Supporting Information

Economic and Sustainability impacts of yield and composition variation in bioenergy crops: *Panicum virgatum L.*

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Supporting information contains nine tables and seven figures over fourteen pages with 12 additional references.

Switchgrass Yield and Cost

Figure S1 shows the results of the feedstock cost model as a function of commercial-scale switchgrass yield, for a fixed annual biorefinery demand and density of fields in switchgrass production. The components of total delivered switchgrass costs include marginal land rental, planting, annual land maintenance, harvest, transport, storage, and grinding. Harvest, transport, and land maintenance costs decrease the most as the switchgrass yield increases from 5 to 17 Mg ha^{-1}. An increase in yield reduces the land requirement which affects the harvest and land maintenance cost while the reduced supply shed footprint affects the transport cost. However, total costs become much less sensitive to yield above 18 Mg ha^{-1}, with the rate of change in total cost per megagram when increasing the yield by 1 megagram per hectare is less than two percent. It should be noted that this is not the price that a biorefinery would pay for feedstock at the refinery gate, but rather is a techno-economic cost that would be incurred if the refinery managed the feedstock supply chain up to the beginning of the conversion processes or the first “reactor throat” or the beginning of the conversion processing. We can assume that if the refinery was purchasing the feedstock from local growers, then the purchase cost would be based on the incurred cost plus a factor for grower profit.

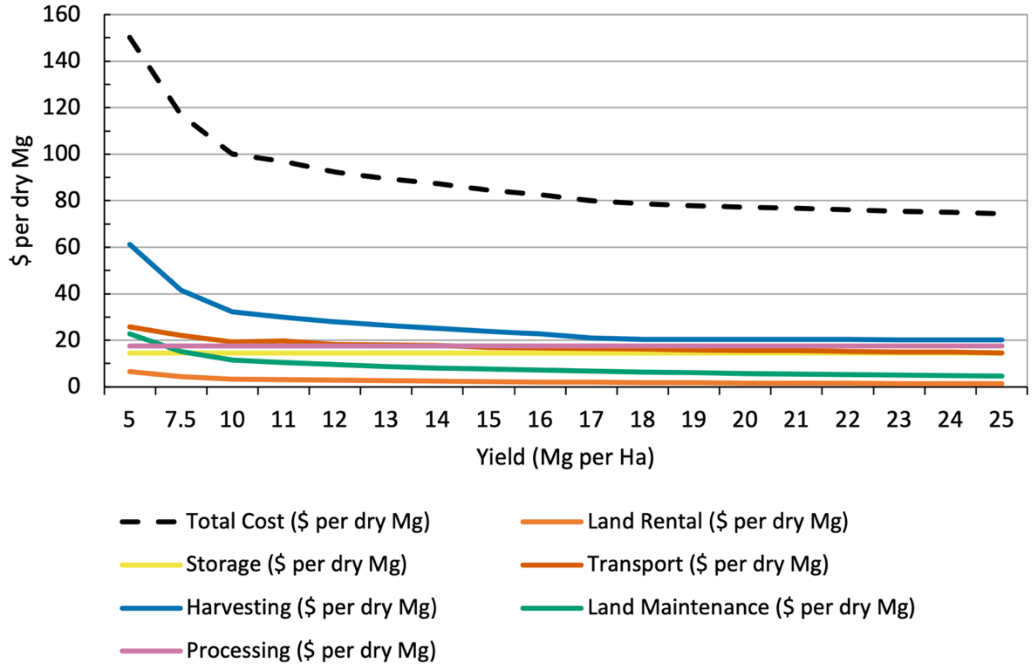

Figure S1. Feedstock delivered costs ($ per dry Mg) as a function of switchgrass yield.

Composition

Table S1. Percent Composition Statistics for 331 analyzed switchgrass samples selected from the population (% w/w)

	Glucose	Xylose	Galactose	Arabinose	Lignin	S/G Ratio
Average	40	25	1.4	2.5	18.8	0.68
Minimum	35	22	0.8	1.4	15.4	0.47
Maximum	46	28	2.5	4.1	21.4	0.92

Prediction Error	±3	±2	±0.6	±0.4	N/A*	N/A*
Std. Dev.	±2	±1	±0.3	±0.4	±0.96	±0.02

** Lignin and syringyl/guaiacyl ratio (S/G) were not determined via models but predicted relative to standard response, hence no model error reported, see Decker et al., 2018* for analysis details[1].

