Validation of an agroecosystem process model (AGRO-BGC) on annual and perennial bioenergy feedstocks

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Abstract

Corn (*Zea mays* L.) residues and perennial C₄ grasses are two Midwest bioenergy feedstock candidates due to their compatibility with agricultural infrastructure and potential for ecosystem service delivery. We validated the ecosystem process model AGRO-BGC by comparing model estimates with empirical observations from corn and perennial C₄ grass systems across Wisconsin and Illinois under no-tillage, nitrogen fertilized, and unfertilized management. Validation parameters included soil organic carbon (SOC), total soil nitrogen (N) to 1.2 meters, aboveground net primary productivity (ANPP), net ecosystem productivity (NEP), and leaf area index (LAI). We parameterized AGRO-BGC to represent ecophysiological characteristics of corn and perennial prairie grasses, and constructed scenarios to represent corresponding edaphic, climate, and management conditions. Unfertilized annual model estimates had normalized mean average errors relative to field measurements of 0.3, 23, and 4 t ha⁻¹ for ANPP, SOC, and N, respectively. Fertilized simulations erred from observations by 0.6, 29, 5 t ha⁻¹ for ANPP, SOC, and N, respectively.

We also estimated long-term implications of varying residue removal rates on SOC. Model estimates compared to field data tested the hypothesis that long-term increased residue removal decreases SOC. Field observations showed 0.17, 0.09, and a -0.17 tC ha⁻¹ yr⁻¹ change for control, harvest, and bare grass residue removal treatments, respectively. Simulated SOC loss was greatest for the most intensive residue removal scenarios (-0.48 and -0.68 tC ha⁻¹ yr⁻¹ for corn and grass, respectively), compared to no-harvest scenarios that increased SOC by 0.05 tC ha⁻¹ yr⁻¹ for both corn and grass. AGRO-BGC estimated a 0.07 tC ha⁻¹ yr⁻¹ loss under corn residue harvest, while estimating 0.09 tC ha⁻¹ yr⁻¹ loss for grass. Results suggest long-term increased corn and grass residue harvest (beyond grain) for biofuel feedstock will decrease SOC and soil productivity by approximately 15% in corn and 21% in grass systems over 47 years.

Keywords: agroecosystem process model, AGRO-BGC, soil organic carbon, switchgrass, corn stover, bioenergy

1. Introduction

Agricultural residues are estimated to provide 350 million dry tons of bioenergy feedstock, 70% of which could come from corn (*Zea mays L.*) stover or corncob biomass. These residues are poised for bioenergy feedstock because of their ample supply, low cost, and widespread availability in the Upper Midwest (Perlack & Stokes, 2011). The 2007 Energy Independence and Security Act (EISA) set forth provisions to promote the use of renewable energy through the Renewable Fuels Standard (RFS). This mandate calls for the production of 36 billion gallons per year (BGY) of renewable fuels by 2022, 16 of which are to come from cellulosic biofuels and 14 BGY from advanced biofuels (Perlack & Stokes, 2011).

The USDA estimates that crop yields will increase by 9.5% over the next ten years, generating the potential for increased amount of crop residues available for allocation to bioenergy production (Perlack & Stokes, 2011). While the production potential of crop residues is great, there is still uncertainty around how much residue can be harvested to meet bioenergy feedstock demands without decreasing long-term soil productivity (Mann *et al.*, 2002; Lal, 2005; Blanco-Canqui & Lal, 2007; Wilhelm *et al.*, 2007; Cruse & Herndl, 2009; Surendran Nair *et al.*, 2012).

Changing land cover from natural vegetation to agriculture results in an initial, large loss of CO₂ from the soil to the atmosphere (Schlesinger, 1997). Continued cultivation results in chronic low-levels of CO₂ released to the atmosphere due to reduced inputs of plant detritus and increased decomposition rates compared with pre-cultivation vegetation conditions (Jenkinson & Coleman, 1994). Carbon release is further intensified by current competing agricultural practices

that include harvest for livestock bedding, silage, and manure-stover slurry, in addition to the potential harvest for bioenergy feedstock. When left on the field, residues provide erosion protection and carbon (C) and nitrogen (N) inputs to soils. Some research suggests that long-term removal of residues will create plant nutrient deficiencies unless N is replaced by alternative inputs (Wilhelm *et al.*, 2004; Lal, 2005). Another concern is that residue removal will decrease soil organic matter (SOM) stocks in agroecosystems (Lal & Pimentel, 2007), which would likely result in decreased nutrient content, diminished biological activity, and degraded soil structure. The removal of crop residues can alter these processes by changing energy balances and leaving soil surfaces exposed to wind and water impacts. These can significantly degrade soil quality and contribute to soil loss, which is detrimental to agricultural systems and environmental quality.

One major uncertainty surrounding bioenergy feedstock production is the long-term sustainability of soil fertility, and the amounts of crop residues that can be sustainably harvested from agroecosystems to meet US bioenergy needs. Field studies provide useful insights into the short-term effects of different management practices on soil productivity, however SOC and N are slow to respond to external change (Jenkinson & Coleman, 1994) and empirical data on long-term residue manipulation studies for agroecosystems are rare, particularly for bioenergy feedstocks. An alternative is to employ a long-term SOC dataset from an annually managed experimental prairie site as a proxy to explore the effects of residue manipulations in agroecosystems. Using ecosystem process modeling tools such as AGRO-BGC (Di Vittorio *et al.*, 2010) validated with empirical field data can help elucidate the long-term implications of residue management policies (Peckham & Gower, 2011). We applied AGRO-BGC to a Wisconsin system to estimate the effects of residue harvest over the long term.

The application of ecosystem process models, such as AGRO-BGC, BIOME-BGC, CENTURY and AGRO-IBIS (Parton *et al.*, 1987; Kucharik, 2003; Wang *et al.*, 2005; Di Vittorio

et al., 2010; Peckham & Gower, 2011), on natural and managed ecosystems improves understanding of the functions and dynamics of complex ecosystems. They improve understanding of the magnitude and variability of management effects over time scales (i.e. multiple decades) that are rarely captured by existing empirical research studies (Peckham & Gower, 2011). Interactions among management practices, erosion, SOM, nutrients, and crop or biomass yields are complex, and the use of AGRO-BGC can assist in clarifying these interactions over the long-term.

