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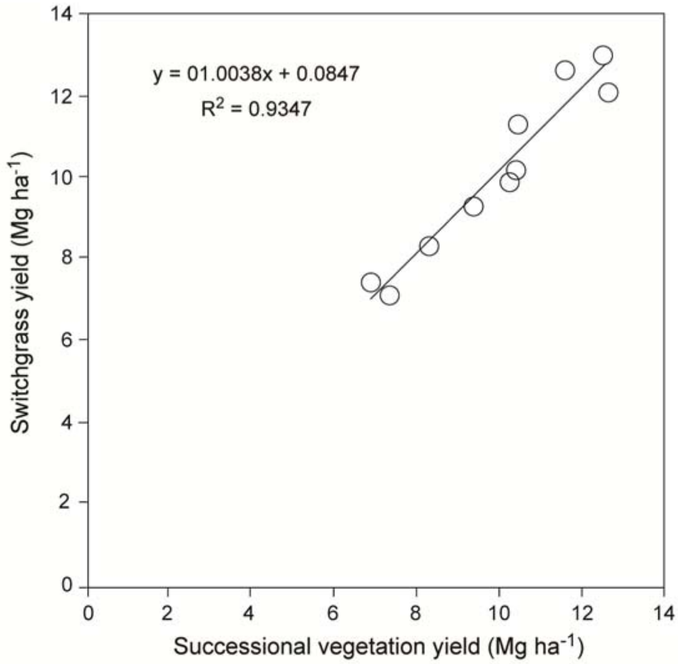
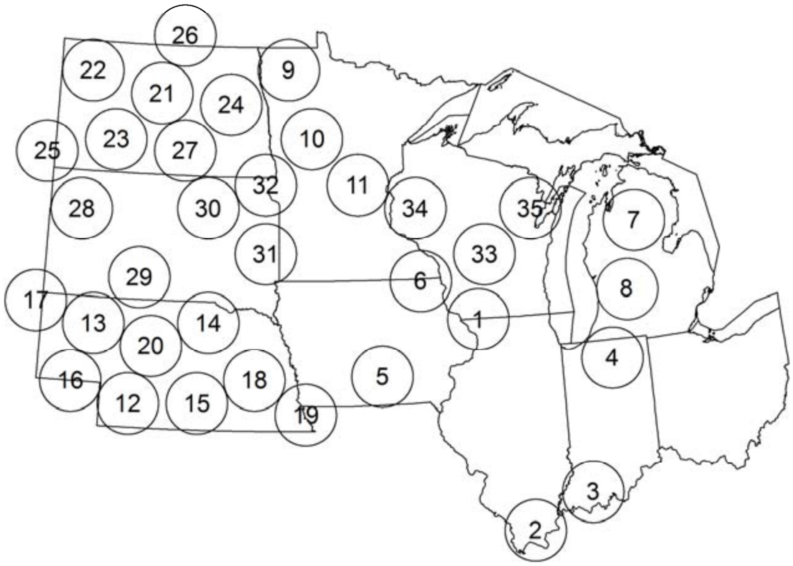
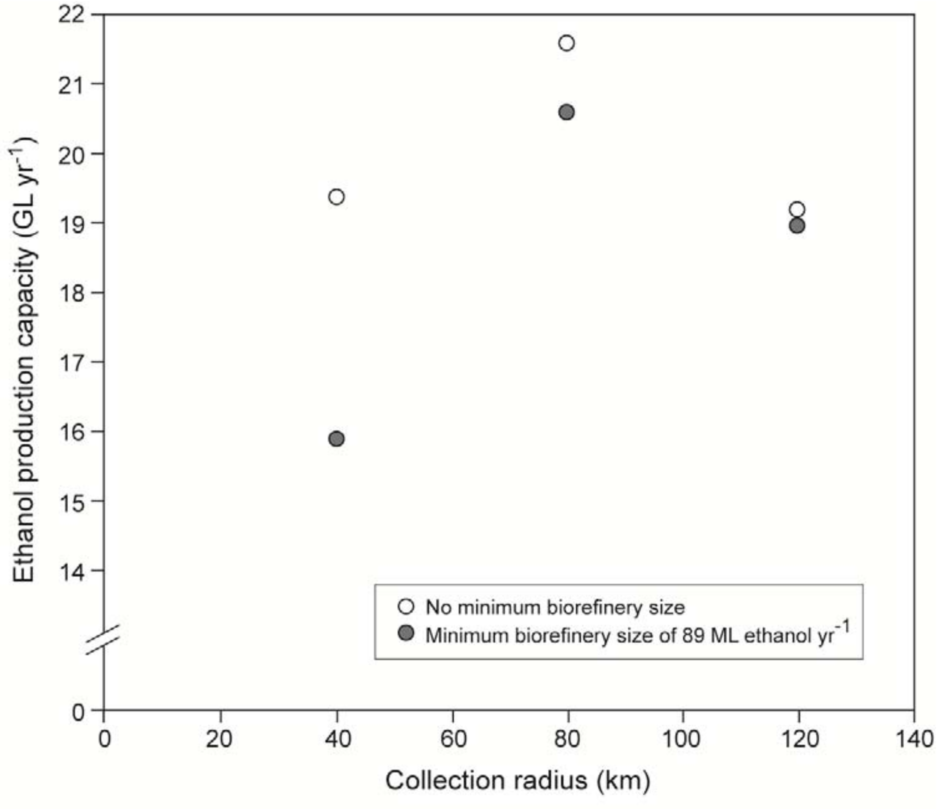
Supplementary Figures



