Supporting Information:

Greenhouse Gas Footprint, Water-Intensity, and, Production Cost of Bio-Based Isopentenol as a Renewable Transportation Fuel

Nawa Raj Baral [a,b], Olga Kavvada [a,c], Daniel Mendez Perez[a,b], Aindrila Mukhopadhyay[a,b], Taek Soon Lee[a,b], Blake A. Simmons[a,b], Corinne D. Scown*[a,b,c]

[a]Joint BioEnergy Institute, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States

[b]Biological Systems and Engineering Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States

[c]Energy Analysis and Environmental Impacts Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, United States.

*Corresponding author, E-mail: cdscown@lbl.gov

Number of pages: 22

Number of tables: 4

Number of figures: 13

S1. Data sources

S1.1. Input parameters and required material and energy for feedstock supply system

Table S1. Major input parameters used in the feedstock supply model

Parameter	Unit	μ	a	b	σ	Probability distribution
Required dry biomass (assumed)	t/day	2,000.0	-	-	-	None
Biorefinery working days (assumed)	days/yr	330.0	-	-	-	None
Moisture content[1–3]	%	59.7	40.0	70.0	10.7	Triangular
Safety stock[4]	%	12.5	8.0	25.0	8.8	Triangular
Dry matter loss (supply chain)[4,5]	%	11.6	4.2	25.0	6.6	Lognormal
Dry matter loss (forage harvester)[6,7]	%	2.4	0.8	4.0	-	Triangular
Harvest window[8]	*days/yr*	31.5	15.0	75.0	14.6	Triangular
Harvesting hours[λ]	*h/day*	16.0	8.0	24.0	8.0	Triangular
Land utilization for sorghum farming[ω]	%	5.0	2.0	10.0	-	Triangular
Road winding factor[9–12]	-	1.5	1.1	3.5	0.4	Normal
Nitrogen[3,13–16]	kg/ha	121.24	48.0	217.0	51.88	Triangular
Phosphorus[3,13,15]	kg/ha	23.89	9.30	67.25	16.74	Triangular
Potassium[3,13,15]	kg/ha	168.09	20.00	293.66	-	Triangular
Price of nitrogen[17–21]	$/kg	1.06	0.60	1.40	0.34	Triangular
Price of phosphorus[17–21]	$/kg	1.01	0.82	1.20	0.15	Triangular
Price of potassium[17–21]	$/kg	1.09	0.91	1.26	0.14	Triangular
Herbicides[22–24]	kg/ha	3.13	1.79	5.60	-	Triangular
Herbicides[22–25]	$/ha	62.12	24.46	111.2	-	Triangular

[λ] Assumed based on the current harvesting practices of biomass sorghum.

[ω] Percentage of the total area (including land, water bodies, and others) around the biorefinery.

Note: **μ** = average value; **a** = minimum value; **b** = maximum value; **σ** = standard deviation

Selection of probability distribution: The probability distribution is selected based on the data gathered from several sources or historical data. In the case of the limited data sources, either triangular or uniform probability distribution is selected. The uniform probability distribution is chosen if the input parameter is dependent on the types of process technology or operating conditions.

Table S2. Material and energy data generated from the feedstock supply model[26]

Lifecycle stage	Materials	Units	μ	a	b	σ
Nutrient	N	kg/t-DBS	7.35	2.03	22.39	4.18
	P	kg/t-DBS	1.45	0.12	9.92	1.54
	K	kg/t-DBS	10.19	0.99	54.62	7.28
Chopping	Diesel	L/t-DBS	3.09	1.10	9.36	1.29
Infield transportation	Diesel	L/t-DBS	0.38	0.21	0.77	0.09
Biorefinery transport	Diesel	L/t-DBS	3.18	0.99	9.61	1.32
Storage at depot	Tarp	m^2/t-DBS	4.30	2.78	8.26	0.79
	Gravel	m^2/t-DBS	3.51	2.27	6.74	0.65

Note: *μ: baseline (average) value; a: minimum value; b: maximum value; and σ: standard deviation. DBS refers to the dry biomass sorghum delivered to the biorefinery*