The ability to simulate the dynamics of an annual cropping system is constrained by our understanding of underlying agroecosystem dynamics, access to accurate climate and edaphic information, and our ability to assign correct ecophysiological values to vegetation subroutines of models. AGRO-BGC simulates C, N, and water cycles, and their interactions, and allows users to simulate ranges of irrigation inputs, annual seed planting, fertilizer application, and harvest practices (Di Vittorio *et al.*, 2010). The predecessor of AGRO-BGC, BIOME-BGC, has been validated extensively against eddy covariance flux tower data (Turner *et al.*, 2005) and against long-term empirical field data sets across evergreen and deciduous forests (Turner *et al.*, 2002; Peckham & Gower, 2011). Both models have been validated in perennial grass systems and BIOME-BGC has been validated in an annual corn cropping system in China (Wang *et al.*, 2005), but neither has been applied to annual corn cropping systems in the Upper Midwest under the context of bioenergy feedstock production.

The two objectives of this research were to i) validate AGRO-BGC by comparing simulated results with empirical observations from multiple agricultural field sites across Wisconsin and Illinois, and to ii) use the model to explore long-term implications of residue removal on soil productivity. Metrics of evaluation included comparing model estimates of state variables and magnitude of fluxes with field measurements. Because agroecosystems are highly

modified through varying management practices and desired production outputs, a realistic and robust ecosystem process model should be able to capture the effects of these practices on soil dynamics.

2. Materials and Methods

We modeled C and N dynamics for one experimental agricultural system in south central Wisconsin, for one active farm in central Illinois, and for two perennial grassland systems (i.e. prairie restorations) also in south central Wisconsin. The experimental agricultural system was in continuous corn production, while the farm validation site was in annual soybean (*Glycine max*) - corn crop rotation. The prairie sites consisted of mixed perennial grasses. All AGRO-BGC simulations were conducted as either continuous corn or perennial grass ecosystems, and detailed information on modeling phase characteristics is in Section A of the Supplementary Information.

2.1 Validation Site Descriptions

Validation field sites were selected to evaluate the model's performance in four specific areas: seasonal phenology (i.e. how well the model captures maxima, minima, and changes throughout the growing season), carbon allocation (i.e. how accurately the model distributes carbon to above ground plant pools), how well the model estimates carbon pools and fluxes, and how accurately the model captures the above soil and plant variable responses to repeated annual harvests (Table 1).

Table 1. Site location, average climate, and soil variables for validation field sites.

Site Name	Air Temp (°C)	Vegetation	Location	PPT (cm)	Soil Particle-size Distribution (% sand/silt/clay)	Elevation (m)
Arlington, WI	Max: 13.5 Min: 2.0	Continuous Corn	Lat: 43.283, Lon: -89.366	94	16/59/25	305
Goose Pond, WI*	Max: 13.5 Min: 2.0	Mixed Prairie	Lat: 43.283, Lon: -89.366	94	16/59/25	305
Bondville, IL	Max: 17.0 Min: 5.6	Corn/Soybean	Lat: 40.006, Lon: -88.291	99	16/57/27	215
Madison, WI	Max: 13.7 Min: 2.1	Mixed Prairie	Lat: 43.038, Lon: -89.430	93	9/65/26	288

Air Temp, mean daily air temperatures, Lat, latitude; Lon, longitude, PPT, precipitation. *Goose Pond Sanctuary is situated <2.5 km from the Arlington Research Station, and is comprised of similar edaphic and climate variables.

The pre-settlement dominant land cover type in Southern Wisconsin was a mixture of prairie and oak (*Quercus spp.*) savannah (Cottam & Loucks, 1965). Following settlement, arable land was put into agriculture production for growing wheat (*Triticum aestivum*), oats (*Avena sativa*), tobacco (*Nicotiana tabacum*), and hops (*Humulus lupulus*), or put into pasture for livestock or dairy. The late 1800s brought about annual row crop production, particularly corn and soybeans (Schaefer, 1922).

The Arlington (AG) dataset provides a robust quantitative assessment of C stocks and fluxes in a corn agroecosystem, particularly metrics for productivity including SOC, total soil N, and ANPP (Kucharik *et al.*, 2001; Brye *et al.*, 2002). The Arlington dataset also provides a robust water budget to supplement the C simulations, including estimates of evapotranspiration (ET; Brye *et al.*, 2000). This site is situated in the University of Wisconsin-Madison's Arlington Agricultural Research Station in Arlington, WI (Latitude: 43.283, Longitude: -89.366). The AG site was on a Plano silt loam (fine-silty, mixed, superactive, mesic Typic Argiudoll) that

developed in loess over glacial till (Brye *et al.*, 2002). The corn study, established in the spring of 1995, consisted of four replicate test plots (9.1 x 12.2 m) of continuous corn under various management practice combinations, with an annual fall grain harvest and crop residues left on the field. Specific management practices included conservation (no-tillage) and conventional (chisel plow) tillage treatments. Nitrogen fertilizer treatments included optimal N-fertilization (180 kg N ha⁻¹ yr⁻¹ applied post planting) and deficient N-fertilization (no N fertilizer application after a small starter N application).

The Goose Pond (GP) prairie restoration site is situated less than 2.5 km from the Arlington agricultural research station and was retired from agricultural use in June 1976 when mesic tallgrass prairie restoration began. The prairie study also consisted of four replicate test plots (7 x 7 m) established in the spring of 1995. Dominant vegetation includes big bluestem (*Andropogon gerardi* Vitman), indiangrass (*Sorghastrum nutans*), switchgrass (*Panicum virgatum*), purple coneflower (*Echinacea purpurea*), goldenrod (*Solidago spp.*), and black-eyed Susan (*Rudbeckia hirta*) (Brye *et al.*, 2002). Management at the prairie included burning approximately every three years since 1976. Data at both AG and GP sites were collected during a C and N budget study from 1995 to 1999. Prior to the C (Brye *et al.*, 2002) and water budget studies (Brye *et al.*, 2000), the prairie was burned in April 1998 (day of year (DOY): 108). Parameters measured in this study include annual SOC, ANPP, N, peak annual LAI, daily ET, and daily LAI. Biomass sampling and biophysical measurement methods are described in Brye *et al.*, 2002.

