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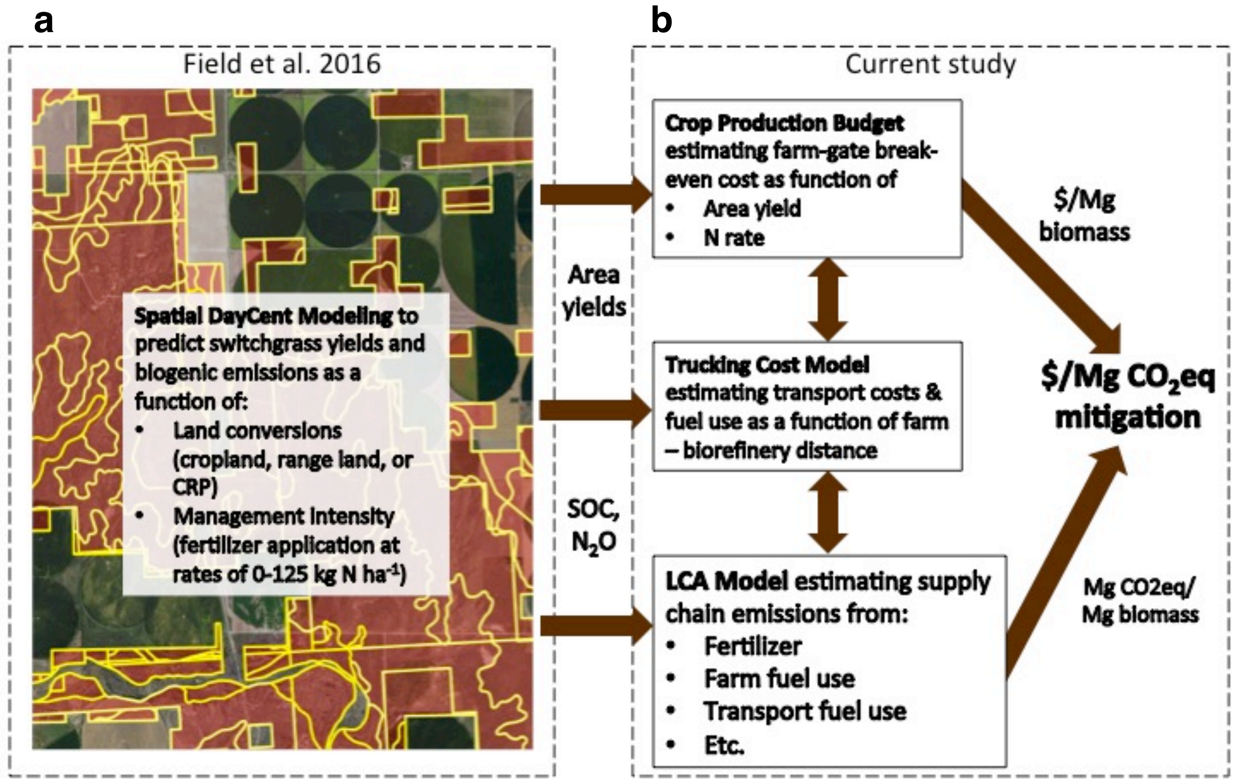
High-resolution techno–ecological modelling of a bioenergy landscape to identify climate mitigation opportunities in cellulosic ethanol production

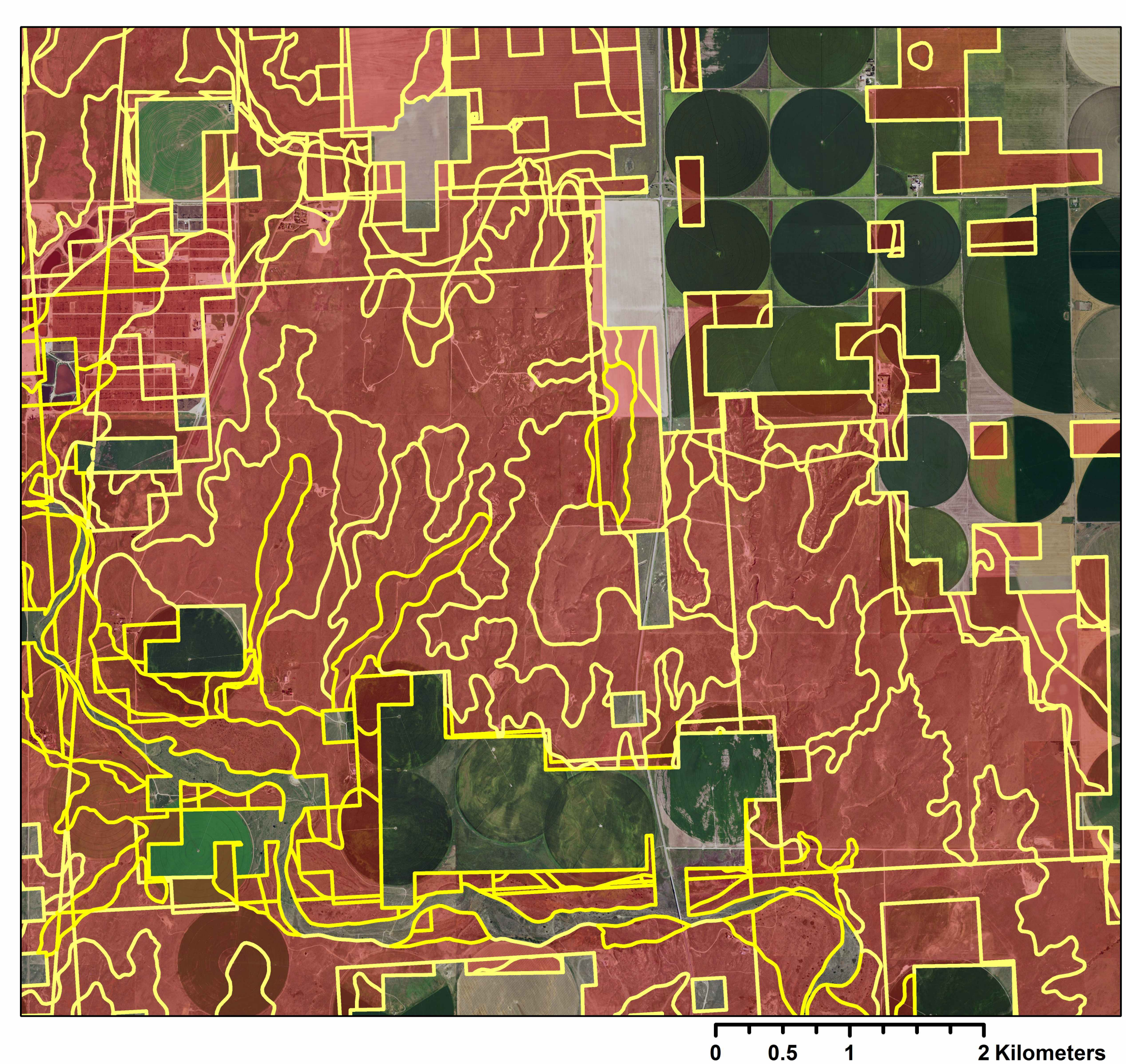
John L. Field[1,2*], Samuel G. Evans[3], Ernie Marx[1], Mark Easter[1], Paul R. Adler[4], Thai Dinh[5], Bryan Willson[2] and Keith Paustian[1,6]