S1.2. Major operating and process parameters used to develop the downstream process model

Table S3. Modeling inputs and their probability distributions

Parameters	Units	μ	a	b	σ	Probability distribution
Cost of sorghum biomass[26]	$/t-dry	101.8	60.00	137	4.82	Lognormal
Sorghum biomass composition[27–34]						
Acetate	wt%	2.20	0.90	2.90		Constant
Ash	wt%	7.70	2.20	10.94	3.49	Lognormal
Cellulose	wt%	35.80	20.50	44.02	5.31	Lognormal
Hemicellulose	wt%	22.92	14.50	29.79	3.80	Lognormal
Lignin	wt%	16.52	9.89	20.29	2.70	Lognormal
Proteins	wt%	4.39	3.88	5.16	0.68	Constant
Ionic liquid (IL) Pretreatment						
Solid loading rate[35–37]	wt%	30.00	20.00	40.00		Triangular
IL loading rate[36]	kg/kg-biomass	0.29	0.25	0.35		Triangular
IL-cost [36,38]	$/kg	2.00	1.43	5.00		Triangular
Sulfuric acid loading[36,38]	kg-/kg-IL	0.16	0.15	0.17		Triangular
Sulfuric acid price[35,39,40]	$/kg	0.14	0.03	0.28	0.11	Triangular
Lignin to soluble lignin[36,38]	wt%	65.00	60	70		Constant
Pretreatment time [36,38]	h	3.00	2.5	3.4		Triangular
Enzymatic hydrolysis[36–38]						
Enzyme loading rate	mg-protein/g-glucan	20.00	7	20		Uniform
Initial solid loading rate	wt%	20.00	20	30		Uniform
Cellulose to glucose	wt%	84.00	84	95		Uniform
Xylan to xylose	wt%	80.00	75	90		Uniform
Hydrolysis time	h	48.00	36	72		Triangular
Enzyme price	$/kg-protein	5.00	4	6		Triangular
Bioconversion						
Aeration rate (aerobic) [41–43]	VVM	1.00	1.00	2.00		Triangular
Aeration rate (micro-aerobic) [41,42,44,45]	VVM	0.5	0.2	1.5		Triangular
Power consumption (aerobic) [46]	kW/m^3	3.00	2.00	5.00		Triangular
Power consumption (micro-aerobic) [46]	kW/m^3	0.35	0.2	0.6		Triangular
Power dissipation to heat (aerobic) [46,47]	%	80.00	70.00	100.00		Triangular
Power dissipation to heat (micro-aerobic) [46,47]	%	40.00	30.00	50.00		Triangular
Bioconversion time[48–50]	h	72.00	48.00	84.00		Uniform
Glucose to isopentenol[48–50]	wt%	20.45	14	40.9		Uniform
Xylose to isopentenol[48–50]	wt%	20.45	14	40.9		Uniform
Corn steep liquor price[35,39,40]	$/kg	0.06	0.05	0.07		Triangular
DAP price[35,39,40]	$/kg	0.97	0.69	1.10		Triangular
Recovery and separation						
Recovery of isopentenol (assumed)	wt%	95	95	99		Uniform
IL-recovery[36,37,51]	wt%	97	85.00	99.0		Triangular
Wastewater treatment						
Organic matter to biogas conversion[35]	wt%	86.00	85	91		Triangular
Onsite energy generation						
Boiler chemicals price[35]	$/kg	5.00	4.00	6.00		Triangular
Natural gas price[b]	$/kg	0.22	0.10	0.44	0.10	Lognormal

Note: *μ: baseline (average) value; a: minimum value; b: maximum value; and σ: standard deviation.* Unless otherwise specified data summarized in this table were gathered from recent studies.[36–38] The uncertainty analysis for each product yield scenario was run by fixing the product yield and considering variabilities present in other input parameters. The probability distribution is selected based on the data gathered from several sources or historical data. In the case of the limited data sources, either triangular or uniform probability distribution is selected. The uniform probability distribution is chosen if the input parameter is dependent on the types of process technology or operating conditions.