The Bondville, IL (BV) research site has been in agricultural production for approximately 100 years, the last 30 of which have been in a corn-soybean rotation. Before this, the farm was in small grain and hay production (J. Reifsteck, personal communication). This site is underlain by a combination of Flanagan silt loam (fine, smectitic, mesic Aquic Argiudoll) and

Drummer silty clay loam (fine-silty, mixed, superactive, mesic Typic Endoaquoll). This dataset provides daily measurements of NEP, daily LAI, and daily leaf C (Meyers & Hollinger, 2004; Hollinger *et al.*, 2005). Site observations were used to assess the model's ability to simulate accurate C allocation within the plant (leaf C) and to compare against model estimates of seasonal CO₂ fluxes between the canopy and the atmosphere (Turner *et al.*, 2002, 2005; Turner, 2003). The site consists of multiple agricultural fields in a no-tillage corn-soybean rotation stratified across 15 farms within a 25 km² study area, and research was established in 1996 (Meyers & Hollinger, 2004; Turner *et al.*, 2005). Field data used in this study included only the corn years of the corn-soybean rotation. Validation data are from a C and N budget study using field measurements of leaf C and LAI representing mean averages for cornfields across the study area (Campbell *et al.*, 1999; Turner *et al.*, 2005). Daily NEP flux tower data were collected for corn crops at one farm field within the study area (years 1997, 1999, 2001, 2003, and 2005) and aggregated over the growing season to determine whether the crop is a C source or C sink. Details on sampling and measurement methods are referenced in Meyers & Hollinger (2004) and Turner *et al.* (2005).

According to 1834 public survey land records, the University of Wisconsin-Madison's Arboretum (AB) site was covered with burr oak (*Quercus macrocarpa*) and black oak (*Quercus velutina*) timber stands, and rolling hills of grass (Wisconsin Public Land Survey Records, 2013). The section of the arboretum where Curtis Prairie currently resides was home to a private farm from unknown origin until 1932, when the land was acquired for the UW-Madison Arboretum. Prairie restoration of the site began between 1935 and 1940 (Nielsen & Hole, 1963). This site is underlain by a Wacousta silty clay loam (fine-silty, mixed, superactive, mesic Typic Endoaquoll).

The Curtis Prairie biomass and residue removal study provides measurements of prairie SOM during a 47-year period (Nielsen & Hole, 1963; VanRooyen, 1973). Vegetation was

established at the Curtis Prairie site in 1940, and residue manipulation treatment plots were established in 1956. Initial prairie vegetation consisted of a mixture of big bluestem, indiangrass, and switchgrass, quack grass (*Agropyron repens*), dandelion (*Taraxacum officinale*), and bluegrass (*Andropogon sp.*), among other prairie grass species. Three treatments were used; an undisturbed (control), vegetation cut and removed in fall (harvest), and vegetation frequently cut and removed to minimize accumulation of above and belowground vegetation and residue (bare). Data on soil C and bulk density in the top 10 cm were recorded in 1959, 1971, 1997, and 2006 (Nielsen & Hole, 1963; VanRooyen, 1973; Lajtha *et al.*, 2014).

2.2 AGRO-BGC Description

AGRO-BGC simulates C, N, and water fluxes and stocks on a daily time step. AGRO-BGC is modified from BIOME-BGC with additional functions for simulating agricultural management practices such as annual seeding, fertilizer application, harvest, and irrigation (Di Vittorio *et al.*, 2010) (Figure 1). Model estimates can be aggregated to monthly or annual time steps for analysis and interpretation. This study uses daily, monthly, and annual aggregations of the model estimates to correspond with the field validation datasets. Variables of interest to this study included SOC and N, NEP, ANPP, and LAI.

Figure 1. Carbon and Nitrogen fluxes and pools as simulated by AGRO-BGC, where solid lines denote carbon fluxes, and dashed lines denote nitrogen fluxes.

AGRO-BGC uses daily maximum and minimum temperature, total precipitation, average vapor pressure deficit, total solar radiation, and daylength for each study site to simulate C, water, and N fluxes. Climate data from 1980 to 2011 were cycled throughout the simulations over each study site (Di Vittorio *et al.*, 2010; Peckham & Gower, 2011), and were provided by DAYMET (<http://daymet.ornl.gov>) through the National Center for Atmospheric Research (<http://ncar.ucar.edu/>). Growing degree-day (GDD) units for corn were included in the

parameterization, specifically for emergence, stem elongation, and flowering using values from the literature (Ritchie & Hanway, 1993; Kucharik & Twine, 2007).

Model spin-up was necessary to equilibrate the terrestrial C and N pools with the atmospheric C and N pools (Thornton & Rosenbloom, 2005). We accomplished this by recycling the annual climate data until steady state conditions were met, then following with managed agroecosystem simulations (Di Vittorio *et al.*, 2010; Peckham & Gower, 2011). Simulations for the four sites were constructed to mimic general land cover and land use patterns in the region (Table 2), and detailed information on modeling phase characteristics is in Section A of the Supplementary Information.

Table 2. Information for validation sites and modeling scenarios used in this study

Crop	Site	Time Period	Treatment	Validation Parameters	References
Corn	Arlington, WI (AG)	1995-1999	Annual grain harvest	Annual SOC	Brye <i>et al.</i> , 2000
			Two nitrogen levels (0, 72 kgN ha ⁻¹ yr ⁻¹)	Annual ANPP	Brye <i>et al.</i> , 2002
				Annual Soil N	Kucharik <i>et al.</i> , 2001
				Annual Peak LAI	
				Daily LAI	
				Daily Evapotranspiration	
Perennial C₄ Grass	Bondville, IL (BV)	1999-2000	Annual grain harvest	Daily Leaf C	Meyers & Hollinger, 2004
				Daily LAI	Hollinger <i>et al.</i> , 2005
					Turner <i>et al.</i> , 2005
	Goose Pond, WI (GP)	1995-1999	Annual grain harvest	Daily NEP	
			Annual aboveground biomass harvest		Brye <i>et al.</i> , 2000
					Brye <i>et al.</i> , 2002
	Madison, WI (AB)	1956-2009			Kucharik <i>et al.</i> , 2001
			Three levels of harvest:	Annual SOC	Nielsen & Hole, 1963
			Control: no harvest		Van Rooyen, 1973
			Harvest: Annual aboveground biomass harvest		Lajtha <i>et al.</i> , 2014
			Bare: Annual aboveground biomass, litter, fine root harvest.		