[1]Natural Resource Ecology Laboratory, Colorado State University, Fort Collins, CO, USA. [2]Department of Mechanical Engineering, Colorado State University, Fort Collins, CO, USA. [3]Department of Environmental Science, Policy, and Management, University of California-Berkeley, Berkeley, CA, USA. [4]Pasture Systems and Watershed Management Research Unit, Department of Agriculture-Agricultural Research Service, University Park, PA, USA. [5]School of Industrial and Systems Engineering, University of Oklahoma, Norman, OK, USA. [6]Department of Soil and Crop Sciences, Colorado State University, Fort Collins, CO, USA. *e-mail: John.L.Field@colostate.edu

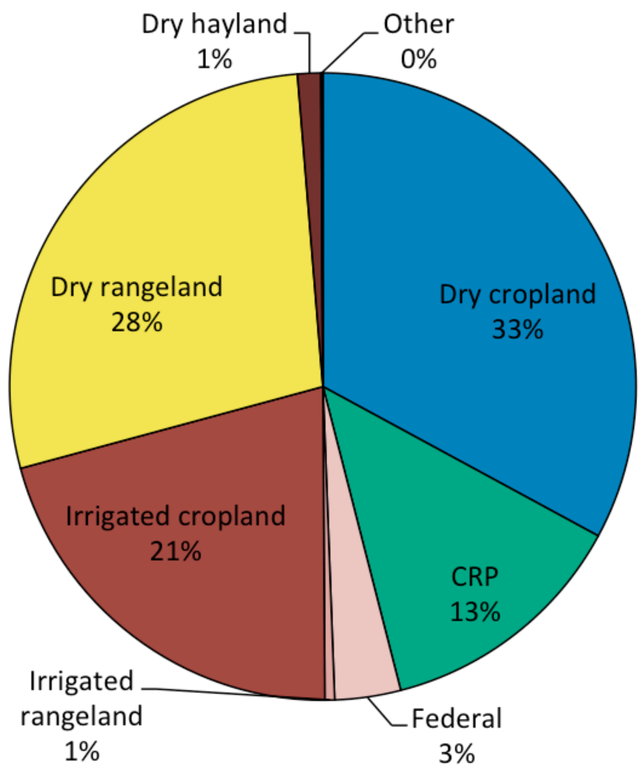
Supplementary Figures



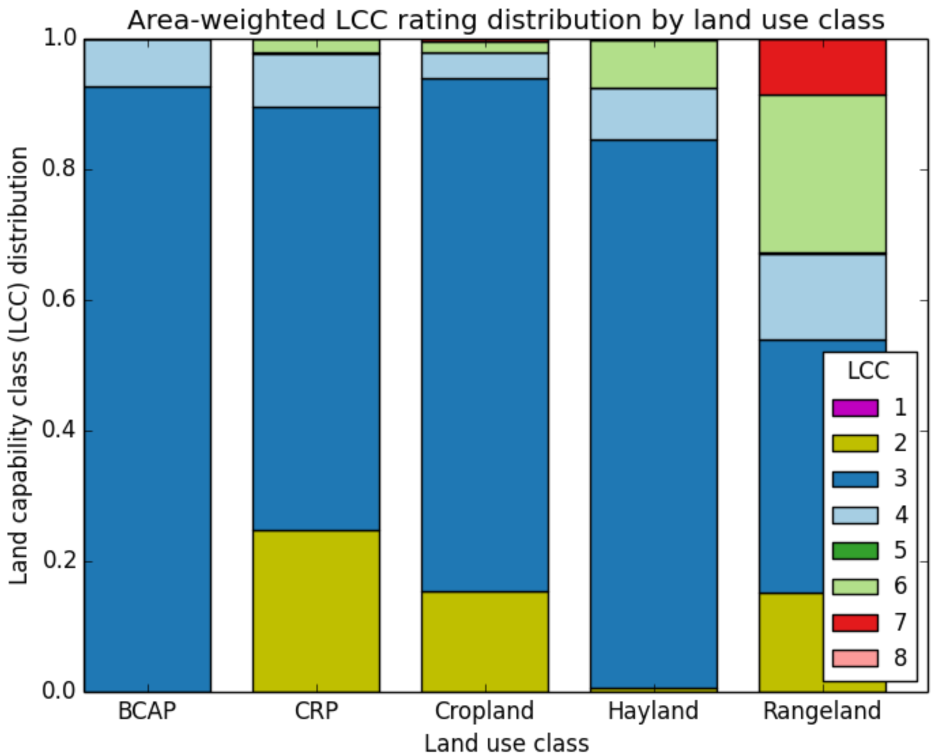
Supplementary Figure 1. Integrated assessment conceptual diagram. **a**, DayCent, a process-based ecosystem model, was previously used[1] to estimate the productivity and biogenic greenhouse gas (GHG) emissions intensity – reflecting net CO_2 flux from changes in soil organic carbon (SOC) and direct and indirect emissions of nitrous oxide (N_2O) – of switchgrass cultivation across our case study area, when managed at different levels of fertilizer application. **b**, In the current analysis these results were integrated with a crop production budget to estimate farmer break-even production costs, a simple biomass transport model to estimate farm – biorefinery transport costs and emissions, and a lifecycle assessment framework to estimate the total lifecycle GHG footprint of the resulting cellulosic biofuel. The resulting fuel production cost and lifecycle GHG footprint estimates were then optimized to assess cost × GHG tradeoffs in bioenergy landscape design. Background aerial imagery is from the National Agricultural Imagery Program (NAIP; a product of the USDA-FSA Aerial Photography Field Office).