[b]**https://www.eia.gov/dnav/ng/hist/rngwhhdA.htm**

S1.3. Material and energy data obtained from process model after 5000 trials

Table S4. Outputs from techno-economic model developed in SuperPro Designer

Lifecycle stage	Parameter	Unit	μ	a	b	σ
Feedstock supply (composition)	Acetate	kg/kg-isopentenol	0.21	0.07	0.37	0.04
	Ash	kg/kg-isopentenol	0.72	0.07	3.13	0.30
	Cellulose	kg/kg-isopentenol	3.36	1.35	5.84	0.67
	Extractive	kg/kg-isopentenol	0.98	0.00	4.98	0.67
	Hemicellulose	kg/kg-isopentenol	2.15	0.71	4.10	0.46
	Lignin	kg/kg-isopentenol	1.55	0.44	3.16	0.37
	Moisture	kg/kg-isopentenol	1.04	0.38	1.85	0.22
Feedstock handling	Electricity	kWh/kg-isopentenol	0.07	0.03	0.13	0.02
Pretreatment	Steam 226°C	kg/kg-isopentenol	0.74	0.20	1.43	0.17
	Electricity	kWh/kg-isopentenol	0.08	0.03	0.14	0.02
	Ionic liquid	kg/kg-isopentenol	0.10	0.0002	0.81	0.13
	Sulfuric Acid	kg/kg-isopentenol	0.73	0.25	1.49	0.17
	Water	kg/kg-isopentenol	12.11	4.72	21.98	2.57
Hydrolysis and Bioconversion	Cooling water	kg/kg-isopentenol	214.65	55.12	595.35	60.77
	Steam 180°C	kg/kg-isopentenol	0.57	0.22	1.10	0.12
	Electricity	kWh/kg-isopentenol	5.90	1.56	18.45	1.85
	Corn liquor	kg/kg-isopentenol	0.12	0.04	0.21	0.03
	Diammonium phosphate	kg/kg-isopentenol	0.01	0.01	0.03	0.00
	Enzyme	kg/kg-isopentenol	0.07	0.01	0.10	0.01
	Water	kg/kg-isopentenol	13.03	5.05	24.43	2.83
	Air	kg/kg-isopentenol	218.79	49.17	670.15	86.66
Recovery and separation	Cooling water	kg/kg-isopentenol	1373.65	541.14	2473.26	285.99
	Steam 226°C	kg/kg-isopentenol	26.96	10.29	49.37	5.74
	Steam 180°C	kg/kg-isopentenol	0.93	0.64	1.29	0.10
	Electricity	kWh/kg-isopentenol	0.08	0.03	0.15	0.02
Wastewater treatment	Steam 180°C	kg/kg-isopentenol	0.26	0.07	0.43	0.05
	Electricity	kWh/kg-isopentenol	0.32	0.12	0.60	0.07
	Water	kg/kg-isopentenol	18.82	6.82	33.38	3.97
	Air	kg/kg-isopentenol	26.90	9.75	47.71	5.67
	WWT nutrients	kg/kg-isopentenol	0.01	0.00	0.01	0.00
Onsite energy generation	Cooling water	kg/kg-isopentenol	665.42	239.33	1112.43	135.25
	Electricity	kWh/kg-isopentenol	0.36	0.13	0.60	0.07
	Natural gas	kg/kg-isopentenol	1.86	0.68	3.30	0.39
	Water	kg/kg-isopentenol	73.54	27.31	133.69	15.87
	Air	kg/kg-isopentenol	329.27	119.32	584.08	69.44

Note: *μ: baseline (average) value; a: minimum value; b: maximum value; and σ: standard deviation. 'WWT' refers to wastewater treatment*