We constructed validation test scenarios to reflect the conditions under which field observations were collected in terms of duration, management practices, and environmental conditions (Brye *et al.*, 2002; Turner *et al.*, 2005) (Table 2). Building the scenarios for each site was based on the above records of each site's land cover and land use history. Following the steady-state spin up of an unmanaged C₄ grass system for the Arlington (AG) and Bondville (BV) sites, the model was run from the early 1900s to the 1990s to simulate a managed continuous corn agroecosystem converted from a mixed prairie grass system. For the Goose Pond (GP) simulations, the model was run from the early 1900s to 1976 to simulate a managed continuous corn agroecosystem. Following 1976, the model was run to simulate a perennial C₄ grass system.

The Arboretum (AB) simulations also followed an unmanaged C₄ grass spin up scenario, followed by a 40-year simulation of continuous corn, followed by a C₄ grass simulation to mimic the conditions of a prairie restoration. Residue removal rates were simulated for 50 years to mimic the duration and conditions of the AB residue removal trials. Planting and harvesting dates for these simulations were based on field planting and harvesting date estimates for each site. Both corn and perennial C₄ grass simulations were run for the AB site.

Atmospheric CO₂ concentrations were estimated for both pre and post-industrial periods using values from the Carbon Dioxide Information Analysis Center (<http://cdiac.ornl.gov>). Nitrogen deposition estimates ranged from the pre-industrial values of 0.001 tons N ha⁻¹ yr⁻¹ to 1994 value of 0.005 tons N ha⁻¹ yr⁻¹ (National Atmospheric Deposition Program (<http://nadp.sws.uiuc.edu>)). Edaphic characteristics including rooting depth, when not defined in the literature, were derived from the Soil Survey Geographic (SSURGO) Database (<http://datagateway.nrcs.usda.gov/>) based on the site location (Peckham & Gower, 2011).

All ecophysiological parameters were assigned values from published literature (Bollero *et al.*, 1996; White *et al.*, 2000; Ma & Dwyer, 2001; Wang *et al.*, 2005; Di Vittorio *et al.*, 2010;

Schulze *et al.*, 2011). For corn, mean values for C₄ grasses were used in the absence of species-specific values, and when these were unavailable, general ecophysiological values were used (White *et al.*, 2000) (Table 3). Ecophysiological parameters for perennial grasses were derived from a previous C₄ grass validation study (DiVittorio *et al.*, 2010). Datasets used to parameterize the ecophysiological characteristics were distinct from datasets used to validate the model outputs.

Table 3: Data Inputs for AGRO-BGC

Daily Climate Inputs	Units
Maximum Daily Temperature	°C
Minimum Daily Temperature	°C
Mean Daily Temperature	°C
Precipitation	cm
Vapor Pressure Deficit	Pa
Incoming Solar Radiation	Watts m ⁻²
Daylength	seconds

Edaphic Data Inputs	Units
Effective Soil Depth	m
Sand Percentage by Volume	%
Silt Percentage by Volume	%
Clay Percentage by Volume	%
Site elevation	m
Site Latitude (- for Southern Hemisphere)	decimal degrees
Site Shortwave Albedo	-
Wet and Dry Atmospheric N Deposition	kgN m ⁻² yr ⁻¹
Symbiotic and Asymbiotic N Fixation	kgN m ⁻² yr ⁻¹

Corn Ecophysiological Inputs	Units
New fine root C: new leaf C	1.1 ^a
New stem C: new leaf C	1.7 ^a
C:N of leaves (kgC kgN ⁻¹)	49.0 ^d
C:N of leaf litter (kgC kgN ⁻¹)	49.0 ^d
C:N of fine roots (kgC kgN ⁻¹)	120.0 ^a
Fruit C:N (kgC kgN ⁻¹)	33.0b
Leaf litter labile proportion	0.68 ^c

Leaf litter cellulose proportion	0.23 ^c
Leaf litter lignin proportion	0.09 ^c
Fine root labile proportion	0.34 ^c
Fine root cellulose proportion	0.44 ^c
Fine root lignin proportion	0.22 ^c

Biophysical Inputs	Units
Canopy water interception coefficient ($1 \text{ LAI}^{-1} \text{ day}^{-1}$)	0.0225 ^c
Canopy light extinction coefficient	0.48 ^c
All-sided to projected leaf area ratio	2.0 ^c
Canopy average specific leaf area ($\text{m}^2 \text{ kgC}^{-1}$)	15.0 ^d
Ratio of shaded SLA:sunlit SLA	2.0 ^c
Fraction of leaf N in Rubisco	0.225 ^c
Fraction of leaf N in PEP Carboxylase	0.03 ^e
Maximum stomatal conductance (m s^{-1})	0.012 ^f
Cuticular conductance (m s^{-1})	0.00012 ^c
Boundary layer conductance (m s^{-1})	0.04 ^c
Leaf water potential: start of conductance reduction (MPa)	-0.73 ^a
Leaf water potential: complete conductance reduction (MPa)	-2.7 ^a
Vapor pressure deficit: start of conductance reduction (Pa)	930.0 ^c
Vapor pressure deficit: complete conductance reduction (Pa)	4000.0 ^c

Ecophysiological values are from the following studies: ^aWang *et al.*, 2005, ^bMa and Dwyer

2001, ^cWhite *et al.*, 2000, ^dSensitivity Analysis Results, ^eSugiharto *et al.*, 1990, ^fSchulze *et al.*, 1994

When specific parameter values could not be obtained from the literature, an independent variation sensitivity analysis was conducted to minimize percentage error between observed and simulated variables (White *et al.*, 2000; Xu *et al.*, 2008). This was done to test the effect of varying each parameter by a constant step throughout a known range, independently of all parameters. The simulated results were compared to observed field values and the percent error was calculated. Parameter values obtained from the literature were used in this analysis, and a mean, standard deviation, minimum, and maximum were included (White *et al.*, 2000; Xu *et al.*, 2008). Parameters included in the sensitivity analysis were grouped into biomass allocation (e.g.

fine root C:leaf C), nutrient stoichiometry (e.g. leaf C:N, fine root C:N), and general vegetation characteristics [e.g. rooting depth, flowering GDD, specific leaf area (SLA), fraction of leaf N in Rubisco (FLNR), fraction of leaf N in PEP carboxylase (FLPEP), and maximum stomatal conductance ($g_{S_{max}}$)]. These parameters represent the processes that drive leaf photosynthetic machinery, leaf infrastructure, and the biophysical dynamics of the crop canopy. Methods and results of the sensitivity analysis are described in Section B of the Supplementary Information.