Key Numerical Results for Figures 6, 7, 8, 9 and S6.

Table S2. Life cycle GWP, CED, and AWARE results for all variants, alongside the fermentable carbohydrate mass fraction, on-farm yield, and MFSP values.

VARIANT	**GWP (g CO_2e/L)**	**CED (MJ/L)**	**AWARE (m^3/L)**	**FERM. CARB. MASS FRACTION**	**YIELD (DRY MG/HA)**	**MFSP (USD/L)**
J324-A	474	8.88	46.7	0.655	34.9	0.588
J303-A	549	10.0	49.1	0.659	9.28	0.674
J594-C	492	9.11	47.6	0.653	18.8	0.605
J341-A	540	9.82	48.7	0.651	9.95	0.669
J271-A	498	9.25	47.6	0.650	16.6	0.619
J484-A	492	9.18	47.3	0.658	18.3	0.607
J016-B	523	9.61	47.3	0.676	10.6	0.643
RAMBO 4	476	8.87	46.2	0.669	21.4	0.587
J463-A	466	8.70	46.2	0.658	39.2	0.577
J496-C	497	9.18	48.1	0.649	18.4	0.611
J499-B	508	9.35	48.1	0.655	14.7	0.624
X211-A	484	9.00	46.6	0.669	18.2	0.597
X222-A	477	8.92	46.7	0.661	26.5	0.590
J319-A	483	9.00	46.8	0.662	20.6	0.597
J321-A	493	9.11	47.3	0.667	16.7	0.604
J497-B	536	9.82	49.0	0.656	11.3	0.657
J041-A	542	9.84	48.7	0.655	9.62	0.670
X502-A	522	9.59	47.7	0.663	11.3	0.644
J013-C	533	9.71	48.6	0.651	11.0	0.655
J212-A	586	10.4	51.4	0.619	8.11	0.727
J330-A	474	8.87	46.1	0.673	24.0	0.583
J022-B	557	10.0	49.3	0.642	8.67	0.693
X229-A	537	9.74	48.8	0.643	10.3	0.667
J280-A	521	9.54	49.0	0.640	13.5	0.641
J073-B	500	9.28	47.3	0.657	14.9	0.620
J295-A	477	8.97	46.3	0.669	23.5	0.588
J226-A	516	9.48	48.6	0.643	14.0	0.635
J251-B	549	9.94	50.2	0.615	11.0	0.686
J250-A	585	10.5	50.4	0.641	7.63	0.722

J419-A	514	9.42	48.5	0.640	14.0	0.635
J340-A	510	9.40	49.0	0.633	16.8	0.631
J218-A	488	9.12	47.1	0.656	19.8	0.605
J023-B	554	10.0	50.3	0.619	10.5	0.690
J514-A	500	9.21	48.1	0.643	17.3	0.618
J331-A	567	10.2	49.4	0.648	7.89	0.701
RAMBO 5	501	9.19	48.9	0.621	21.0	0.621
J274-A	506	9.32	48.5	0.628	16.5	0.631
J177-A	507	9.26	49.4	0.615	19.2	0.631
J315-A	514	9.47	48.8	0.628	14.9	0.641
J610-B	505	9.28	48.1	0.647	15.1	0.624
J249-B	541	9.87	48.7	0.647	9.93	0.674
J394-C	531	9.67	48.4	0.645	11.0	0.658
J008-B	553	10.0	49.7	0.638	9.61	0.685
J301-A	487	9.03	47.2	0.656	20.4	0.599
J065-A	490	9.10	47.2	0.656	18.5	0.605
J251-C	481	8.95	47.1	0.647	24.7	0.595
J499-A	517	9.54	49.4	0.632	15.8	0.638
J272-A	497	9.21	47.6	0.657	16.9	0.612
J251-A	470	8.85	45.3	0.688	20.8	0.578
J610-C	575	10.3	49.7	0.648	7.74	0.708
J497-C	497	9.25	48.0	0.654	19.3	0.611
J004-B	486	9.06	46.6	0.667	17.2	0.601
J447-A	580	10.4	50.3	0.638	7.76	0.717
J249-A	538	9.72	49.6	0.620	11.4	0.672
J270-A	554	10.0	48.3	0.669	8.13	0.684
J247-A	499	9.25	48.3	0.634	20.2	0.618
J065-B	510	9.41	48.1	0.645	14.4	0.633
J016-D	534	9.73	48.9	0.648	11.3	0.655
J276-A	548	10.0	49.0	0.648	9.49	0.680
J022-A	468	8.84	45.5	0.674	26.1	0.580
J235-A	559	10.2	48.1	0.676	7.64	0.688
J250-C	534	9.80	47.9	0.667	9.87	0.660
J610-A	546	9.93	48.7	0.662	9.22	0.674
J016-A	490	9.14	47.1	0.668	18.4	0.602
J497-A	497	9.21	47.4	0.663	15.9	0.612
J005-D	524	9.58	47.7	0.669	10.8	0.644
J003-D	515	9.49	47.5	0.666	11.9	0.636
J326-A	495	9.17	47.2	0.661	16.1	0.611
J594-A	558	10.1	48.8	0.660	8.25	0.690
J215-A	498	9.20	48.4	0.640	20.2	0.612
J249-C	483	8.97	47.1	0.647	24.2	0.597
J237-A	502	9.25	48.2	0.643	16.2	0.621