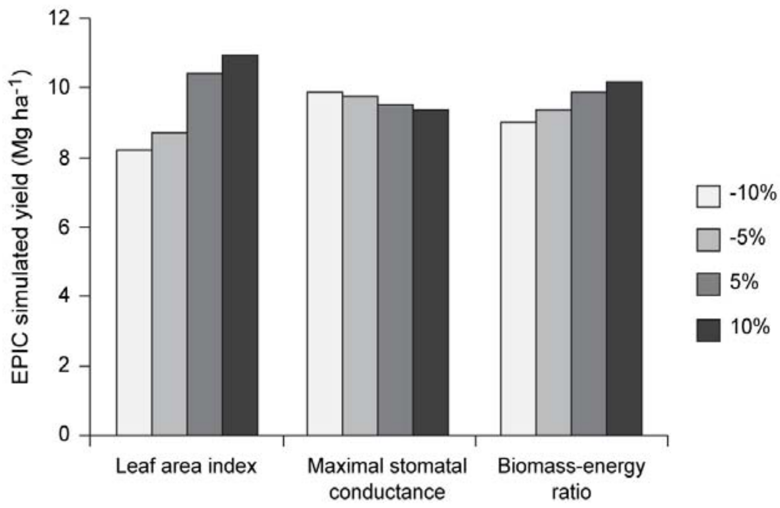
Supplementary Figure 1. Comparison of EPIC-simulated state-level average yields of post-establishment switchgrass (y-axis) and well-established successional vegetation (x-axis) in the US Midwest with nitrogen fertilization at 68 kg N ha^{-1} yr^{-1}. Results are from a sensitivity test of EPIC simulations to vegetation type. We examined the extent to which yields of grass mixes simulated across the 10-state US Midwest related to the simulated yields of N-fertilized switchgrass (*Panicum virgatum*), a model biomass crop also used in the Billion Ton Study[1]. Overall, there was a strong correlation between modeled yields, with R^2 = 0.935, and the Spearman rank-order correlation coefficient (r_S) = 0.952 with a two-tailed p-value of 0.000023. An r_S value above 0 implies positive agreement between the two rankings, suggesting that the KBS successional community can serve as a proxy of other perennial herbaceous systems including switchgrass. In general, we observe that modeled switchgrass yields at the state level in the Dakotas and Nebraska compare favorably with reported on-farm yields observed on marginal lands[2].



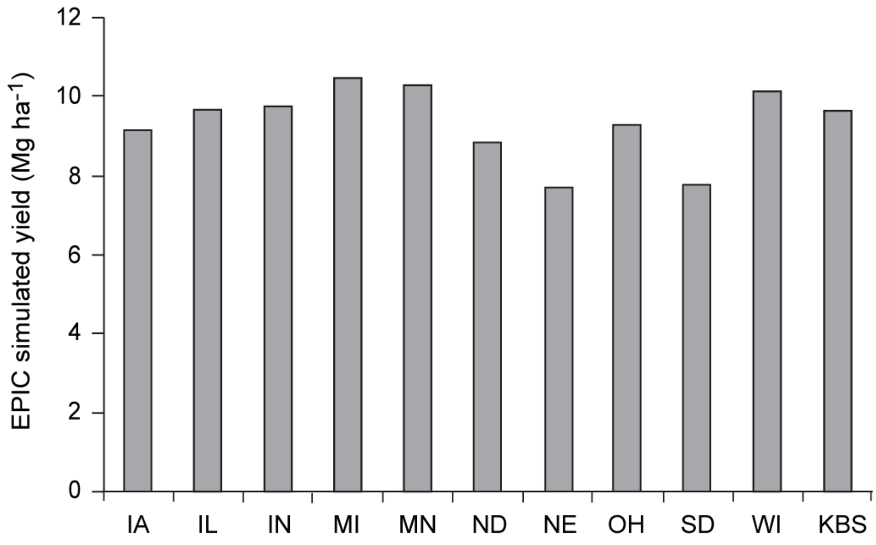
Supplementary Figure 2. The placement of biorefineries for cellulosic biomass production from marginal lands in ten US Midwest states with identification numbers corresponding to entries in Supplementary Table 3. Each circle represents an 80 km radius area with sufficient biomass resources to produce at least 89 ML ethanol yr^{-1} based on quantitative simulation of yields from non-forested marginal lands at a 60×60 m resolution.



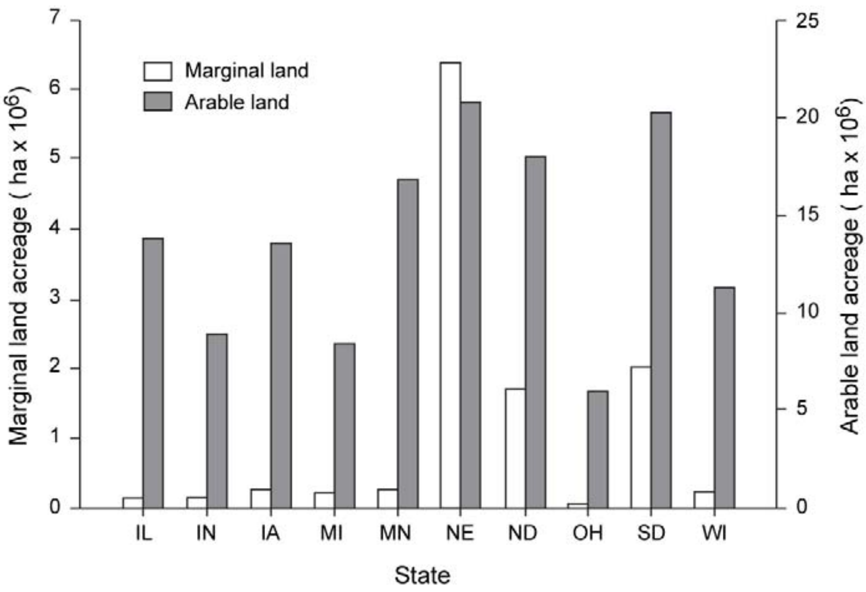
Supplementary Figure 3. Estimates of regional ethanol production as affected by the size of the biomass collection area (collection radius). Open circles denote production with no constraint on minimum biorefinery size; closed circles constrain collection areas to those with enough biomass to support a biorefinery producing at least 89 ML ethanol yr^{-1}. Note discontinuous y-axis.



Supplementary Figure 4. Sensitivity of EPIC modeled results at KBS to three key model parameters: leaf area index (LAI), maximal stomatal conductance, and biomass-energy ratio. These model parameters were varied by ±5% and ±10%. Results are from a sensitivity test of EPIC simulations to crop parameters. The EPIC model has been shown to be sensitive to a variety of crop and soil parameters[3,4]. Based on these studies, we selected three crop parameters (biomass-energy ratio, LAI, and stomatal conductance) to perform sensitivity tests of EPIC under KBS conditions by varying these parameters from -10% to +10% in 5% increments. EPIC yields showed the greatest sensitivity to changes in LAI and similar levels of sensitivity to changes in biomass-energy ratio and stomatal conductance.