S2. Capital and operating costs for isopentenol production system

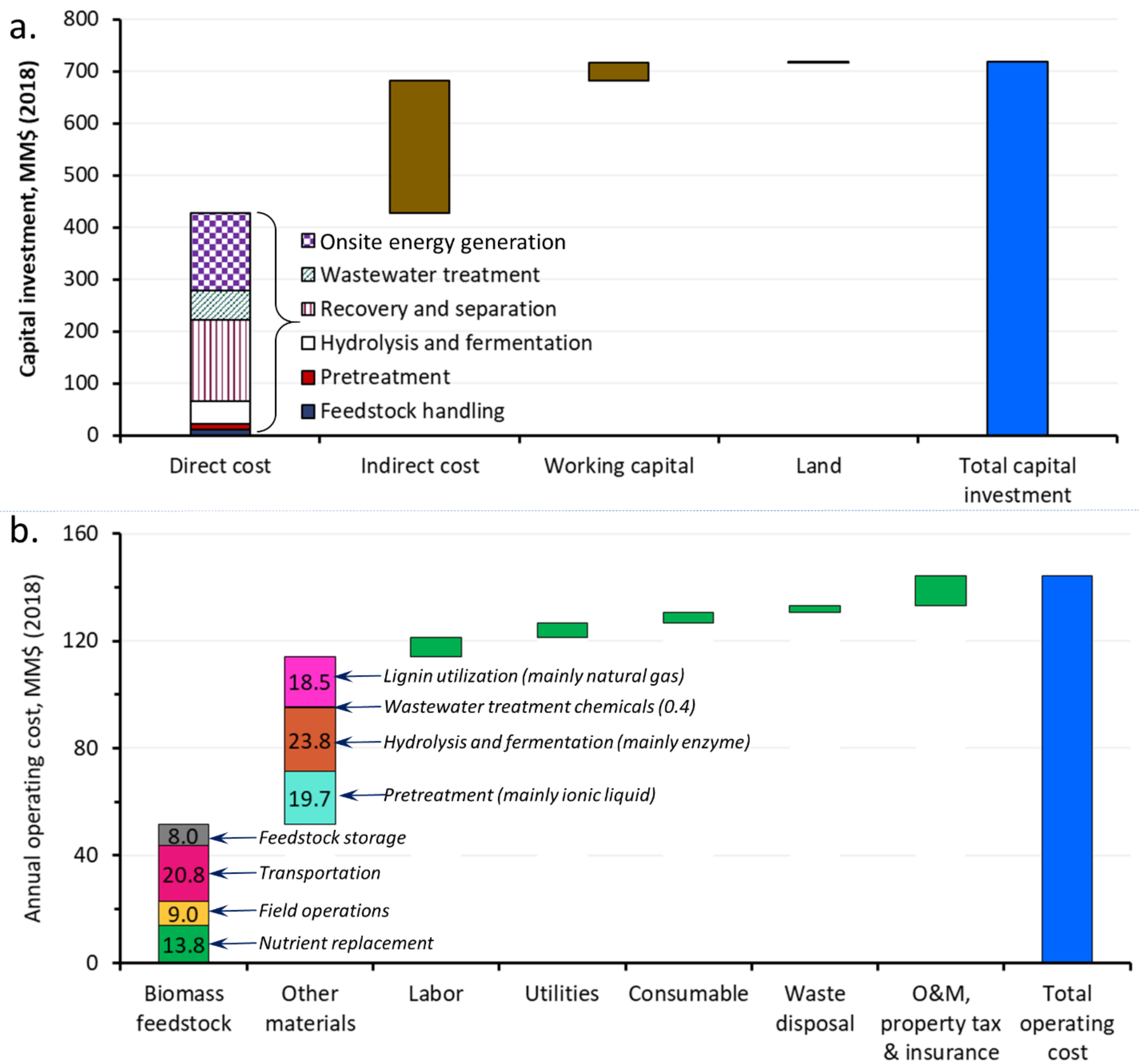


Figure S1. Capital investment (a) and annual operating cost (b) for isopentenol production system. The biorefinery utilizes 2000 dry metric ton of biomass sorghum per day and operates 330 days per year and 24 hours per day.