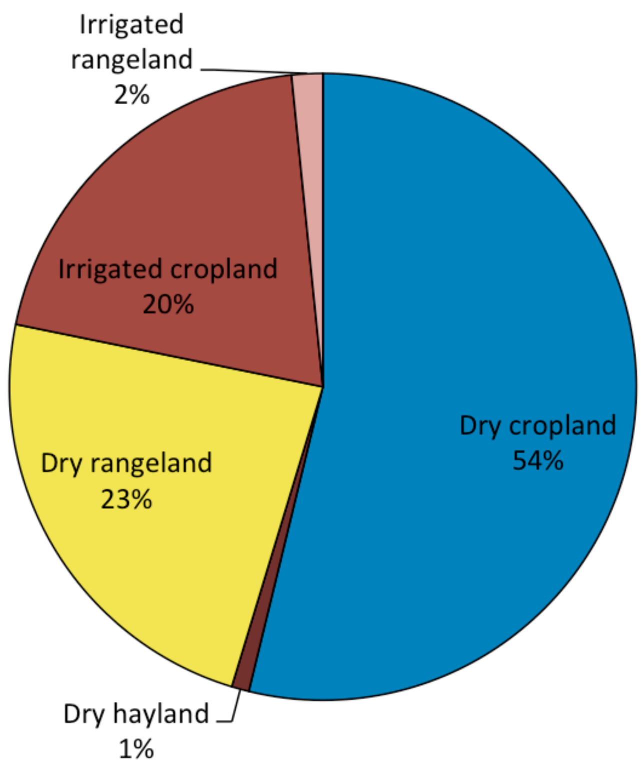
Supplementary Figure 2. GIS analysis polygons overlaid on aerial imagery for a portion of the case study area to qualitatively illustrate the spatial resolution of the assessment. The polygon boundaries (yellow) reflect an intersection of the North American Regional Reanalysis database[2] (NARR), 2011 National Land Cover Database[3] (NLCD), the MODIS Irrigated Agriculture dataset[4] (MIrAD-US, supplemented with center-pivot location data where available), and the Soil Survey Geographic database[5] (SSURGO). Shaded polygons were included in the analysis, and other areas were excluded due to their classification as irrigated, developed, open water, federally-owned, etc. Background aerial imagery is from the National Agricultural Imagery Program (NAIP; a product of the USDA-FSA Aerial Photography Field Office).



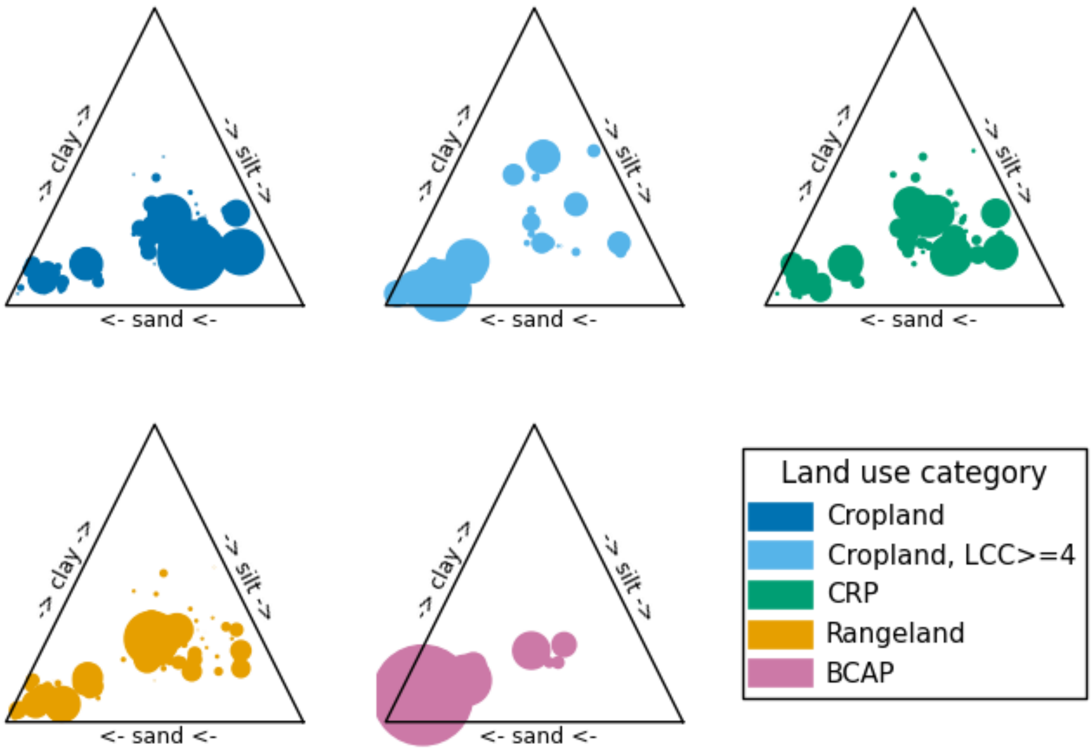
Supplementary Figure 3. Current land use within the 7-county case study area as per intersection of the NLCD and MIrAD-US GIS layers, as well as a proprietary coverage of Conservation Reserve Program (CRP) enrollments. The case study landscape is dominated by non-irrigated cultivated lands (NLCD cropland and hayland), followed by non-irrigated rangeland (NLCD herbaceous grassland and shrubland), irrigated cropland, and CRP enrollment areas. The presence of a small amount of implausible land use combinations (e.g., irrigated rangeland) gives some indication of the quality of the resulting spatial data intersection.