Supplementary Figure 5. Sensitivity of EPIC modeled results at KBS to climatic variations and soil drivers. The North America Regional Reanalysis (NARR) climate record closest to the centroid of each state was used to run the EPIC model for KBS. EPIC simulations were performed with KBS management and soil properties under 10 representative climates, one from each state. EPIC yields were sensitive to climatic drivers as suggested by a 2.8 Mg ha^{-1} yield range. To examine model sensitivity to soil properties, we ran EPIC with KBS weather and management and all the soils present in the surrounding KBS area. Average yield was 10.4±0.9 Mg ha^{-1} (n=10). Variation in total soil profile organic carbon was the most important factor contributing to yield; it explained 71% of the total variation simulated (y = 275.0x - 2644).



Supplementary Figure 6. Marginal lands acreage ($\times10^6$ ha) in 10 states of the US Midwest, as modeled by EPIC (left Y axis, note the difference in scale between left and right Y axis; open bars) and arable land acreage (right Y axis; shaded bars) from Cropland Data Layer of 2008. States names given by standard abbreviation; IL – Illinois, IN – Indiana, IA – Iowa, MI – Michigan, MN – Minnesota, NE – Nebraska, ND – North Dakota, OH – Ohio, SD – South Dakota, WI – Wisconsin.

Supplementary Tables

Supplementary Table 1. Average yields of studied ecosystems (mean ± s.e., n = 6); C=corn, S= soybean, W=wheat. †

System	Corn yield	Wheat yield	Soybean yield	Cellulosic biomass*
	Mg ha^{-1} yr^{-1} dry mass			
Conventional tillage C-S-W	4.9 (0.4)	3.1 (0.1)	2.0 (0.1)	4.8 (0.1)
No-till C-S-W	5.4 (0.1)	3.3 (0.1)	2.3 (0.0)	4.8 (0.1)
No-till C-C	5.9 (0.6)			1.0 (0.6)
Alfalfa ‡	-	0.2 (0.0)	-	6.4 (0.2)
Poplar	-	-		3.8 (0.4)
Successional ¶	-	-	-	3.3 (0.2) – 5.4 (0.4)
Successional + N ¶	-	-	-	4.8 (0.4) – 7.9 (0.6)

† Grain yield dry mass is calculated from yields reported at standard moisture (soybean and wheat at 13% moisture, corn at 15.5% moisture). Stover and straw biomass calculations for annual crops are based on standard harvest indices (HI = grain / [grain + stover]); HI for Conventional tillage corn and wheat are 0.51 and 0.39, respectively, and for No-till 0.52 and 0.41, respectively. For C offset calculations, the relative contribution of rotational crop yields were used: over 20 years of KBS LTER management corn has been planted 40% of the time, soybean 35%, and wheat 25%. For potential bioenergy production we used all produced grain (corn, soybean, wheat) and straw (wheat). We did not use corn stover production in order to maintain soil organic matter, which in SW Michigan requires stover inputs of 5.2 Mg ha^{-1} yr^{-1} for continuous corn and 7.8 Mg ha^{-1} yr^{-1} for corn–soybean rotations[5,6]; these management practices have maintained soil carbon concentrations over last 20 years (see Supplementary Table 10, and [7]). For the No-till continuous corn rotation scenario we used average corn yields of 7.7±0.8 Mg ha^{-1} yr^{-1} from Kalamazoo County, MI (2007 – 2009, average), less a 10% yield reduction penalty typical for continuous vs. rotational corn[8].

* Cellulosic biomass includes wheat straw.

‡ Includes wheat grain and straw production during the grain break year prior to periodic re-establishment of the alfalfa stand due to weed encroachment and self-toxicity. The average yield for grain break years (3.2 ± 0.1 Mg dry mass ha^{-1} yr^{-1}) was calculated as the average wheat yield of conventional tillage and No-till systems, with one grain break year during the studied period. For alfalfa yields estimation we used machine harvest yields from the KBS LTER site for years 1995, 2002 – 2004, and 2006.

¶ For estimation of harvestable cellulosic biomass we used average ANPP from Successional treatments of the KBS LTER site between years 2000 and 2009, after initial stabilization of biomass produced by these plots between 1989 and 2000 (dataset: http://lter.kbs.msu.edu/datatables/40; Fig. 1). From the dataset used for estimation of Successional ANPP we removed a small "standing dead" biomass pool due to our inability to attribute "standing dead" to biomass produced during a given season. The ANPP for this period averaged 598±44 g dry matter m^{-2} yr^{-1}. For the Successional + N treatment we estimate an ANPP of 879±64 g dry matter m^{-2} yr^{-1} based on the yield ratio between the fertilized and unfertilized sub-plots (average ANPP for 1989-2009, n = 6; Fig 1 inset). Successional harvestable biomass reflects a 55% contemporary and 90% potential harvest efficiency[9,10,11].

Supplementary Table 2. Average biomass and ethanol yields for 78,184 parcels of marginal land as modeled by EPIC for three levels of N fertilizer application and two harvest efficiencies. Values in parentheses are standard deviations. Ethanol yields are based on a conversion factor of 380 L Mg^{-1} of cellulosic biomass (Supplementary Eq. 1).

Factor	Average Yields	
	Biomass	Ethanol
	Mg ha^{-1} yr^{-1}	$L \times 10^3$ ha^{-1} yr^{-1}
Harvest efficiency (*%*)		
55	4.3 (1.7)	1.6 (0.6)
90	6.0 (2.6)	2.3 (1.0)
N Fertilization (*kg* ha^{-1} yr^{-1}) †		
0	6.0 (2.6)	2.3 (1.0)
68	8.2 (2.7)	3.1 (1.0)
123	8.9 (2.8)	3.3 (1.0)

† Simulations under different N fertilization regimes with assumed 90% harvest efficiency.

Supplementary Table 3. EPIC modeled biomass and cellulosic ethanol production by potential refineries within a given state assuming 90% harvest efficiency and two N-fertilization levels (0 and 68 kg N ha^{-1}). Refineries are numbered in states with more than one refinery.

