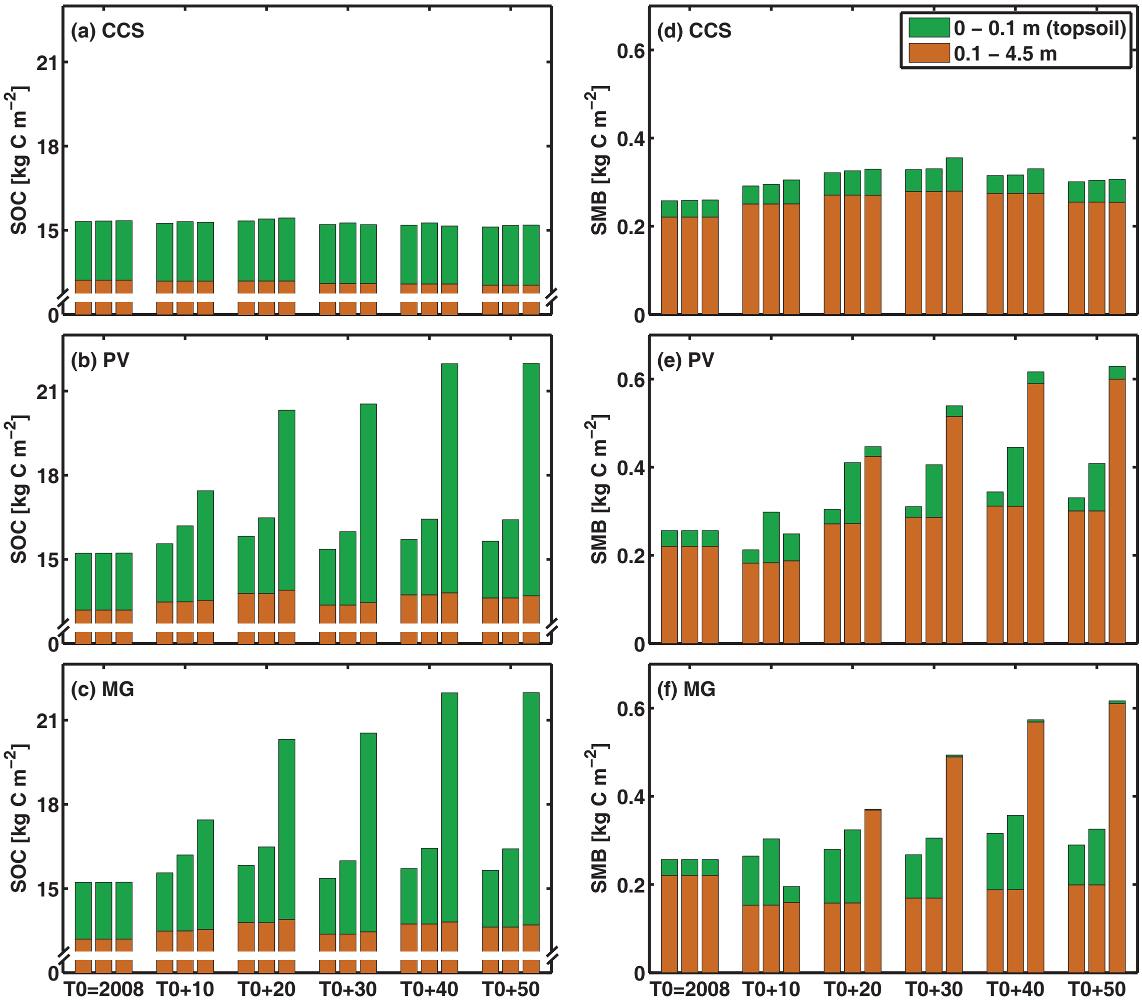

Figure S7. Projected (a–c) soil organic carbon (SOC), and (d–f) microbial biomass (SMB) for corn–corn–soybean rotation (CCS), switchgrass (PV), and miscanthus (MG) every 10 years from T0=2008 to T0+50. The bars at left, middle, and right in a given year represent scenario I, II, and III, respectively.

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