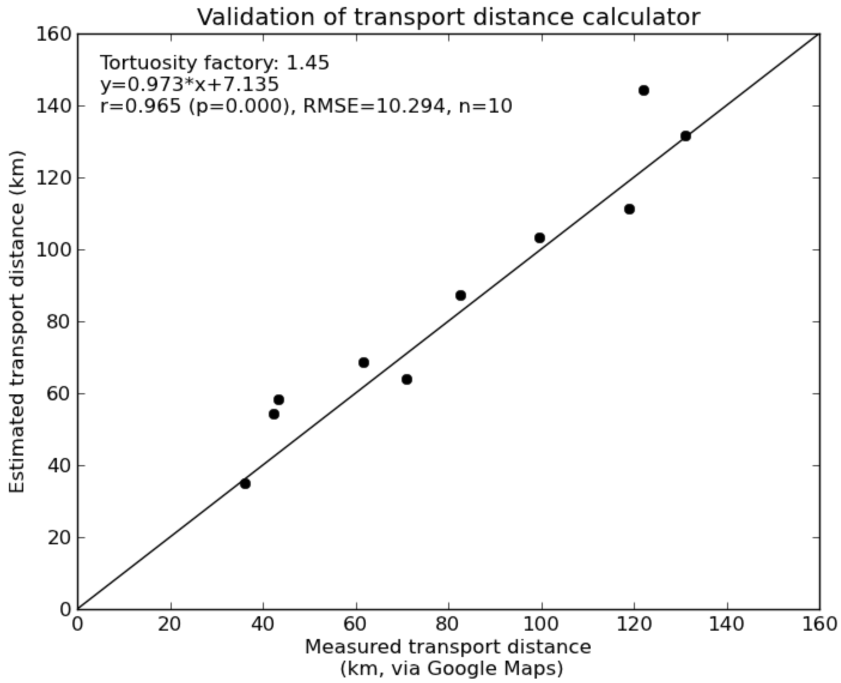
Supplementary Figure 4. Distribution of Natural Resource Conservation Service Land Capability Classification system[6] (LCC) ratings for lands in our case study area grouped by current land use, including both CRP and Biomass Crop Assistance Program (BCAP) enrollment areas. LCC ratings reflect land use limitations due to challenging soils (extreme texture, shallow, rocky, etc.), erosion susceptibility, unfavorable local climate, or tendency towards water-logging. An LCC rating of I indicates prime cropland with no limitations on agricultural use, whereas LCC=VIII indicates extremely marginal land unsuitable for cultivation.



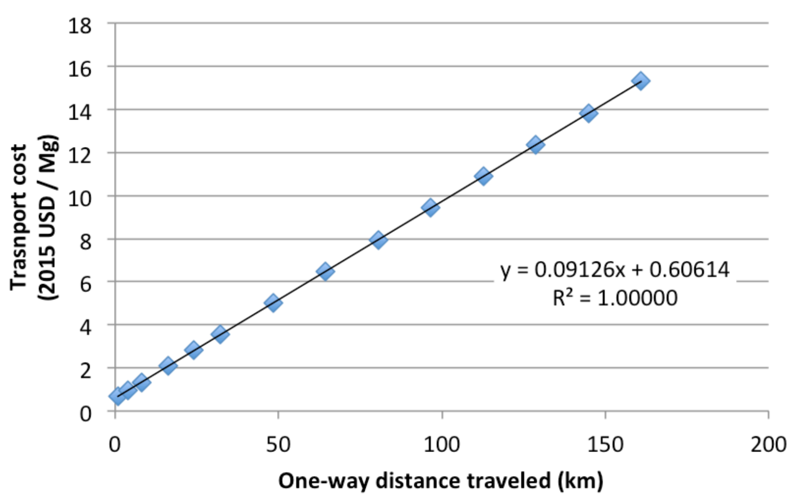
Supplementary Figure 5. Prior land use of BCAP enrollment areas, as per NLCD and MIrAD-US.