ID[§]	*State*	Total biomass production per biorefinery area *Mg × 10^6*		Total cellulosic ethanol production *GL yr^{-1}*		Total fossil fuel offset *Mg $CO_2e \times 10^6$*		Grazed land[††] *%*	Total biomass production without grazed land *Mg × 10^6*		Total fossil fuel offset without grazed land *Mg $CO_2e \times 10^6$*	
		F*=0	F=68	F=0	F=68	F=0	F=68		F=0	F=68	F*=0	F=68
1	Illinois 1[‡]	1.35	1.88	0.18	0.26	0.38	0.46	62.3	0.51	0.71	0.16	0.20
2	Illinois 2	0.67	0.80	0.09	0.11	0.20	0.23	46.3	0.36	0.43	0.11	0.12
3	Indiana 1[‡]	1.18	1.43	0.16	0.19	0.29	0.33	52.7	0.56	0.68	0.17	0.19
4	Indiana 2[‡]	0.77	0.96	0.11	0.13	0.25	0.27	31.1	0.53	0.66	0.16	0.19
5	Iowa 1	1.67	2.27	0.23	0.31	0.54	0.64	70.6	0.49	0.67	0.15	0.19
6	Iowa 2[‡]	0.87	1.17	0.12	0.16	0.27	0.33	46.4	0.47	0.63	0.14	0.18
7	Michigan 1	1.78	2.29	0.24	0.31	0.52	0.58	6.8	1.66	2.13	0.51	0.61
8	Michigan 2	1.63	1.97	0.22	0.27	0.27	0.33	29.4	1.15	1.39	0.36	0.39
9	Minnesota 1	2.38	2.55	0.32	0.35	0.52	0.64	63.5	0.87	0.93	0.27	0.26
10	Minnesota 2	0.86	1.10	0.12	0.15	0.52	0.66	68.9	0.27	0.34	0.08	0.10
11	Minnesota 3	0.90	1.11	0.12	0.15	0.27	0.31	68.8	0.28	0.35	0.09	0.10
12	Nebraska 1	13.72	19.13	1.88	2.62	4.78	5.91	<0.1	13.72	19.13	4.25	5.43
13	Nebraska 2[‡]	10.44	14.66	1.43	2.01	3.26	4.19	0.2	10.42	14.63	3.23	4.15
14	Nebraska 3[‡]	9.75	13.83	1.33	1.89	3.01	3.92	<0.1	9.75	13.83	3.02	3.92
15	Nebraska 4	8.89	11.54	1.22	1.58	2.24	3.11	2.5	8.67	11.25	2.68	3.19
16	Nebraska 5	6.43	9.01	0.88	1.23	1.7	2.14	<0.1	6.43	9.01	1.99	2.56
17	Nebraska 6[‡]	4.05	5.33	0.55	0.73	1.36	1.6	<0.1	4.05	5.33	1.25	1.51
18	Nebraska 7	2.55	3.40	0.35	0.46	0.61	0.73	0	2.55	3.40	0.79	0.96
19	Nebraska 8[‡]	1.68	2.30	0.23	0.31	0.41	0.54	0.6	1.67	2.29	0.52	0.65
20	Nebraska 9	0.61	0.80	0.08	0.11	0.18	0.23	17.1	0.51	0.66	0.16	0.19
21	N. Dakota 1	5.48	7.50	0.75	1.03	1.34	1.74	5.8	5.16	7.07	1.60	2.00
22	N. Dakota 2	4.01	5.19	0.55	0.71	1.18	1.45	23.9	3.05	3.95	0.95	1.12
23	N. Dakota 3	3.75	5.12	0.51	0.7	1.25	1.47	0.4	3.74	5.10	1.16	1.45
24	N. Dakota 4	3.59	4.62	0.49	0.63	1.11	1.31	4.5	3.43	4.41	1.06	1.25
25	N. Dakota 5[‡]	1.52	1.89	0.21	0.26	0.36	0.41	45.9	0.82	1.02	0.25	0.29
26	N. Dakota 6	1.28	1.8	0.17	0.25	0.29	0.35	1.4	1.26	1.77	0.39	0.50
27	N. Dakota 7[‡]	0.74	0.95	0.1	0.13	0.23	0.27	12.0	0.65	0.84	0.20	0.24
28	S. Dakota 1	7.22	10.97	0.99	1.5	2.76	3.28	0.4	7.19	10.93	2.23	3.10

29	S. Dakota 2‡	4.25	6.07	0.58	0.83	1.99	2.57	<0.1	4.25	6.07	1.32	1.72
30	S. Dakota 3	1.97	2.77	0.27	0.38	0.79	0.95	30.0	1.38	1.94	0.43	0.55
31	S. Dakota 4‡	1.86	2.42	0.26	0.33	0.61	0.79	37.1	1.17	1.52	0.36	0.43
32	S. Dakota 5‡	0.93	1.22	0.13	0.17	0.38	0.52	16.9	0.77	1.01	0.24	0.29
33	Wisconsin 1	1.64	2.03	0.22	0.28	0.75	0.73	41.9	0.95	1.18	0.30	0.33
34	Wisconsin 2‡	1.20	1.58	0.16	0.22	0.48	0.54	49.8	0.60	0.79	0.19	0.23
35	Wisconsin 3‡	0.53	0.65	0.07	0.09	0.18	0.23	39.8	0.32	0.39	0.10	0.11
	Total	*112.2*	*152.3‡‡*	*15.3*	*20.8*	*35.3*	*43.8*		*99.7*	*136.4*	*30.9*	*38.7*

* N fertilizer application in kg N ha^{-1}
‡ Biomass collection area crosses state boundaries.
§ Biorefinery placements associated with biorefinery ID are presented in Figure S2.
†† Maximum currently grazed lands are estimated from 2008 CDL data.
‡‡ Total biomass production 261.7 Mg×10^6

Supplementary Table 4. EPIC modeled biomass and cellulosic ethanol production and calculated biofuel offset credits for three different collection radii without inclusion of grazing lands, assuming 90% harvest efficiency and fertilization level of 68 kg N ha^{-1}.

Collection Radius	Biomass production	Fossil fuel offset
km	*Mg×10⁶*	*Mg CO₂e×10⁶*
40	108.0	30.8
80	136.4	38.7
120	120.9	34.3

Supplementary Table 5. Comparison of state-wide biomass production estimated by EPIC's simulation of successional biomass on unfertilized marginal lands vs. the Billion Ton Study's[1] extrapolation of upland switchgrass to marginal and arable lands. The R^2 value is 0.0079 and the Spearman rank-order correlation coefficient (r_s) is -0.0061 with a two-tiled p-value of 0.98. An r_s value below 0 implies negative agreement between the two rankings.