S3. Contributions of capital and operating costs to isopentenol selling price

Figure S2 indicates the contributions of major capital and operating expenses to overall minimum selling price of isopentenol in the baseline scenario (assuming 50% of theoretical yield). The detailed capital and operating costs are provided in the Figure S1. The total capital investment equates to $10/L of production capacity ($37.8/gal), which is 5.3 times greater than the dilute-acid-based cellulosic ethanol production facility studied by NREL,[35] due to both the difference in bioconversion route/yield and pretreatment process. Recovery and separation of the IL and isopentenol (including capital-intensive pervaporation[52]), along with the combined heat and power (boiler and steam turbine[35]) section, are the major contributors to direct fixed capital cost. Improved, lower-cost pervaporation systems or alternative IL recovery strategies could reduce the direct capital cost associated with recovery and separation. The direct fixed capital cost accounts for 59.4% of the total fixed capital. Indirect costs (engineering, construction, and overheads) account for 35.6% of the total capital investment (Figures S1 and S2).

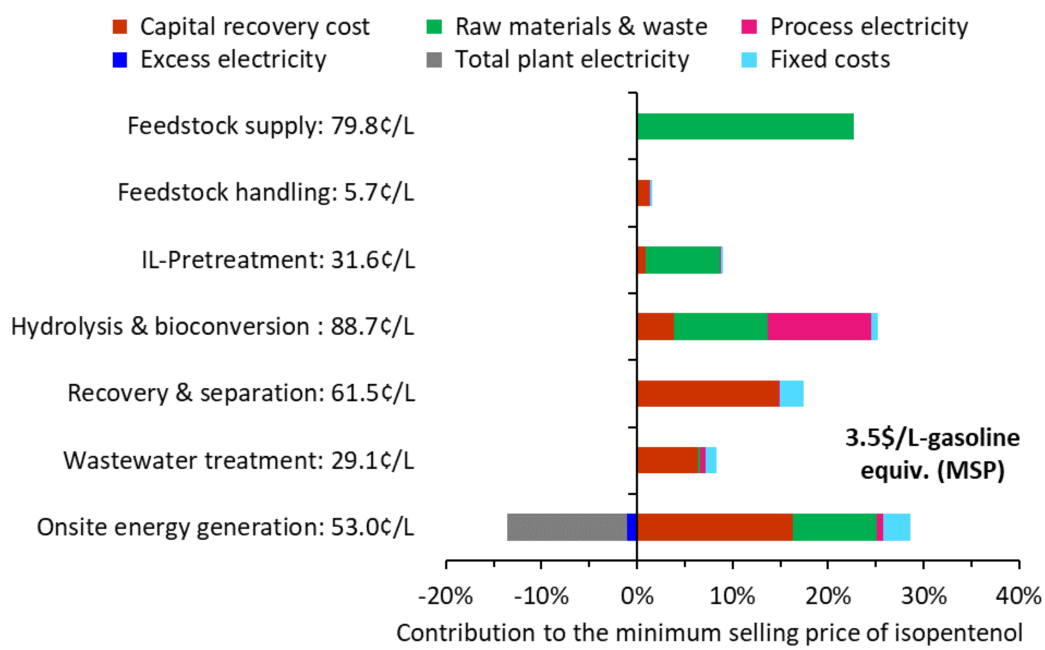


Figure S2. Baseline scenario costs for each stage of isopentenol production system, including capital and operating costs normalized on a per-liter basis.

Biomass feedstock supply is the single largest contributor to operating cost (35.7%), and other material inputs comprise another 43.3% (Figure S1). The major contributors to the feedstock supply cost are transportation and on-field nutrient inputs (Figure S1). Similarly, enzymes, the IL, and natural gas are major contributors to annual operating cost (Figures S1 and S2). Increasing the IL recovery rate and decreasing the enzyme loading can reduce the required makeup IL and enzymes, respectively, thus lowering operating costs. Additionally, switching from aerobic to a micro-aerobic process can eliminate the natural gas input (because lignin and biogas are sufficient fuel sources to provide the required electricity and process steam in the microaerobic case). Others, including labor, utilities, consumables, and overheads, account for about 20% of the total operating cost (Figures S1 and S2).