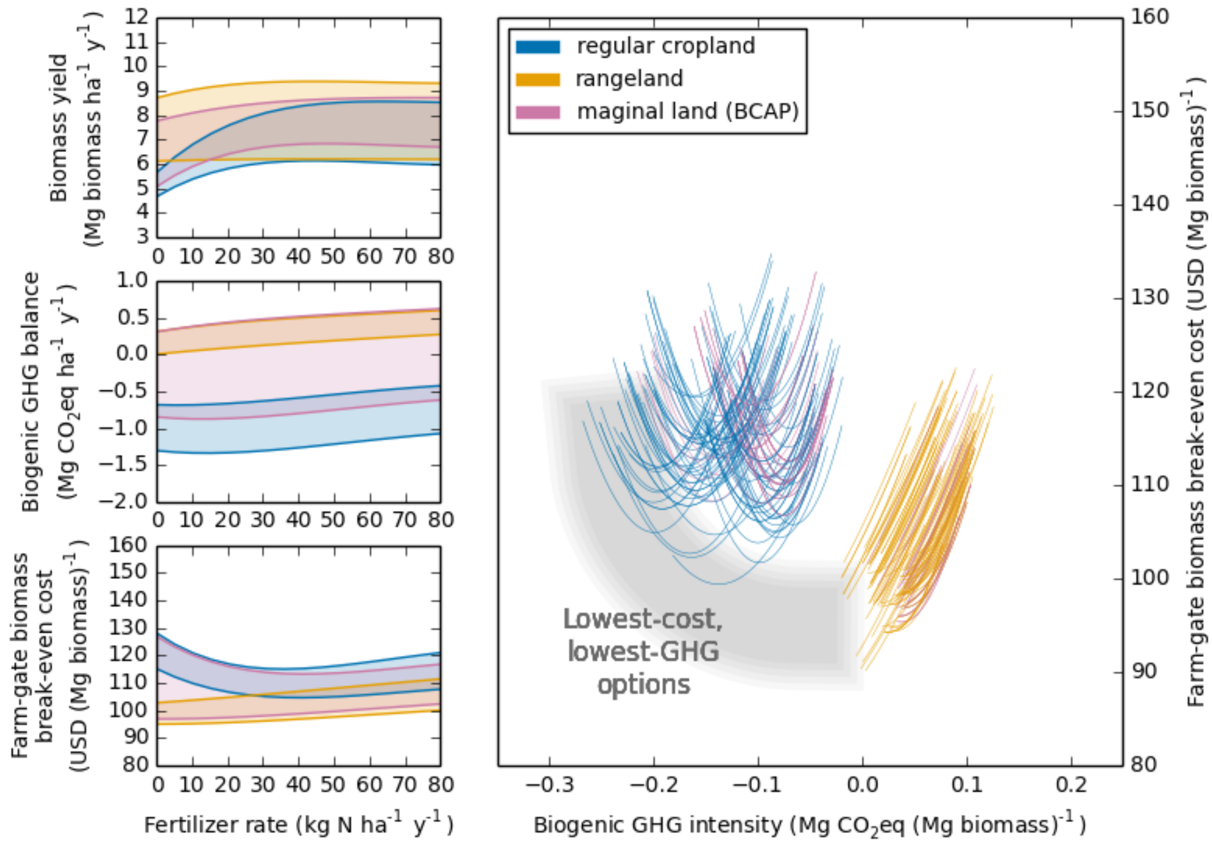
Supplementary Figure 6. Distribution of soil surface textures across our case study area grouped by current land use, including the subset of cropland with LCC rating IV or greater. Point size qualitatively indicates area-weighted prevalence.



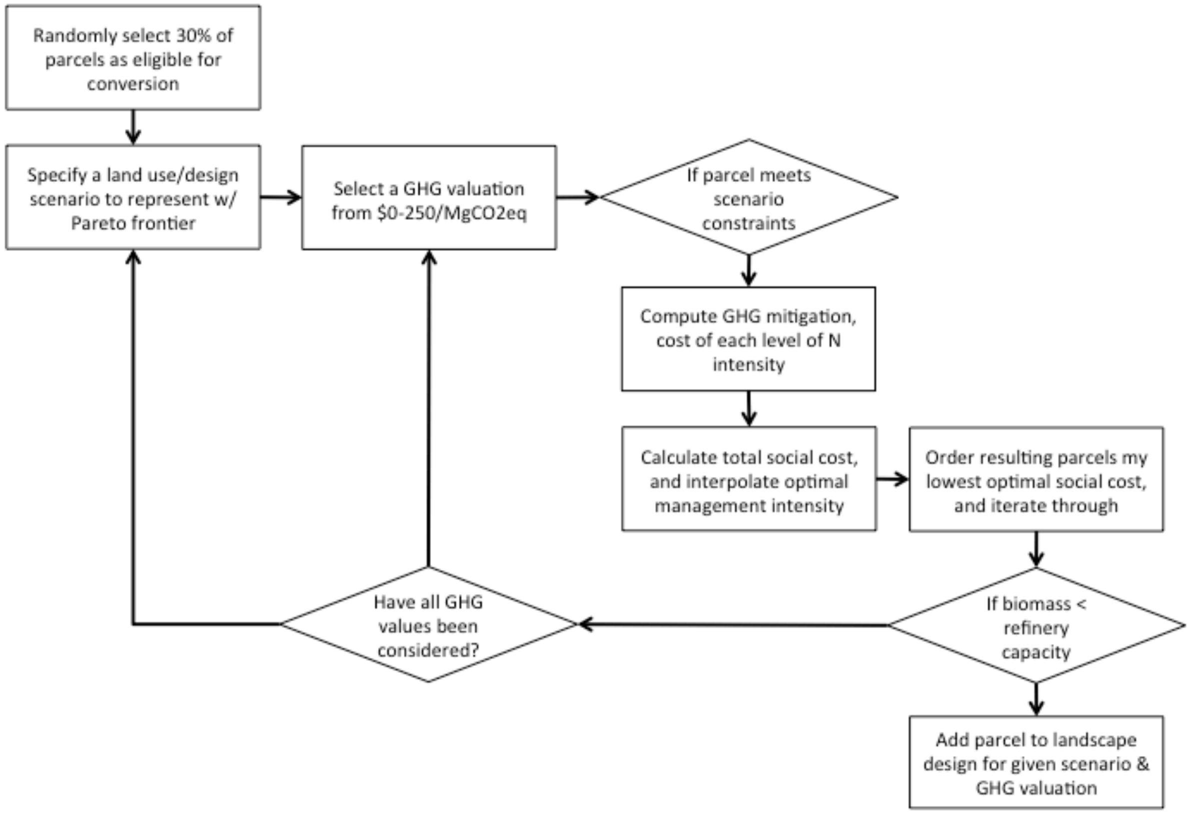
Supplementary Figure 7. Determination of a tortuosity factor representative of the road network in our case study area.