	Average Biomass Production	
State	EPIC model	Billion Ton Study
	Mg ha^{-1}	
Illinois	8.16	12.50
Indiana	8.35	13.07
Iowa	7.81	11.73
Michigan	9.98	7.44
Minnesota	10.63	6.04
Nebraska	6.01	8.87
North Dakota	5.55	4.59
Ohio	7.16	14.03
South Dakota	4.75	7.59
Wisconsin	8.96	9.23
Area-weighted average	6.00	8.81

Supplementary Table 6. Estimates of CO_2-equivalent emissions from fuel used for field operations[†]; all fuel is assumed to be diesel with a carbon content of 85%.

Field Operation	Fuel Consumption	CO_2e Emission	Source
	L ha^{-1}	*g CO_2 m^{-2} yr^{-1}*	
Plowing [‡]			
Moldboard	21.8	5.6	*12*
Chisel	10.1	2.6	*13*
Soil finishing	7.4	1.7	*13*
Fertilizer application	9.8	2.6	*12*
Herbicide application	1.8	0.5	*13*
Cultivation	5.1	1.3	*13*
Rotary hoe	2.6	0.7	*13*
Planting	4.9	1.3	*12*
Harvest			
Baling (round)	7.4	1.9	*13*
Mowing [¶]	1.3	0.4	*14*
Forage raking	2.2	0.6	*13*
Alfalfa baling [¶]	1.2	0.3	*14*
Hay cut [*]	4.1	1.1	*15*
Haylage [*]	13.1	3.4	*15*
Soybean	11.1	2.9	*12*
Wheat [§]	11.1	2.9	*13*
Corn	11.5	3.0	*13*
Forage	17.4	4.5	*13*
Poplar	21.3	5.5	*16*

[†] All reported values were converted to L ha^{-1} if reported otherwise. The diesel energy content was assumed to be 36.4 MJ L^{-1} [17].

[‡] Moldboard plowing was conducted during 1989-1997, and chisel plowing during 1997-2009.

[¶] Fuel usage depends on crop yield; value given per yield of Mg ha^{-1}.

[*] Equipment used in calculation: for chopped forage (hay silage) a pull type pickup head 12 ft; for hay a rotary mower-conditioner 12 ft.

[§] Wheat and soybean harvest operations were assumed to consume equivalent amounts of energy.

Supplementary Table 7. Estimates of CO_2-equivalent (CO_2e) emissions associated with farming inputs other than fuel (see Supplementary Table 6).

Input	CO_2e emissions	Active ingredient	Source
	kg CO_2e kg^{-1}	*g L^{-1}*	
Fertilizer			
N	4.5		*18*
P	0.7		*13*
K	0.6		*12*; *13*
Lime	0.4		*12*
Herbicides †			
Accent	3.5	750	
Assure II	0.5	105	
Atrazine	2.3	479	
Basagran	2.3	479	
Bladex	4.2	900	
Broadstrike + Dual	4.3	925	
Buctril Gel	2.3	479	
Callisto	2.3	479	
Canopy	3.5	750	
Dimate 4E	2.3	479	
Dual II Magnum	3.9	824	
Dual Magnum	3.9	837	
Galaxy	2.3	490	
Goal	4.5	954	
Harmony Extra	0.0	10	
Lexar	1.9	404	
Lorox	2.4	500	
Marksman	1.8	393	
Princep	2.0	420	
Poast Plus	0.6	130	
Roundup	2.5	490	
Stinger	1.9	409	
Sevin 80	3.8	800	
Sencor	3.5	750	
First Rate	3.9	840	
Seeds			
Alfalfa	9.6		*12*
Wheat	0.4		*12*
Soybean	0.9		*12*
Corn	3.9		*12*
Red clover‡	6.3		*12*
Rye grass‡	2.0		*12*

† We assume emission of 4.7 kg CO_2 kg^{-1} herbicide active ingredient (*13*). Active ingredients concentrations were obtained as g L^{-1} or percent from the manufacturer's labels:

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Dual II Magnum – Syngenta (2010) Dual II Magnum herbicide material safety data sheet, Syngenta Crop Protection Inc. P.O. Box 18300, Greensboro, NC 27419 USA. Available at www.syngentacropprotection.com/pdf/labels/SCP818AL1N0809n.pdf. Accessed February 23, 2012.

Dual Magnum – Syngenta (2010) Dual Magnum herbicide material safety data sheet, Syngenta Crop Protection Inc. P.O. Box 18300, Greensboro, NC 27419 USA. Available at www.syngentacropprotection.com/pdf/labels/SCP816AL1U1210.pdf. Accessed February 23, 2012.

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‡ Cover crops

Supplementary Table 8. Estimates of total CO_2e emissions associated with farming of individual crops in areal (g CO_2e m^{-2} yr^{-1}) and energy intensity (g CO_2e MJ^{-1}) units. Emissions per areal unit are based on Supplementary Tables 6 and 7. Emissions per unit of energy for annual crops are calculated from GREET Version 1.8d.1, except for soybean. Soybean and perennial systems energy intensities are calculated from measured values at KBS. Average rotational values of CO_2e emissions (g CO_2e m^{-2} yr^{-1}) for the corn-soybean-wheat rotation appear in Table 1 of the main text.

Tillage	Corn	Soybean	Wheat	Poplar	Alfalfa	Suc*	Suc+N*
			g CO_2e m^{-2} yr^{-1}				
Conventional	73.0	10.2	41.5	-	-	-	-
No-till	72.9	11.1	40.3	7.1	39.9	4.4	63.1
			g CO_2e MJ^{-1}				
Conventional	37.7	7.1	37.8	-	-	-	-
No-till	34.7	6.8	35.6	2.3	8.0	1.0	9.9

* CO_2e emissions include harvest, feedstock transportation, and (for Successional + N) N fertilizer application.

Supplementary Table 9. Greenhouse gas (GHG) fluxes in the studied ecosystems (1989 – 2010, except as noted)*. Results shown are mean (± standard error), n = 4 replicate blocks. Statistically significant differences (ANOVA repeated measurements, $p < 0.05$) within columns are indicated by different letters.