AGRO-BGC simulates photosynthesis based on the DePury and Farquhar two-leaf model (White *et al.*, 2000; Golinkoff, 2010), which estimates canopy area (LAI) prior to partitioning light to the sunlit and shaded canopy components. LAI is the product of leaf carbon and the user prescribed specific leaf area (SLA) and is calculated preceding any daily photosynthetic activity. Each gross primary production calculation is conducted for both sunlit and shaded leaves, and the amount of C assimilated is summed at the end of the day. After accounting for metabolic demands estimated by vegetation specific allometric equations, the photosynthetically accumulated C is allocated to the various plant (e.g. leaves, stem, and fine roots) and soil pools according to allocation parameters (White *et al.*, 2000; Di Vittorio *et al.*, 2010). Nitrogen concentrations of tissue pools are characterized by C:N ratios, and these drive new growth, plant respiration rates, photosynthetic capacity, and litter type. The calculation for NPP is the gross primary productivity (GPP) minus maintenance and growth respiration, where a positive value reflects net biomass accumulation. Evapotranspiration is simulated in AGRO-BGC using a modified Penman-Monteith equation, and takes into account evaporated canopy intercepted water, photosynthetic transpiration, and soil evaporation (Di Vittorio *et al.*, 2010; Golinkoff, 2010).

Net ecosystem productivity is the net quantity of C accumulated by the system, accounting for C loss through autotrophic, growth and heterotrophic respiration, erosion, and

consumption by herbivory. In the model, NEP is calculated by subtracting heterotrophic respiration from NPP, as erosion is not accounted for in AGRO-BGC.

AGRO-BGC's disturbance function simulates agroecosystem management practices through prescribed addition, removal, or allocation of N and C to plant and soil pools. Practices such as grain and residue harvest, N fertilizer application, and residue removal were simulated using this function. Crop management practices documented in the field studies were replicated in the AGRO-BGC simulations including the proportion of biomass removed from the system, frequency of residue removal, and the duration of the biomass removal (Di Vittorio *et al.*, 2010; Peckham & Gower, 2011). For this research, all annual cropping management practices were assumed to be no-tillage, as all agricultural validation data used were from no-tillage systems (Brye *et al.*, 2002; Hollinger *et al.*, 2005) and AGRO-BGC currently lacks the capacity to simulate tillage. Annual corn harvest was simulated by assuming 100% grain removal with all remaining residue (e.g. stem, leaf, and fine roots) transferred to the litter pool. Fertilizer application was simulated by assigning the amount of fertilizer to be added into the available soil mineral N pool (Di Vittorio *et al.*, 2010) in specific quantities at a specific time. A N uptake efficiency of 40% (Cassman *et al.*, 2002) was assumed and the amount of applied N during the AG field study of $180 \text{ kgN ha}^{-1} \text{ yr}^{-1}$ that was taken up by the crop was calculated to be $72 \text{ kgN ha}^{-1} \text{ yr}^{-1}$.

For C_4 grass simulations at the AB site, harvest was simulated by 100% removal of above ground biomass, but leaving the litter pool and fine roots on site, while the bare simulations removed the litter pool in addition to all above ground biomass. Control simulations of the grass systems experienced no disturbance.

2.3 Validation Parameters

Annual SOC and N pools were selected to evaluate AGRO-BGC's ability to simulate the long-term effects of residue management on soil productivity. All aboveground biomass (e.g. leaves, stems, roots, fruit) was either harvested (i.e. removed from the system), transferred to litter pools during senescence and mortality, or left on the soil surface as residue following harvest. The litter pool fragments the detritus into different pools with differing recycling rates based on litter composition, temperature, and moisture content. Upon decomposition, the C and N in the transient detritus pools are transferred into the SOM pools, where the quantity of SOC and N can each be calculated.

Leaf area index is a measure of the amount of leaf surface area exposed to light interception and attenuation, and it is a driver of photosynthesis in the plant canopy (Meyers & Hollinger, 2004). Leaf area index acts as an indicator of AGRO-BGC's ability to capture annual plant phenology in a managed annual cropping system. In AGRO-BGC, LAI drives the absorption of photosynthetically active radiation, interception of precipitation, photosynthesis, and the amount and type of litter deposited into detritus pools (White *et al.*, 2000; Golinkoff, 2010).

2.4 AGRO-BGC Modeling Scenarios

2.4.1 Arlington (AG): We constructed two scenarios to simulate continuous corn under conservation tillage management and under two N fertilizer treatments from 1995 to 1999. Each harvest scenario experienced an annual fall grain harvest with residue left on the soil. The base scenario (NTNF0) consisted of an annual grain harvest, no-tillage, no fertilizer application, and the fertilized scenario (NTF0) consisted of the same practices but with an annual fertilizer application of $72 \text{ kgN ha}^{-1} \text{ yr}^{-1}$.

2.4.2 Goose Pond Prairie Sanctuary (GP): We constructed one scenario to simulate a perennial grass system restored from agricultural land use. The system experienced a burn disturbance every three years from 1976 to the beginning of the C budget study in 1995, then one additional burn in the spring of 1998.

2.4.3 Bondville (BV): We constructed one scenario to simulate a continuous corn system under conservation tillage management, with no fertilizer application for years 1999 to 2000 for comparison with daily leaf C and LAI measurements. We constructed an additional scenario to simulate a continuous corn system from 1997 to 2006 under conservation tillage management with no fertilizer treatment for comparison with FLUXNET tower NEP measurements. Each harvest scenario experienced an annual fall grain harvest with residue left on the soil.