J503-A	577	10.3	51.7	0.616	8.92	0.714
J294-A	524	9.58	49.1	0.632	13.2	0.649
J327-A	559	10.1	49.7	0.644	9.05	0.690
J020-C	526	9.66	49.3	0.632	13.6	0.651
J008-D	534	9.78	49.5	0.633	12.2	0.661
J268-A	542	9.90	49.9	0.618	11.7	0.676
J305-A	514	9.43	48.8	0.630	14.7	0.639
J322-A	509	9.40	48.8	0.630	16.8	0.631
J293-A	562	10.2	50.7	0.611	9.90	0.705
J001-A	515	9.45	48.1	0.650	12.9	0.636
J587-B	484	9.02	47.1	0.653	22.7	0.599
J323-A	490	9.06	47.7	0.640	22.0	0.606

Statistical Summary of Numerical Results

Table S3. Statistical summary of ethanol life cycle impacts observed in this study.

	GWP (Gco$_2$e/L)	**CED (MJ/L)**	**AWARE (m^3/L)**
Mean	517	9.50	48.3
Minimum	466	8.70	45.3
Maximum	586	10.5	51.7
Standard Deviation	30.6	0.445	1.27

Inventory Comparison to Other Studies

Table S4. Agricultural inputs comparison between GREET (2021)[2], and this study, adapted from Supplementary Table 8 of Field et al (2018)[3]. Where values are given as ranges, the exact values used for a variant were dependent on the estimated switchgrass yield projected from the single plant yields. While the units here are reported in metric or English units as in the cited studies, all were converted in SI for the calculations.

Agricultural Input	**Units**	**GREET (2021)[2]**	**Field et al (2018)[3]**	**This Study**
Seed	kg/dry U.S. ton	-	-	0.030 – 0.110
N fertilizer	kg N/dry U.S. ton	4.30	5.67	5.51
P$_2$O$_5$ fertilizer	kg P/dry U.S. ton	0.221	3.56	1.88 – 2.28
K$_2$O fertilizer	kg K$_2$O/dry U.S. ton	2.80	15.0	11.9 – 12.5
CaCO$_3$ fertilizer	kg CaCO$_3$/dry U.S. ton	5.10	-	-
Atrazine	kg chemical/dry U.S. ton	0.0467 (generic herbicide)	0.066	0.021 – 0.069
2,4D	kg chemical/dry U.S. ton		0.267	0.113 – 0.368
Insecticide	kg chemical/dry U.S. ton	0	-	-

Farm operations diesel use	BTU/dry U.S. ton	5.94 x 10^4 (farming and harvest)	3.90 x 10^4	6.30 x 10^3 – 2.05 x 10^4
Harvest operations diesel use	BTU/dry U.S. ton		1.28 x 10^5	1.61 x 10^5 – 3.07 x 10^5

Table S5. Biorefinery inputs and coproduct comparison between GREET (2021)[2] and this study. Where values are given as ranges, the exact values used for a variant were dependent on switchgrass composition.