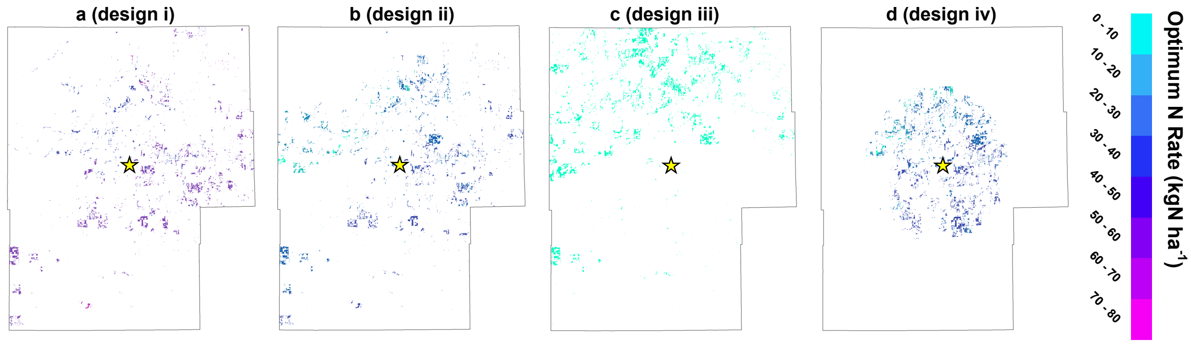
Supplementary Figure 8. Trucking Cost Model[7] results regression, showing the transport cost per metric tonne of biomass as a function of farm-to-biorefinery one-way transport distance (though price accounts for the return trip as well).



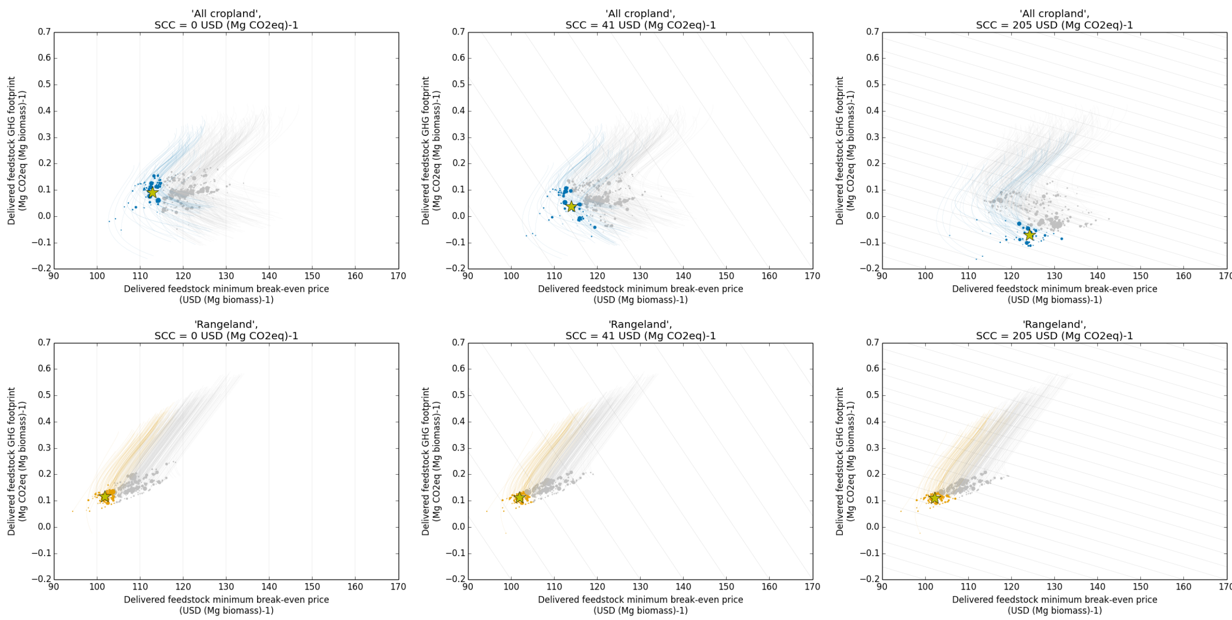
Supplementary Figure 9. Representative ecosystem modeling results illustrating 10-90th percentile ranges of yield, GHG, and cost response to increasing N fertilizer application, and associated cost × GHG tradeoffs. Note that for clarity only subset of the various analysis scenarios are shown here.



Supplementary Figure 10. Landscape optimization sequence. The GHG footprint of feedstock production (Mg CO_2eq (Mg biomass)$^{-1}$) simulated for each land parcel at every N application rate is valorized at a given carbon price (USD (Mg CO_2eq)$^{-1}$). The N rate minimizing the total social cost of switchgrass production is then identified for each parcel, the set of polygons minimizing total social costs while meeting the feedstock demand of the biorefinery determined, and associated fuel costs and GHG footprints for the resulting cellulosic ethanol estimated. Pareto-optimal tradeoff frontiers are constructed for each scenario by stepping through a range carbon price, and determining the associated set of optimal fuel cost and GHG footprint results.



Supplementary Figure 11. Cultivation locations and associated management intensities (N fertilizer application rates) for landscape designs ***i***, ***ii***, ***iii***, and ***iv***. BCAP and CRP locations are confidential, and not shown. Biorefinery location marked with a small yellow star.



Supplementary Figure 12. Optimization routine detail, illustrating the determination of optimal bioenergy landscape designs and performance considering switchgrass cultivation on cropland (top row) or rangeland (bottom row) at carbon prices of 0, 41, and 205 USD (Mg CO_2eq)$^{-1}$ (shown left to right). The full range of interpolated feedstock cost and GHG footprint outcomes for each land parcel as N application rate is adjusted from 0 – 150 kg N ha^{-1} is illustrated with a line (only 10% of parcels are plotted, for clarity). The optimal cost and GHG footprint under the specified carbon price is shown with a marker along each line, with marker area scaled to reflect the total amount of feedstock supplied by that parcel. Parcels that are selected for inclusion in the optimized bioenergy landscape are shown in color, and those that are excluded in grey. Average landscape performance across all included parcels is marked with a small yellow star. These averaged results are then converted to a per-unit-fuel basis and used to construct the Pareto tradeoff curve (Fig. 4 in the main manuscript).