2.4.4 Arboretum (AB): We constructed six scenarios to simulate 1) an annual continuous corn and 2) a perennial C₄ grass system under conservation tillage management, no fertilizer application, and under three residue manipulations from 1956 to 2009. The “control” scenarios simulated both systems with no annual harvest or residue removal. The “harvest” scenarios simulated both systems with an annual fall removal of aboveground biomass and no additional residue removal. For the corn simulation, this meant a 100% grain removal with remaining plant residues left on the soil. For the C₄ grass simulation, this meant a 100% removal of above ground plant material. The “bare” scenarios simulated both systems with annual fall harvest and complete residue removal.

2.5 Evaluation Methods

We compared model outputs with field and eddy-covariance measurements from several C budget and biophysical studies to evaluate the model's ability to accurately simulate the ecosystem C and N dynamics. Annual model estimates were compared to each site's respective field data, and the normalized mean absolute error (NMAE) between simulated and observed values was calculated using the following equation:

$$\text{NMAE} = \Sigma [(SIM - OBS)/(n \text{ } OBS_{mean})] \quad (1)$$

Where OBS indicates observed measurements, SIM indicates modeled estimates, n is the sample size, and OBS_{mean} refers to the mean of all observed values in the sample set. Perfect agreement between the model and observations results in $\text{NMAE} = 0$ (Schwalm *et al.*, 2010, Yang *et al.*, 2014), and negative values reflect model underestimates while positive values reflect model overestimates.

Annual NPP (ANPP) for the corn system was estimated from the annual above ground biomass accumulated and compared with field measurements of above ground biomass harvested in the fall. Within the R programming environment, linear regression analysis was used to compare simulations of daily LAI with both corn and prairie LAI measurements throughout the growing season for the duration of the Arlington study (Pineiro *et al.*, 2008). AGRO-BGC requires a static planting date that is repeated yearly for the duration of the simulation, so it is unable to capture the variation in planting dates that producers deal with every year. Model outputs were shifted to reflect actual planting dates for each simulated growing season, when available.

Soil C and N estimates consisted of the summation of organic soil C and total soil N pool fractions at the end of the simulation year, respectively. These estimates were compared with field measurements to 1.2 m at the Arlington site, and to 10 cm at the Arboretum site. The discrepancy between sampling and simulation depths is a result of the depth to which SOC

samples were taken across the 47-year field study, and the depth to which AGRO-BGC can feasibly simulate an annual corn system. The Arlington soil C and N measurements were calculated as the average of the mean content for spring and fall. The Arboretum soil C estimates were estimated from the fall sampling period.

Simulated and measured SOC was compared for 1959, 1971, 1997, and 2006 to assess the model's ability to estimate response to residue manipulations at the Arboretum site. Total SOC loss under the varying residue manipulations was estimated as the difference between initial and final SOC content.

To evaluate the model's ability to accurately simulate NEP, model estimates were compared to eddy-covariance flux tower measurements at the Bondville field using linear regression (Pineiro *et al.*, 2008). Carbon flux measurements during the growing season were summed to measure the C storage of the crop for corn years where the growing season was defined as the time period between planting and harvest.

3. Results

3.1 Carbon and Phenology Validation Results

Estimated corn ANPP for NTNF0 and NTF0 treatments at Arlington averaged approximately 5 and 8 tC ha⁻¹yr⁻¹ respectively over the 1995 to 1999 simulation. AGRO-BGC overestimated ANPP on average by 0.3 t ha⁻¹ for the unfertilized treatment, and underestimated ANPP by 0.6 t ha⁻¹ for the fertilized treatment (Table 4). Daily simulated ET averaged 2.4 and 2.5 mm day⁻¹ for the no-tillage corn (AG) and prairie system (GP) respectively, across the 1995 to 1999 study period.

Table 4. Annual summary of simulated and observed peak leaf area index (PeakLAI), aboveground net primary productivity (ANPP), total soil organic carbon (C), and total soil nitrogen (N) for no-tillage and unfertilized (top) and fertilized (bottom) treatments at the Arlington corn site (AG), and accumulated normalized mean absolute error (NMAE) over 1995-1999.

Year	Simulated [t ha ⁻¹]				Observed [t ha ⁻¹]				NMAE [t ha ⁻¹]			
	Peak LAI	ANPP	Soil C	Soil N	Peak LAI	ANPP	Soil C	Soil N	Peak LAI	ANPP	SoilC	Soil N
1995	3.9	5	170	17	3.4	5	179	14	1.7	0.3	22.5	3.8
1996	4.9	5	170	17	3.2	5	160	13				
1997	4.7	5	170	17	3	6	153	13				
1998	5.9	6	169	17	3.1	5	132	12				
1999	-	5	170	-	-	4	131	-				

Year	Simulated [t ha ⁻¹]				Observed [t ha ⁻¹]				NMAE [t ha ⁻¹]			
	Peak LAI	ANPP	Soil C	Soil N	Peak LAI	ANPP	Soil C	Soil N	Peak LAI	ANPP	SoilC	Soil N
1995	6.6	7	194	-	3.8	7	179	-	4.4	-0.6	29.2	4.5
1996	7.6	8	194	19	3.9	9	191	14				
1997	7.7	8	195	19	3.3	9	166	14				
1998	9.9	9	194	19	3.3	10	146	17				
1999	-	7	195	-	-	8	146	-				

When model estimates were adjusted for variable planting dates, early season growth was captured by the model for both the AG (Figure 2) and BV (Figure 3a) field sites. In general,

simulated and measured LAI increased during the early growing season, reached a peak LAI on average around late August (DOY: 232 to 234), then decreased as the corn canopy senesced.

Figure 2. Daily leaf area index (LAI) model outputs compared with field observations for no-tillage, unfertilized (NTNF0) scenario (a) and no-tillage, fertilizer applied (NTF0) scenario for AG field site (b).

Figure 3. Daily leaf area index (LAI) model outputs compared with field observations for no-till, unfertilized scenario (a), and daily leaf carbon content (b) compared with field observations for no-till unfertilized scenario for the BV site.