Biorefinery Input	**Units**	**GREET (2021)[2]**	**This Study**
Switchgrass, bone dry	kg/gal ethanol	11.3	9.56 – 10.8
Sulfuric acid		0.300	0.227 – 0.256
Ammonia		0.048	0.140 – 0.158
Corn steep liquor		0.136	0.155 – 0.175
Diammonium phosphate		0.015	0.017 – 0.019
Sodium hydroxide, 100%		0.103	0.271 – 0.304
Lime		0.065	0.085 – 0.111
Glucose		2.73 x 10^{-4}	0.305 – 0.343
Sulfur Dioxide		1.63 x 10^{-3}	2.07 x 10^{-3} – 2.33 x 10^{-3}
Sorbitol		4.50 x 10^{-3}	5.14 x 10^{-3} – 5.78 x 10^{-3}
Host Nutrients		6.88 x 10^{-3}	0.008 – 0.010
Boiler Chemicals		-	2.81 x 10^{-5} – 3.27 x 10^{-5}
Cooling Tower Chemicals		2.50 x 10^{-4}	2.41 x 10^{-4} – 2.97 x 10^{-4}
Makeup water		-	15.8 – 19.5
Electricity coproduct	kWh/gal ethanol	1.79	0.878 – 1.95

Process Contribution Analysis

A process contribution analysis (PCA) provides more detailed insight into environmental hotspots, which are processes involved in ethanol production which may be producing a disproportionate level of impacts. This analysis can be a first step towards identifying and prioritizing research areas that could reduce total life cycle impacts. For this study, the objective of the PCA is to identify any trends that may exist in process-specific impacts due to variability in FCMF or in switchgrass yield. Variants were selected for PCA based on five percentiles of the FCMF values and of the yield values represented in the study. After calculating the FMCF percentiles, the five variants with FCMF values closes to those percentiles were selected for PCA, and five variants representing the switchgrass yield percentiles were chosen analogously. Figure S2 shows box-and-whisker plots of the five percentiles for FCMF (A) and for yield (B), with percentiles labeled with the corresponding variant names in gray.

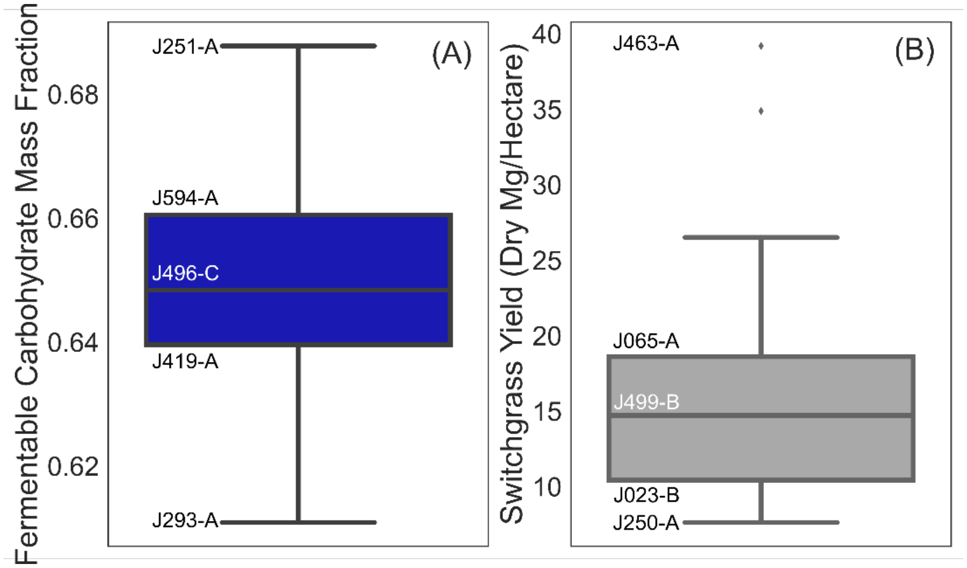

Figure S2. Box-and-whisker plots showing (A) five fermentable carbohydrate mass fraction percentiles and (B) five switchgrass yield percentiles, with the switchgrass variants nearest to each percentile labeled in gray. The process contribution analysis was performed on these ten variants.

The ethanol life cycle was divided into five process categories for the PCA. Four of these categories cover switchgrass agriculture and logistics: site preparation and planting, chemicals and application operations, harvest operations, and transport to biorefinery. The final category consists of inputs to the biorefinery.