Supplementary Tables

Supplementary Table 1. Summary of previous spatial sustainability assessments and bioenergy landscape design studies, focusing on assessment scope and key methodological details. Adapted from Whitaker et al.[8]

					Environmental assessment scope				System-level complexity & integration					
Study	**Site**	**Feedstock**	**Model**	**Spatial reso-lution[a]**	**Land quality explicitly defined?**	**Full soil GHG balance (incl. N2O)?**	**Water quality or quantity?**	**Erosion?**	**Variable crop management considered?**	**Upstream supply chain emissions?**	**Costs?**	**Land costs adjusted for productivity?**	**Indirect leakage?**	**Optimization algorithm applied?**
Zhang et al. (2010)[9]	SW Michigan, USA	Variety of 1st & 2nd gen	EPIC	ND[b]	X		X	X	X	X				X
Wu et al. (2012)[10]	James River Basin, USA	Corn, switch-grass	SWAT EPIC	~1,500 ha			X		X					X
Davis et al. (2012)[11]	USA corn-growing areas	Switch-grass, Miscanthus	Day-Cent	ND		X	X		X					
Gelfand et al. (2013)[12]	Midwest USA	Variety incl. native mix	EPIC	ND	X	X			X	X				
Yu et al. (2014)[13]	TN, USA	Switch-grass	Day-Cent	ND		X				X	X	X		X
Gramig et al. (2013)[14]	Wildcat Creek IN, USA	Corn stover	SWAT Day-Cent	ND		X	X	X	X		X	X		X
This study	SW Kansas, USA	Switch-grass	Day-Cent	~410 ha	X	X			X	X	X	X	X	X

[a] Total analysis area divided by number of unique model strata

[b] Not determined

Supplementary Table 2. The Cropland Data Layer[15] (CDL) was used to determine the dominant crop rotations on arable land within the case study area. A total of fifty points were randomly selected across the landscape, and the associated CDL-identified crops coded by hand for all years of data availability (typically 2006-2013). These cropping data points were then categorized within various potential crop rotations consisting of all simple combinations of corn, winter wheat, sorghum, and fallow (excluding any combination containing both corn and a fallow period or containing wheat or sorghum without a fallow period). Wheat–fallow and more intensive wheat–sorghum–fallow rotations are both common on non-irrigated areas, whereas corn–wheat rotations are most common where irrigation is available.

Rotation	Est. incidence on non-irrigated cropland	Est. incidence on irrigated cropland
continuous corn	5%	5%
corn–wheat	5%	40%
corn–sorghum	0%	5%
wheat–fallow	30%	20%
sorghum–fallow	5%	0%
corn–wheat–sorghum	10%	5%
wheat–sorghum–fallow	45%	15%

Supplementary Table 3. Summary of land conversion scenarios included in the analysis, specifying how each land class was designated, typical associated soil properties, and land use history assumptions used for DayCent model spin-up. Land use history is assumed to be homogeneous within each land class except for current switchgrass plantings (BCAP enrollment areas), for which NLCD and MIrAD-US can identify land use prior to switchgrass planting (Supplementary Fig. 5), and parcel land use histories can be customized accordingly.

Land conversion scenarios	**A. Cropland (all)**	**B. Marginal cropland**	**C. Current switchgrass plantings**	**D. Conservation easements**	**E. Rangeland**
Land class designation details	'cultivated crops' or 'pasture/hay' as per NLCD[3]; non-irrigated as per MIrAD-US[4]	Subset of (A) with NRCS LCC[6] rating >III	Areas enrolled in the BCAP program as per proprietary USDA FSA spatial data	Areas enrolled in the CRP program as per proprietary USDA FSA spatial data	'dwarf shrub', 'shrub/ scrub', 'grassland/ herbaceous', or 'sedge/ herbaceous') as per NLCD[3]
Soil summary (see Supplementary Fig. 6 above)	Mostly silty or clay loams, with a small fraction of sandy soils	Heavily skewed towards sandy soils and clays, very few loams	Almost entirely sandy soils, with a few loams	Very similar to (A), but skewed somewhat away from silty loams towards clay loams and sandy soils	Mostly clay loams, medium loams, and sandy soils
Land use history & business-as-usual management	Non-irrigated wheat-fallow rotation, no residue removal	Same as (A)	Combination of (A) and (E) depending on prior land use (see Supplement. Fig. 5 above)	Same as (A) prior to 1990; Unmanaged, unharvested mixed C3:C4 temperate grass thereafter	Unmanaged mixed C3:C4 temperate grass subject to seasonal low-intensity livestock grazing

Supplementary Table 4. Schedule of area-scaled switchgrass agricultural inputs and field operations, assuming tilled establishment and a 10-year replanting cycle.

Input	Units	Y1 rate	Y2 rate	Y3-10 rate	Notes
Seed	kg ha^{-1}	6.39	1.60	0	Assuming 25% re-seed
N	kg ha^{-1}	0	variable	variable	No N on newly-planted areas
P*	kg ha^{-1}	34.8	8.7	0	Assuming 25% re-seed
K*	kg ha^{-1}	56.1	14.0	0	" "
Atrazine	L ha^{-1}	3.5	0.88	0	Assuming 25% re-seed
2,4D	L ha^{-1}	1.78	1.78	1.78	
Chisel plow	pass ha^{-1}	1	0	0	Field preparation
Harrow	pass ha^{-1}	1	0	0	" "
Grass seeder	pass ha^{-1}	1	0.25	0	Assuming 25% re-seed
Chemical app.	pass ha^{-1}	1	1	1	Same schedule as 2,4D
Bulk fert. spread	pass ha^{-1}	0	0.75	1	" "
Mower	pass ha^{-1}	0	1	1	No estab. year harvest
Raking	pass ha^{-1}	0	1	1	" "

*initial area-scaled application of P and K is supplemented with yield-scaled applications of 1.88 and 12.8 kg (Mg biomass)$^{-1}$, respectively, for each subsequent harvest

Supplementary Table 5. Prices for switchgrass inputs and field operations, adjusted to 2015 USD using the US Consumer Price Index.