System	N_2O-N	CH_4-C
	g ha^{-1}d^{-1}	
Conventional tillage C-S-W †	2.0 (0.3) [a]	-0.7 (0.1) [a]
No-till C-S-W	2.0 (0.2) [a]	-0.7 (0.1) [a]
Alfalfa	1.9 (0.2) [a]	-0.8 (0.0) [b]
Poplar	1.0 (0.2) [b]	-0.6 (0.0) [a,b]
Successional	0.6 (0.0) [c]	-0.9 (0.1) [b]
Successional + N ‡	1.6 (0.3) [a]	-1.0 (0.4) [a,b]

* Average fluxes are calculated from fluxes measured when soils are unfrozen (March to November/December). We assume negligible fluxes during January – February when soils are mostly frozen: (1) fluxes measured in March immediately after soil thaw are the same or significantly lower than average March-December fluxes except for the Successional site; March fluxes were: Conventional tillage 1.0±0.2 (n=8 dates); No-till 1.3±0.2 (n=8); Alfalfa 2.0±0.8 (n=7); Poplar 0.7±0.2 (n=13); and Successional 1.3±0.1 (n=8) g N_2O-N ha^{-1} d^{-1}. Likewise, average pre-frost fluxes in November/December were similar (2 sites) or lower (5 sites) than the March-December average: Conventional tillage 0.7±0.1; No-till 0.8±0.1; Alfalfa 1.1±0.2; Poplar 0.5±0.2; and Successional 0.5±0.1 g N_2O-N ha^{-1} d^{-1} (n=16 dates for all sites). (2) Average soil concentrations of NO_3^--N to 25 cm during March and December were low relative to peak concentrations during the growing season (July) in all systems but the Successional: Conventional tillage N concentrations were 1.2±0.1, 1.8±0.1, and 9.9±0.7 μg NO_3^--N g^{-1} soil for December, March, and July, respectively; corresponding values for No-Till were 0.9±0.1, 1.4±0.1, and 8.0±0.7; for Poplar 0.3±0.1, 0.5±0.1, and 2.1±0.3; for Alfalfa 3.2±0.2, 2.3±0.1, and 5.6±0.2; for Successional 0.4±0.1, 0.6±0.1, and 0.5±0.1.

† Corn-Soybean-Wheat rotation

‡ GHG fluxes from fertilized Successional system plots were measured in fertilized micro-plots within the Successional plots between the years 2008 – 2010.

Supplementary Table 10. Annual soil carbon change in A/Ap horizon and GHG impact (Supplementary Equation 2) over the period 1989 – 2001. There were no significant soil carbon changes in deeper horizons to 1m. Results are shown as mean difference from the conventional system, ±s.e., n = 6. From (*7*).

System	Soil carbon [†]	GHG impact
	kg C m^{-2}	*g* $CO_2e\ m^{-2}\ yr^{-1}$
Conventional tillage C-S-W	0.0 (0.1)[a,‡]	0.0 (30.6)
No-till C-S-W	0.4 (0.1)[b]	-122.2 (30.6)
Alfalfa	0.4 (0.3)[a,b]	-122.2 (91.7)
Poplar	-0.2 (0.5)[a,b]	61.1 (152.8)
Successional[¶]	1.3 (0.1)[c]	-397.2 (30.6)

[†] Positive values mean soil carbon gain and negative values carbon loss.
[‡] Statistically significant differences in SOC concentration (ANOVA repeated measurements, $p < 0.05$) are indicated by different letters within column.
[¶] Successional and Successional + N ecosystems assumed to be equal.

Supplementary Table 11. Fossil fuels offset credits.

System	Corn grain	Wheat grain	Soybean grain	Wheat straw	Alfalfa	Poplar	Suc	Suc + N
				g $CO_2e\ MJ^{-1}$				
Conventional C-S-W	25.9	21.4	225.6	108.3	-	-		-
No-till C-S-W	28.9	23.2	225.9	108.3	-	-		-
Cellulosic feedstock	-	-	-	-	103.3	105.0	107.3	98.4

Supplementary Table 12. Distribution of different slopes (%) across Land Capability Classes (LCC) IV – VII in the US Midwest as a percentage of the total acreage in each LCC. Because sloped marginal lands (LCC V-VII) are of a similar extent (20.1%) to cropped arable lands in LCC IV (20.9%), slope per se should pose little impediment to potential use for perennial cellulosic crops.

Slope	Land Capability Class			
	IV	V	VI	VII
%	% of LCC Area			
0 – 10	79.2	99.9	81.8	71.6
11 - 15	14.0	0.1	10.4	16.1
16 - 19	6.9	0.0	7.8	12.3

Supplementary Equations

Supplementary Eq 1: Ethanol production from marginal lands in regional simulations by EPIC

We used the following equation to convert biomass yields into liters of ethanol:

$$\text{Ethanol production} = \text{Biomass Yield} \times 0.06\ \text{km} \times 0.06\ \text{km} \times 380.0\ \text{L Mg}^{-1} \times 100 \quad \text{(Eq 1)}$$

$$= \text{Biomass Yield} \times 136.8$$

where Biomass Yield (Mg ha^{-1}) is biomass production, 0.06 × 0.06 km is the cell size of the model, 380.0 L Mg^{-1} is the conversion factor for converting cellulosic biomass to ethanol[2], and 100 is number of hectares in 1 km^2.

Supplementary Eq 2: Soil Carbon CO_2e calculation

CO_2e for soil C change was calculated from carbon in soil cores collected in 2001 (Supplementary Table 10 and [7]):

$$CO_2e(SOC)\ g\ CO_2 \times m^{-2}\ yr^{-1} = \frac{(x_1 - x_2)\ kg\ C}{m^2 \times x_3\ yr} \times \frac{44\ kg\ CO_2}{12\ kg\ C} \times \frac{10^3\ g\ CO_2}{1\ kg\ CO_2} \quad \text{(Eq 2)}$$

where x_1 is soil C in the target system (in kg C m^{-2}), x_2 is soil C in the original reference system (Conventional tillage), and x_3 is the period of C accumulation (yr since transition; or 12 yr).