PCA results are shown in Figures S3, S4, and S5 for GWP, CED, and the AWARE indicator, respectively. Numerical PCA results are listed in Tables S6 and S7. In each PCA figure, results for the FCMF percentile variants are given in sub-figure (A) and the yield percentile variants are in sub-figure (B). A lighter shade indicates a higher percentile. For all three impacts, increased FCMF does not correspond to a uniformly increased or decreased impact in any of the five process categories, while increased yield does correspond to decreased impacts for all categories except site preparation and planting.

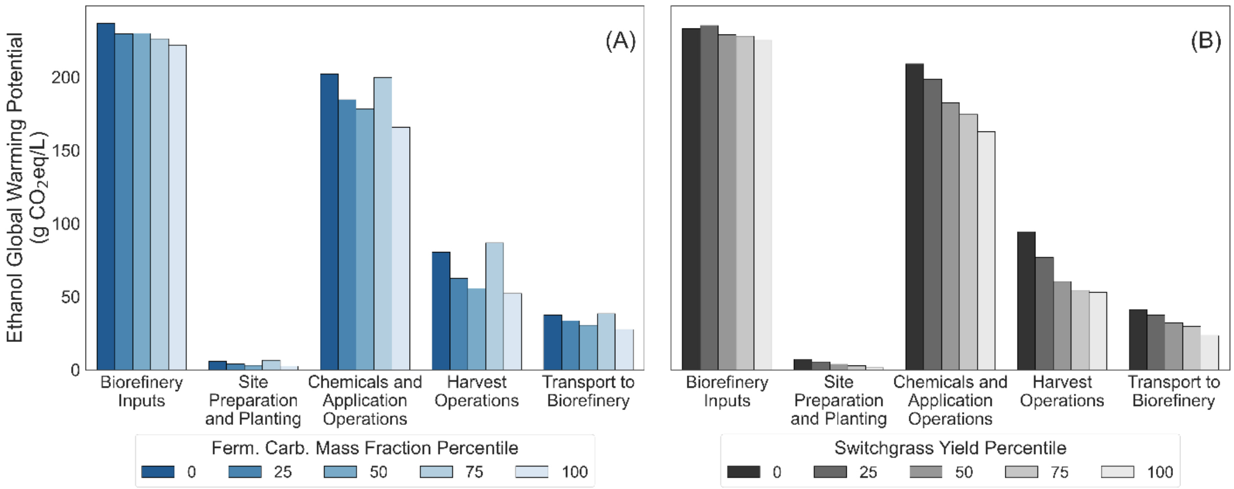

Figure S3. Global warming potential for 1 L ethanol disaggregated by process category and shown for selected variants based on carbohydrate fraction percentiles (A) and yield percentiles (B).

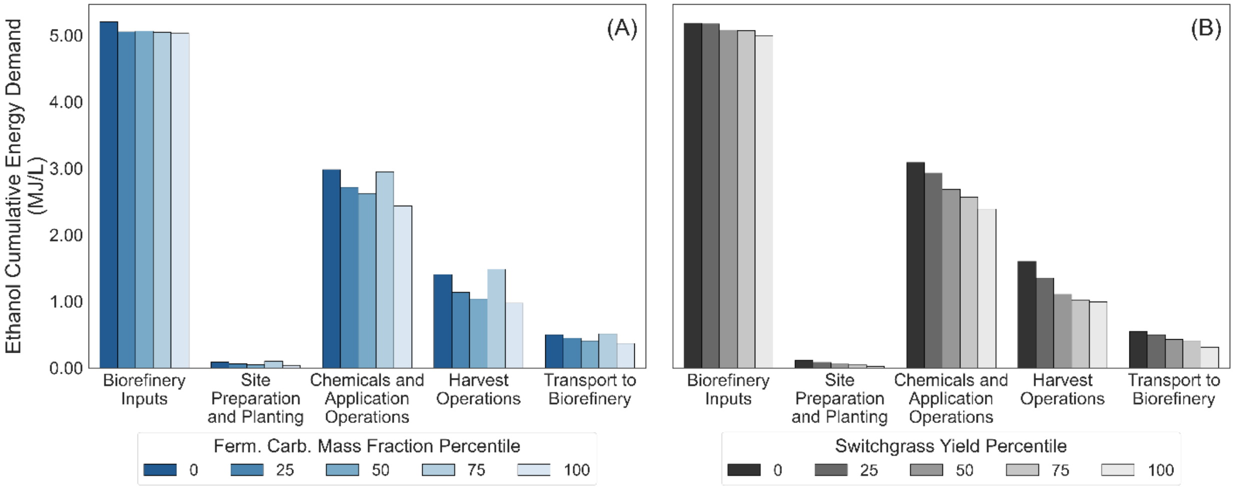

Figure S4. Cumulative energy demand for 1 L ethanol disaggregated by process category and shown for selected variants based on carbohydrate fraction (A) and yield percentiles (B).