Input	Price	Units	Source
Seed	24.98	USD kg^{-1}	James et al. 2010[16]
N	0.66	USD kg^{-1}	USDA Fertilizer Use and Price database[17]
P	1.23	USD kg^{-1}	USDA Fertilizer Use and Price database[17]
K	0.93	USD kg^{-1}	USDA Fertilizer Use and Price database[17]
Atrazine	3.95	USD L^{-1}	Agricultural Chemical Solutions Inc.*
2,4D	4.56	USD L^{-1}	Agricultural Chemical Solutions Inc.*
Chisel plow	41.76	USD $(pass\ ha)^{-1}$	2015 Iowa Farm Custom Rate Survey[18]
Harrow	23.10	USD $(pass\ ha)^{-1}$	2015 Iowa Farm Custom Rate Survey[18]
Grass seeder	30.39	USD $(pass\ ha)^{-1}$	2015 Iowa Farm Custom Rate Survey[18]
Chemical application	18.29	USD $(pass\ ha)^{-1}$	2015 Iowa Farm Custom Rate Survey[18]
Bulk fertilizer spreader	13.34	USD $(pass\ ha)^{-1}$	2015 Iowa Farm Custom Rate Survey[18]
Mower	35.21	USD $(pass\ ha)^{-1}$	2015 Iowa Farm Custom Rate Survey[18]
Raking	16.06	USD $(pass\ ha)^{-1}$	2015 Iowa Farm Custom Rate Survey[18]
Baling	26.56	USD $(Mg\ biomass)^{-1}$	2015 Iowa Farm Custom Rate Survey[18]
Staging	8.15	USD $(Mg\ biomass)^{-1}$	2015 Iowa Farm Custom Rate Survey[18]
Storage	21.01	USD $(Mg\ biomass)^{-1}$	Duffy 2008[19]

*current market quote from http://www.agchemicalsolutions.com/, accessed June 9, 2016

Supplementary Table 6. Adjustment of land rental rates for productivity, in USD ha^{-1} except where noted.

	Non-irrigated cropland rental rate	Rangeland rental rate[a]	CRP rental payment
Adjustment factors			
$C_{rent,j}$	77.84	24.71	81.22
$\dot{Y}_{BAU,j}$ (Mg ha^{-1})	0.74[b]	0.34[c]	0.75[d]
Resulting distributions			
Minimum	24.19	17.44	29.24
Median	73.63	23.98	77.97
Maximum	139.89	40.70	144.03

[a] Using pastureland as a proxy, as estimated by K-State Research & Extension[20]
[b] Average simulated winter wheat yield within a wheat–fallow rotation
[c] Average simulated biomass grazed annually
[d] Average simulated winter wheat yield prior to CRP conversion

Supplementary Table 7. Estimated diesel fuel use for farm operations included in our switchgrass production budget (excluding bailing) for a 10-year replanting cycle, assuming no biomass harvest in the first year of the rotation.

Operation	Frequency per harvest	Fuel use (BTU ha^{-1})	Fuel use (BTU ha^{-1} $harvest^{-1}$)
Chisel plow	0.111	349,000	38,800
Harrow[a]	0.111	286,000	31,700
Grass seeder[b]	0.139	127,000	17,600
Chemical application[c]	1.111	31,700	35,300
Bulk fertilizer spreader	0.972	47,600	46,300
Mower	1.000	95,200	95,200
Raking	1.000	79,300	79,300
Total			**344,300**

[a] Based on fuel use for a 'Seedbed conditioner'[21]
[b] Based on fuel use for a 'Planter- seed only'[21]
[c] Based on fuel use for a 'Sprayer- trailer type'[21]

Supplementary Table 8. Harmonization of the GREET default switchgrass production pathway and our switchgrass production budget. Discrepancies reflect different input rates per area of farmland, and different switchgrass area yield assumptions.

Input	Units	GREET values*	Baseline value used	Notes
Seed	kg (short ton)$^{-1}$	-	-	Not included in GREET
N fertilizer	kg (short ton)$^{-1}$	8.30	5.67	GREET assumes mix, we assumed anhydrous ammonia
P_2O_5 fertilizer	kg (short ton)$^{-1}$	0.114	3.56	
K_2O fertilizer	kg (short ton)$^{-1}$	0.227	15.0	
Atrazine	kg (short ton)$^{-1}$	-	0.066	
2,4D	kg (short ton)$^{-1}$	0.0318	0.267	Simply 'herbicide' in GREET
Farm operations diesel use	BTU (short ton)$^{-1}$	50,000	39,000	
Harvest operations diesel use	BTU (short ton)$^{-1}$	127,700	127,700	

Supplementary Table 9. Sensitivity of harmonized GREET cellulosic ethanol pathway GHG footprint estimate to perturbations in various key model parameters.

Parameter	Symbol	GREET result sensitivity (% Δ footprint/ % Δ parameter)
Specific total farm energy use	ε_E	0.112
Specific N fertilizer input	ε_N	0.277
Specific SOC emissions	ε_{SOC}	-0.288
Specific N_2O emissions	ε_{N2O}	0.172
Specific iLUC factor	ε_{iLUC}	0.139
Transport distance	ε_{dist}	0.050

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