Measured and simulated daily LAI were positively correlated for AG ($R^2 = 0.85$ for NTNFO and $R^2 = 0.83$ for NTF0) (Figure 4). The NTNFO simulation had a slope coefficient of 0.66

deviating significantly ($p < 0.05$) from zero and unity, while NTF0 also deviated significantly ($p < 0.05$) from both zero and unity with a slope coefficient of 0.50. The intercepts of both regressions deviated significantly from zero ($p < 0.05$). Leaf area index estimates agreed with observations for lower LAI values, but the two estimates increased in deviance from observations for LAI values above 2.5 for NTNFO and above 2.0 for NTF0.

Figure 4. Plot of simulated versus observed daily LAI values for NTNFO (a) and NTF0 (b) treatments for AG research site for 1995-1999. The dashed line represents the 1:1 relationship between simulated and observed LAI measurements, while the solid line represents the linear regression relationship.

On average, the model overestimated annual peak LAI for the NTNFO and NTF0 simulations by 1.7 and 4.4 units, respectively (Table 4). Peak LAI estimates averaged 5 and 8 for the NTNFO and NTF0 simulations (Table 4), respectively. However, for the GP system, measurements of peak LAI aligned with simulated average peak LAI, each averaging at 4. The model also overestimated daily LAI and daily leaf C throughout the growing season at the BV site (Figure 3).

The BV flux tower measurements from years 1997, 1999, 2001, 2003, and 2005 are represented in Figure 5. Measured and simulated NEP were positively correlated for BV (R^2 of 0.51) (Figure 5). The regression equation had a slope coefficient of 1.1 deviating significantly ($p < 0.05$) from zero and deviating insignificantly away from unity ($p > 0.05$), while the intercept was 0.43, deviating significantly ($p < 0.05$) from zero. AGRO-BGC captured the intra-annual variability of daily NEP, with maximum NEP occurring at full canopy closure during the growing season and negative NEP values outside the growing season (Figure 5). Model estimates of NEP averaged $3 \text{ tC ha}^{-1}\text{yr}^{-1}$, while flux tower measurements averaged at $5 \text{ tC ha}^{-1}\text{yr}^{-1}$, with a mean simulation underestimation of 47% across all corn years.

Figure 5. Linear regression of observed and simulated monthly mean aggregated net ecosystem productivity (NEP) for cornfields across the BV site, corn years only. The dashed line represents the 1:1 relationship between simulated and observed NEP measurements, while the solid line represents the linear regression relationship.

3.2 Soil C and N Validation Results

Simulated SOC content for the AG NTNFO and NTF0 treatments averaged 170 and 195 tC ha⁻¹ during the 5-year simulation, respectively (Table 4). On average in the NTNFO simulations, the model overestimated observed soil C by 23 t ha⁻¹, while NTF0 simulations overestimated soil C by 29 t ha⁻¹.

AGRO-BGC overestimated total soil N for the AG NTNFO and NTF0 treatment by 4 and 5 t ha⁻¹, respectively. Simulated total soil N for the NTNFO and NTF0 treatments averaged approximately 17 and 19 tN ha⁻¹, respectively (Table 4) in the top 1.2 m of the soil profile.

3.3 Long-term SOC Effects

AGRO-BGC corn estimates SOC increased (151 to 153 tC ha⁻¹) during the AB 47-year control simulation at a rate of 0.05 tC ha⁻¹ yr⁻¹, but decreased (151 to 148 tC ha⁻¹) for the harvest simulation at a rate of 0.07 tC ha⁻¹ yr⁻¹. Soil organic C in the bare simulation lost 22 tC ha⁻¹ during the 47-year period, at a rate of 0.5 tC ha⁻¹ yr⁻¹ (Figure 6a).

The results of the AB C₄ grass AGRO-BGC simulations showed an increase in soil C of 0.05 tC ha⁻¹ yr⁻¹ in the control (151 tC ha⁻¹ to 154 tC ha⁻¹), a 0.09 tC ha⁻¹ yr⁻¹ loss in the harvest (151 tC ha⁻¹ to 147 tC ha⁻¹), and a 21% loss in the bare scenario (151 tC ha⁻¹ to 120 tC ha⁻¹) in the top 1.5 m soil profile (Figure 6b). The greatest SOC rate loss was for the bare residue removal treatment, which averaged 0.48 and 0.68 tC ha⁻¹ yr⁻¹ loss for corn and grass simulations, respectively.

Figure 6. Simulated annual soil organic carbon content under varying residue removal rates from 1960 - 2006 for corn (a) and C₄ mixed grasses (b) compared to field observations at the AB field site. SOC was estimated at 1.2 m in AGROBGC, measured SOC at 10 cm at AB.

4. Discussion

Models provide an effective means for understanding the complex dynamics between the terrestrial, vegetation, and atmospheric components of managed agroecosystems, and allow for informed predictions about long-term effects of varying management practices when empirical field studies are unavailable. Models are not perfect predictors of future outcomes and the performance of individual models is limited by the user's understanding of agroecosystem dynamics and intrinsic model factors. However, confidence in their predictive power increases when models are validated with long-term field observations.

Capturing all simultaneous processes of a managed agroecosystem within a single model is an impossible undertaking, particularly in agricultural systems that undergo frequent and significant disturbance. However, demonstrating AGRO-BGC's ability to approximate the C and N stocks and responses to bioenergy feedstock harvest is a significant contribution to the modeling community. Further application of AGRO-BGC can contribute to developing sound bioenergy feedstock management policies by improving our understanding of the magnitude and variability of the effects of management practices over time scales that are rarely captured by existing empirical field studies.

4.1 Comparison of Model Simulations with Empirical Data

AGRO-BGC results demonstrate reasonable agreement between simulations and empirical data, with NTNFO and NTF0 annual biomass falling within 0.3 and 0.6 tC ha⁻¹, respectively, and soil C pool estimates falling within 23 and 29 tC ha⁻¹ of field observations, respectively. Brye *et al.* (2002) measured ANPP at 5 and 9 tC ha⁻¹ for a continuous corn cropping system under NTNFO and NTF0 management, respectively at the AG site, and reported SOC at 151 and 166 tC ha⁻¹, respectively.

While AGRO-BGC overestimated annual peak LAI under fertilized scenarios at the AG site, the model captured the seasonal minima and canopy phenology in both the fertilized and non-fertilized scenarios. Daily simulated ET averages aligned well with field observations reported by Brye *et al.* (2000), matching fluxes of 2.4 and 2.5 mm day⁻¹ for the no-tillage corn (AG) and prairie system (GP) respectively. AGRO-BGC simulations also showed good agreement with field measurements of C₄ grass peak LAI.