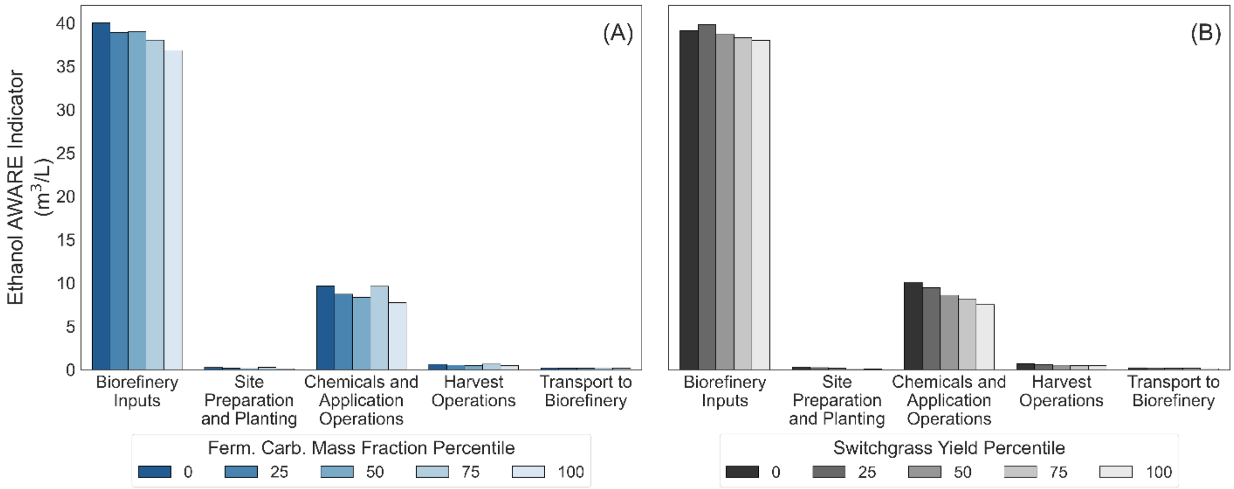

Figure S5. Available water remaining indicator for 1 L ethanol disaggregated by process category and shown for selected variants based on carbohydrate fraction (A) and yield percentiles (B).

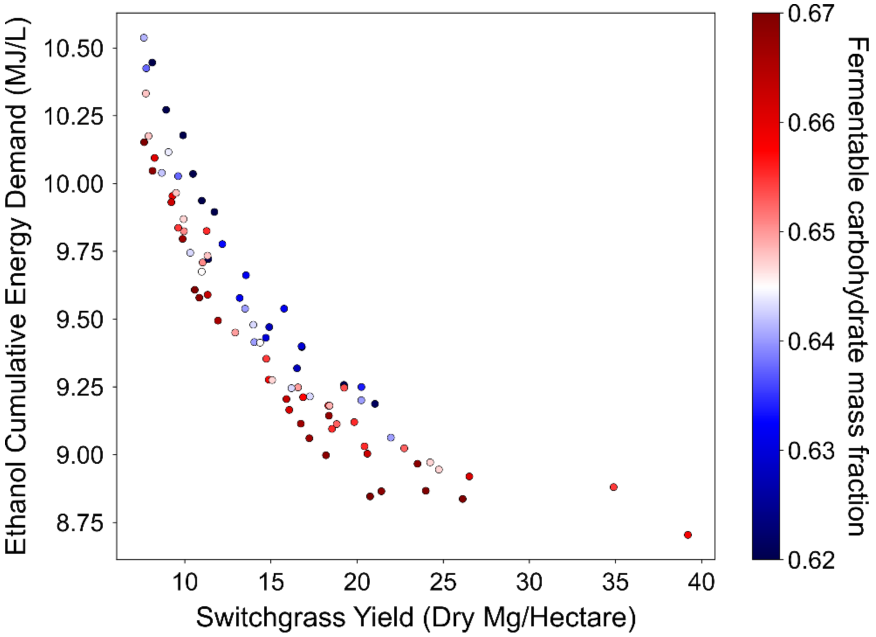

Figure S6. Ethanol cumulative energy demand (MJ/L) shows a strong negative correlation (R^2 = 0.77) with switchgrass yield.