Supplemental Eq 3 and 4: N_2O and CH_4 CO_2-equivalents calculation

The CO_2-equivalents (g CO_2e m^{-2} yr^{-1}) for N_2O and CH_4 emissions were calculated using the IPCC 100-year horizon factors (298 for N_2O and 25 for CH_4)[19]:

$$CO_2e(N_2O) = \frac{x_1\ g\ N_2O - N}{ha \times d} \times \frac{44\ g\ N_2O}{28\ g\ N_2O - N} \times \frac{365\ d}{1\ yr} \times \frac{1\ ha}{10^4\ m^2} \times \frac{298\ g\ CO_2}{1\ g\ N_2O} \quad \text{(Eq 3)}$$

$$CO_2e(CH_4) = \frac{x_2\ g\ CH_4 - C}{ha \times d} \times \frac{16\ g\ CH_4}{12\ g\ CH_4 - C} \times \frac{365\ d}{1\ yr} \times \frac{1\ ha}{10^4\ m^2} \times \frac{25\ g\ CO_2}{1\ g\ CH_4} \quad \text{(Eq 4)}$$

where x_1 is the average daily N_2O-N emission rate (g N ha^{-1} d^{-1}) and x_2 is the average daily CH_4-C emission rate (g C ha^{-1} d^{-1}). Average fluxes of N_2O and CH_4 for all studied systems are given in Supplementary Table 1. Measurements of soil GHG fluxes were performed bi-weekly using a static-chamber method; for details see[18]. Cumulative emissions of N_2O (g N_2O – N ha^{-1}) and CH_4 (g CH_4 – C ha^{-1} d^{-1}) for each plot were determined by interpolating daily fluxes between sampling days over the course of the entire growing season from first thaw until the onset of frozen soils during 1989 - 2010. Average daily flux (g N_2O – N or CH_4 – C ha^{-1} day^{-1}) for each plot was calculated by dividing the cumulative emissions for that plot by number of days in the year (365), assuming negligible fluxes to occur during winter when soils remain mostly frozen, but see Table S9 for details on fluxes during the soil thawing period. Average daily fluxes in row crop rotations were determined from rotational averages. For this we calculated cumulative emissions for each crop year as above and divided cumulative emissions by number of days in a given crop year.

Supplementary Eq 5: Farming CO_2 emissions equivalents

We assume 100% oxidation of diesel fuel (represented by the formula $C_{16}H_{34}$) to CO_2[18]:

$$CO_2e(\text{diesel}) = \frac{x_1\,\text{L}\,C_{16}H_{34}}{\text{ha}\times\text{yr}} \times \frac{832\,\text{g}\,C_{16}H_{34}}{1\,\text{L}\,C_{16}H_{34}} \times \frac{192\,\text{g}\,C}{226\,\text{g}\,C_{16}H_{34}} \times \frac{44\,\text{g}\,CO_2}{12\,\text{g}\,C} \times \frac{1\,\text{ha}}{10^4\,\text{m}^2} \qquad \text{(Eq 5)}$$

where x_1 is average annual diesel use for the field operation (L ha^{-1} yr^{-1}).

Supplementary Eq 6: Energy Equivalent calculation

$$\text{Energy Equivalent}(\text{MJ ha}^{-1}\,\text{yr}^{-1}) = \text{DM} \times X\frac{\text{kg Fuel}}{\text{kg DM}} \times Y\frac{\text{L Fuel}}{\text{kg Fuel}} \times \text{Biofuel}_{\text{energy}} \qquad \text{(Eq 6)}$$

where DM is dry mass of biomass yield (kg ha^{-1} yr^{-1}; Supplementary Table 2), X is the conversion factor for biofuel production from grain, straw, stover, or cellulosic feedstocks, Y is a factor accounting for fuel specific density, and $\text{Biofuel}_{\text{energy}}$ is biofuel energy content (MJ L^{-1}).

Supplementary Eq 7-8: GHG emission intensity of biofuel energy production

The GHG emission intensity (g CO_2e MJ^{-1}), defined here as the net CO_2e balance per unit of biofuel energy produced in the system:

$$\text{GHG emission intensity} = \frac{\text{Net } CO_2e \text{ balance}}{\text{Biofuel energy content}} \qquad \text{(Eq 7)}$$

where Biofuel energy content is the net biofuel energy yield of the system in MJ m^{-2} yr^{-1} and Net CO_2e balance (g CO_2e m^{-2} yr^{-1}) is:

$$\text{Net } CO_2e \text{ balance} = \sum CO_2e(\text{GHG, FF, Farm, Soil C}) \qquad \text{(Eq 8)}$$

where GHG is field fluxes of N_2O and CH_4, FF is fossil fuel offset credit, Farm is emissions associated with farming practices, and Soil C is changes in soil C concentrations under different tillage practices, all in g CO_2e m^{-2} yr^{-1}.

Supplementary Methods

Site-specific EPIC simulations

We used site-scale simulations based on specific data to calibrate the EPIC model before applying it to the regional-scale simulations. For calibration purposes, we used data from two Long-term Ecological Research (LTER) sites, KBS in Michigan (kbs.lternet.edu) and Cedar Creek (CDR) in Minnesota (cdr.lternet.edu), to model aboveground net primary productivity (NPP) of successional vegetation growing on former agricultural fields.

For EPIC simulations of aboveground net primary productivity (ANPP) of successional fields at KBS we used historical weather, terrain characteristics, and soil properties of the site. The Successional treatment at KBS was initiated in 1989 when agricultural management ceased and natural vegetation was allowed to re-establish. Spring burning began in 1997 to inhibit colonization of woody species. Dominant species include *Solidago canadensis*, *Elytrigia repens*, *Poa pratensis*, *Aster pilosus*, *Phleum pratense*, *Trifolium pratense*, *Apocynum cannabinum*, *Daucus carota*, *Hieracium spp.*, and *Rhus typhina* (http://lter.kbs.msu.edu/).