The capacity for bioenergy feedstock systems to store C is represented by NEP. Agroecosystems taking up more C than is released are considered C sinks, while systems that release more C than is taken up are considered C sources. When comparing the BV observations to model predictions, AGRO-BGC captured the growing season net storage of C and the net loss of C during the off season. Before planting and after harvest, greater amounts of C are released through respiration than are stored, because there is no plant biomass photosynthesizing for approximately six months out of the year (Hollinger *et al.* 2005).

Flux towers at the BV unfertilized corn agroecosystem site (Hollinger *et al.*, 2005) measured a mean annual NEP of 6 tC ha⁻¹ yr⁻¹ from 1997 to 2002. AGRO-BGC simulated NEP averaged 3 tC ha⁻¹yr⁻¹ for 1997 to 2006, which suggests that the model overestimated canopy respiration because, as shown at the AG site, the ANPP estimates align with field measurements.

4.2 LAI and Crop Canopy Dynamics

While modeled LAI captured greater than 80% of the variation in the AG field LAI observations and aligned with observations during early and late season canopy dynamics, the model still greatly overestimated peak LAI under both NTNF0 by 1.7 and NTF0 by 4.4. Modeled LAI tended to increase in overestimation above observed LAI values of 2.0, indicating a larger contribution to leaf area at peak canopy closure. When coupling this with accurate ANPP

estimates, it suggests further exploration into the crop canopy algorithms. In AGRO-BGC, LAI is calculated preceding radiation partitioning into the two-layered model. The two-layered model is the unit over which all photosynthetic processes take place, which can account for the disconnect between peak LAI and accurate ANPP predictions. The two-layered model used in AGRO-BGC represents a canopy with increasing SLA with increased canopy depth, which requires assignment of different SLA for both sunlit and shaded canopy layers (White *et al.*, 2000). As the corn canopy grows, lower leaves become shaded by top leaves and by leaves and stems of adjacent densely planted crop rows. In their sensitivity analysis, White *et al.* (2000) assigned a constant 2.0 for the shaded SLA: sunlit SLA (e.g. evergreen needle leaf forests, deciduous broadleaf forests, and grasslands). This static ratio in an agroecosystem does not entirely capture the morphological dynamics of a canopy where crops are densely planted in uniform rows, nor does it account for the productivity effects of full canopy light saturation late in the growing season. Further validation efforts would benefit from daily ANPP field observations with which to compare model predictions.

Overall sensitivity analysis results (see Section B of Supplementary Information) and comparison of estimates with field observations suggest that AGRO-BGC is a competent and suitable modeling tool for estimating C and N dynamics in corn agroecosystems. Further testing against empirical datasets will improve the model's performance and enhance understanding of these dynamics over the long term.

4.3 Residue Removal Effects on SOC

Agricultural soils provide a significant stock of C to terrestrial ecosystems, and when managed appropriately, they can provide a sink for C and improve agricultural soil quality (Paustian *et al.*, 1998; Hollinger *et al.*, 2005). It is important to sustain and enhance SOC and soil

N when managing agroecosystems, particularly as agricultural residues become more viable candidates for bioenergy feedstocks on a commercial scale (Anderson-Teixeira *et al.*, 2009).

Results of varying residue removal rates for the AB simulations showed slight SOC increases in both corn and grass simulations under the control scenarios, while increasing residue removal rates decreased SOC over the duration of the study. This was also observed in the residue manipulation trials in the UW-Madison Arboretum studies (Nielsen & Hole, 1963; VanRooyen, 1973; Lajtha *et al.*, 2014). These results are similar to those reported in empirical field studies regarding land use change and SOC dynamics (Post & Kwon, 2000; Nave *et al.*, 2010; Powers *et al.*, 2011). A meta-analysis conducted across multiple agroecosystems with differing land use histories and residue management regimes showed that SOC is typically depleted under corn residue harvest (Anderson-Teixeira *et al.*, 2009). These results are applicable to any terrestrial ecosystem as residue, an important pre-cursor for SOC, is removed. Similar results have been reported for forests (Peckham & Gower, 2011) and in a wheat grain harvest system (Brye, 2012). This universal pattern suggests a first principle that cannot be ignored: increased residue removal will lead to long-term declines in SOM. Moreover, crop residue removal renders the soil more vulnerable to wind and rain erosion.

In order to maintain and enhance soil C and N pools in a bioenergy cropping system, the aboveground C and N contributions of crop residues must be maintained by additional organic matter amendments, or by increasing N fertilizer application (Chivenge *et al.*, 2007). Our findings show an increase in SOC under the no-harvest scenario, demonstrating that when leaves, stems and stalks are left on the soil surface to decompose, they contribute to SOC pools. Findings of this study support the argument that crop residues are best left on the field for maintaining and improving soil productivity (Anderson-Teixeira *et al.*, 2009).

This effect of removing increased amounts of crop residue for bioenergy poses a contrast with USDA predicted yield increases into the future (Perlack & Stokes, 2011). If agricultural feedstocks like crop residues are to be a substantial contributor to meeting US energy needs while meeting goals of climate change mitigation, it is important that corn systems are managed in such a way that prevents SOC loss and maximizes SOC gain. Future bioenergy guidelines should recommend residue removal rates or other management practices that do not lead to maximum soil C loss (e.g. conservation tillage), or recommend other sources of bioenergy feedstocks such as perennial grasses or short rotation woody crops (Schimel *et al.*, 2001; Hollinger *et al.*, 2005).

The long-term model estimates generated from this study can be used in identifying which residue removal scenarios would stabilize and enhance soil C contents, and prevent loss in soil productivity under a bioenergy management plan. Further research and validation of AGRO-BGC with long-term datasets will allow us to better estimate the capacity of Upper Midwestern farms to sustainably generate the necessary biomass to meet future energy demands. This work lays the foundation to further exploration into estimating the quantities of SOC, productivity, and carbon budget changes across different management practices and on varying landscapes of varying biophysical characteristics to apply in generating sustainable management of agricultural resources.

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