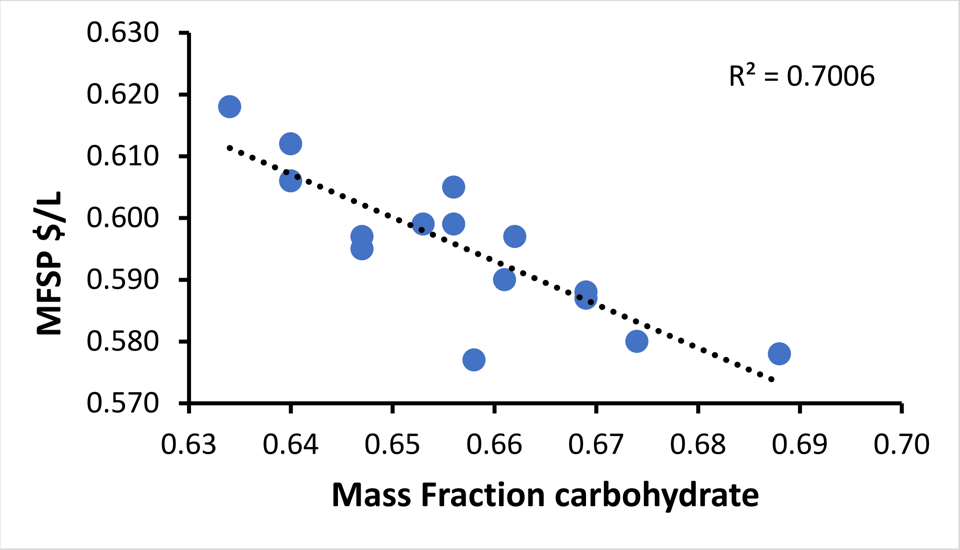

Figure S7: MFSP decreases with increasing fermentable carbohydrate content. (R^2 = 0.70) when considering only the higher yielding switchgrass genotypes (≥ 20 dry Mg/ha)

Table S6. Process contribution analysis results for the fermentable carbohydrate mass fraction percentile variants.

	J293-A (0th)	**J419-A (25th)**	**J496-C (50th)**	**J594-A (75th)**	**J251-A (100th)**
Global Warming Potential ($g\ CO_2e/L$)					
Biorefinery Inputs and Co-Products	237	230	230	226	222
Site Preparation and Planting	5.75	3.94	3.01	6.55	2.51
Chemicals and Application Operations	202	185	178	200	166
Harvest Operations	80.4	62.4	55.6	86.7	52.1
Transport to Biorefinery	37.4	33.5	30.5	38.4	27.6
Cumulative Energy Demand (MJ/L)					
Biorefinery Inputs and Co-Products	5.20	5.05	5.07	5.05	5.03
Site Preparation and Planting	0.088	0.0603	0.0461	0.100	0.0385
Chemicals and Application Operations	2.98	2.72	2.62	2.95	2.44
Harvest Operations	1.40	1.14	1.04	1.49	0.974
Transport to Biorefinery	0.500	0.448	0.408	0.513	0.369
AWARE (m^3/L)					
Biorefinery Inputs and Co-Products	40.0	38.9	39.0	38.0	36.8
Site Preparation and Planting	0.249	0.170	0.130	0.283	0.109
Chemicals and Application Operations	9.66	8.71	8.35	9.62	7.74
Harvest Operations	0.620	0.523	0.487	0.641	0.454
Transport to Biorefinery	0.206	0.185	0.168	0.212	0.152

Table S7. Process contribution analysis results for the switchgrass yield percentile variants.