For EPIC calibration with KBS LTER results, we simulated composition of the successional plant community with three species previously parameterized for EPIC (*Poa pratensis*, *Phleum pratense*, and *Trifolium pratense*) with information on radiation use efficiency, leaf area index, stomatal conductance, and other physiological attributes. Colonization of competing woody species was simulated with a stand of poplar (*Populus* spp.) from 1989 until spring 1998 when it was terminated[20]. Spring burning (3 – 15 April) with 80% efficiency was simulated for the years 1997, 2003, 2004, 2006, and 2008. We simulated ANPP under three different scenarios, one without harvest and N fertilization, and two scenarios with fall harvest, one without N fertilization and one with N fertilization rates of 12.3 g N m^{-2} yr^{-1}. The scenario without fertilization and harvest included woody invasion and spring burning, while scenarios with fall harvest did not. For all scenarios, the EPIC model runs were based on historical records of daily maximum and minimum air temperature and precipitation from the KBS LTER dataset (http://lter.kbs.msu.edu/datatables). Daily solar radiation, relative humidity, wind speed, and missing temperature and precipitation were acquired from Gull Lake NWS weather station (42º 24’ N 85º 23’ W) also at KBS. Soil layer properties used in the simulations were those of the Kalamazoo soil series (fine-loamy, mixed, mesic Typic Hapludalf)[21].

ANPP simulated during EPIC calibration between years 2000 and 2008 averaged 600±110 g m^{-2} yr^{-1} for the scenario without biomass harvest and fertilization, which is similar to the observed average of 598±44 g m^{-2} (Table S2). Similarly, simulated ANPP for the scenario with harvest and fertilization was very close to field-based estimation, 960±80 vs. 879±64 g m^{-2} yr^{-1}.

Further, we validated EPIC model results for ANPP simulations with published field data from CDR. We used simulated weather, terrain characteristics, and soil layer properties to simulate ANPP of a 60-yr chronosequence experiment[22]. The 60-yr chronosequence at CDR was simulated according to the description in[22]. The chronosequence consisted of a series of 14 agricultural fields on Alfic and Typic Udipsamments[21] left unmanaged during periods ranging from one to 60 years. Floristic surveys conducted in 1987 revealed the presence of *Ambrosia artemisiifolia, Andropogon gerardii, Agropyron repens, Agrostris scabra, Polygonum convolvulus, Poa pratensis, and Schizachyrium scoparium*, among others. C_3 species appeared to dominate over C_4 species during the first half of the chronosequence period while an equal mix appeared to prevail during the second. The species composition during secondary succession appears to be consistent with that reported[23]. Due to lack of plant parameters for several species and uncertainty in their temporal occurrence and dominance, we used an equal mix of generic C_3 and C_4 plant parameterizations and simulated daily weather generated from data of the weather station at Rosemount, MN, near CDR. Weather parameters were used to simulate ANPP during a 60-yr period intended to approximate environmental conditions for 1928 – 1987. The only simulated external N addition was 7.7 kg ha^{-1} via wet deposition.

Direct comparisons of biomass productivity results are not possible for the CDR data because the simulations are not time specific. Simulated standing aboveground biomass during the July-August period averaged 513±113 g m^{-2} during the first three years. In comparison, (*22*) observed 509 g m^{-2} in the 1-yr old field and 296 g m^{-2} in the 3-yr old field. Simulated biomass during the last three years of the simulation averaged 767±127 g m^{-2}, while (*22*) observed 783 g m^{-2} in the 60-yr old field. While EPIC failed to capture the decrease in plant productivity observed during the first years of the chronosequence, it did capture the increase in productivity toward the end of the period. Similar to observations, simulated annual biomass productivity correlated moderately well with N mineralization and soil N. However, correlations obtained with observed data (R^2 = 0.78 for potential N mineralization; R^2 = 0.94 for soil N) (*24*) were considerably stronger than those obtained with simulated data (R^2 = 0.34 for net N mineralization; R^2 = 0.32 for soil N).

Overall, EPIC appeared to capture adequately the observed plant productivity patterns from both KBS and CDR LTER sites under different environmental constraints and management scenarios. In addition, (*24*) used EPIC for simulations of the effects of unmanaged grasses on soil carbon accrual on marginal lands in Nebraska, Kansas, and Texas and found good agreement between EPIC predictions and long-term field data, which provides further justification for using the model for large scale simulations.

KBS LTER vs. Regional Yields 1989-2009

Are KBS yields typical for the region? Yields (Mg ha^{-1} at standard moisture of 15.5% for corn and 13% for soybean and wheat) for KBS wheat and soybeans over our 21-year study period were similar to Kalamazoo County yields, which were similar to (soybean) or higher than (wheat) US national average yields (for soybean: 2.6±0.2 for KBS no-till vs. 2.5±0.1 for Kalamazoo County vs. 2.6±0.1 for the entire US; for wheat: 3.7±0.3 for KBS no-till vs. 3.4±0.1 for Kalamazoo County vs. 2.8±0.1 Mg ha^{-1} for the US from 1989-2009)[25].

KBS corn yields were more variable than County or national averages, likely reflecting the greater sensitivity of corn yield to midsummer periods of low rainfall and heat waves[26]. Overall average yields for KBS no-till corn (6.4±0.7 Mg ha^{-1}) were lower than county (7.4±0.2 Mg ha^{-1}) and national (8.4±0.2 Mg ha^{-1}) yields for 1989-2009. KBS corn yields were at or above county and national yields for 4 of the study's 9 corn years and not significantly different from, though lower than county and national yields, in 3 years. In 2 of the 9 corn years KBS yields were significantly lower than county and national averages. However, county and national data include yield from both irrigated and rainfed acreage, and thus would be expected to be higher than rainfed (non-irrigated) KBS yields. About 38% of Kalamazoo County and 15% of total US corn acreage is irrigated[27]. The well-drained loam soils at KBS make corn yields particularly sensitive to interannual variation in precipitation. For example, in 2008 (a drought year at KBS) rainfed yields at KBS were only ~60% of irrigated yields (7.5±0.3 vs. 12.3±0.2 Mg ha^{-1} for rainfed vs. irrigated corn, respectively). In contrast in 2011, a year with high summer precipitation at KBS, rainfed yields at KBS nearly matched irrigated yields (12.3±0.2 Mg ha^{-1} rainfed vs. 13.8±0.1 Mg ha^{-1} irrigated), and were well above the average from Kalamazoo County (10.2 Mg ha^{-1}). These data suggest that KBS corn yields are not atypical of those experienced by Kalamazoo County farmers, and reflect how yields from rainfed corn will vary given the year-to-year variability in local precipitation that is typical for the region.

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