	J250-A (0th)	**J023-B (25th)**	**J499-B (50th)**	**J065-A (75th)**	**J463-A (100th)**
Global Warming Potential ($g\ CO_2e/L$)					
Biorefinery Inputs and Co-Products	233	235	229	228	225
Site Preparation and Planting	7.28	5.40	3.73	2.93	1.38
Chemicals and Application Operations	209	199	182	175	163
Harvest Operations	94.4	76.9	60.4	54.4	52.8
Transport to Biorefinery	41.2	37.3	32.1	29.7	23.4
Cumulative Energy Demand (MJ/L)					
Biorefinery Inputs and Co-Products	5.18	5.17	5.08	5.07	4.99
Site Preparation and Planting	0.111	0.0827	0.0572	0.0448	0.0211
Chemicals and Application Operations	3.09	2.93	2.68	2.57	2.39
Harvest Operations	1.60	1.35	1.11	1.02	0.991
Transport to Biorefinery	0.551	0.499	0.429	0.398	0.313
AWARE (m^3/L)					
Biorefinery Inputs and Co-Products	39.1	39.8	38.7	38.3	38.0
Site Preparation and Planting	0.315	0.233	0.161	0.127	0.0596
Chemicals and Application Operations	10.1	9.47	8.59	8.17	7.51
Harvest Operations	0.685	0.601	0.512	0.477	0.452
Transport to Biorefinery	0.227	0.206	0.177	0.164	0.129

Feedstock Supply Model Details

Our switchgrass transport process included crews of semi-trucks with flatbed trailers moving the bales to storage near the refinery with loaders at both the field and the storage facility. The storage near the refinery consisted of a hybrid storage process with half of the feedstock stored under a tarp on a gravel pad and the other half stored covered under a pole barn. The tarped feedstock would be used first so weather during storage would have minimal effect on the stored feedstock. The system would only keep a few days’ supply of feedstock at the refinery where it is processed by a grinder.

Table S8. Feedstock cost model parameters. While the units here are reported in metric or English units as in the cited studies, all were converted in SI for the calculations.

Description	**Value**
Dry matter loss (DML) during storage	3% [4]
Bale Data (dimension; density; moisture)	8x4x3 ft^3 [5]; 175 dry Kg per m^3 [5];15% [6]
On highway diesel	\$4.10 per gallon [7]
Ag Equipment Operator Labor Rate	\$15.63 per hour [8]
Semi Transport Labor Rate	\$22.66 per hour [8]
Self-Propelled Mower Conditioner	1.8 ha per hour [9];31.2 mg per hour [9]; \$175.3 per hour[10,a]
Tractor and Large Square Baler	1.4 Ha per hour [9]; 25.1 dry Mg per hour [9,11]; \$226.5 per hour [10, b]
Move to field side	72 bales per hour [c]; 34.3 dry mg per hour [5]; \$148.1 per hour [10, d]
Transport Crew with three to four Semi-trailer trucks with flatbed trailers and a loader at the field side	36 Bales per load; 17.1 dry mg per load [5, e]; \$208.89 [f,g]

[a] Using a 235 hp mower conditioner (JD W235M) with a list price of \$184,457

[b] Using a large square baler (JD L341) with a list price of \$198,583 pulled by a 190 hp tractor (JD 6R 195) with a list price of \$247,674.

[c] as suggested by FDC Enterprises.

[d] Assuming a purchase cost of \$202,500 for a 320 hp Stinger Stacker 6500.

[e] Assuming a bale density of 175 dry Kg per m^3 and a moisture of 15%.

[f] Assuming a purchase cost of \$109,835 for a semi-truck, \$49,410 for a flatbed trailer (53 ft. X 102 in.), and \$85,112 for a wheeled loader (JD 204L Wheeled Loader).

[g] Using one loader at the field for each transport crew consisting of three to four semi-trucks with flatbed trailers.

The number of fields required was calculated for each yield scenario using the annual refinery demand of 2000 dry U.S. tons while assuming a 3% dry matter loss (DML) during storage (3), a field size of 60 hectares, and the switchgrass yield set by the scenario which ranged from 5 to 40 Mg ha^{-1}. We assumed a switchgrass supply shed density of 15% which would randomly place one 60-hectare field every four km^2. The road distance from the refinery to the field was assumed to be a factor of 1.4 times the direct distance.

Table S9. Feedstock cost model parameters

Description	Value
Land Rental	\$32.12 per hectare [12]
Planting and Annual Land Maintenance	\$110.56 per hectare per year [13]
Storage Cost	\$14.43 per dry megagram [14]
Short Term Storage at Refinery	\$1.8 per dry megagram [13]
Grinding	\$17.66 per dry megagram [13]

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