S4. Single point sensitivity analysis

S4.1. Minimum selling price

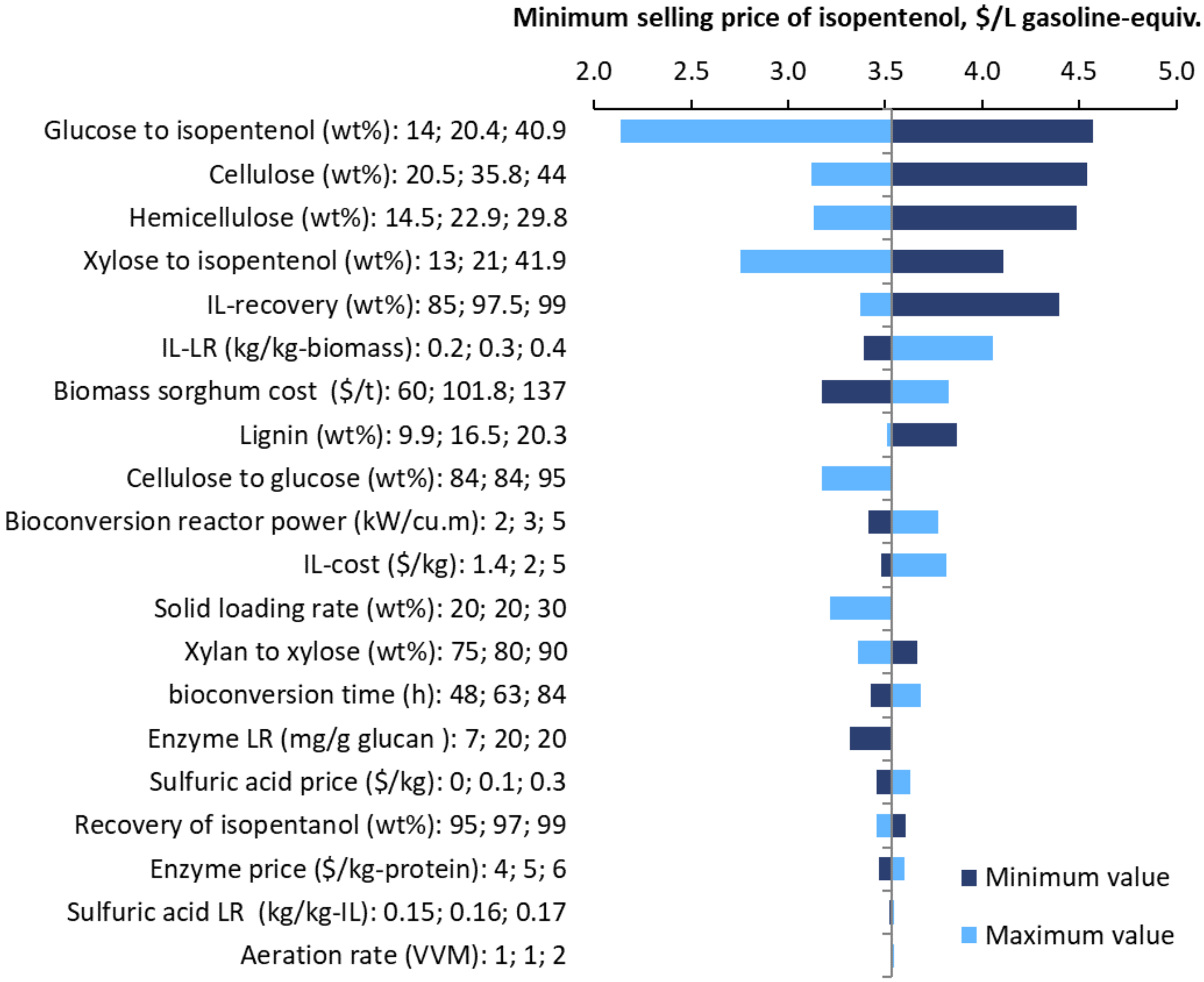


Figure S3. Most influential input parameters to the selling price of isopentenol

S4.2. GHG emissions

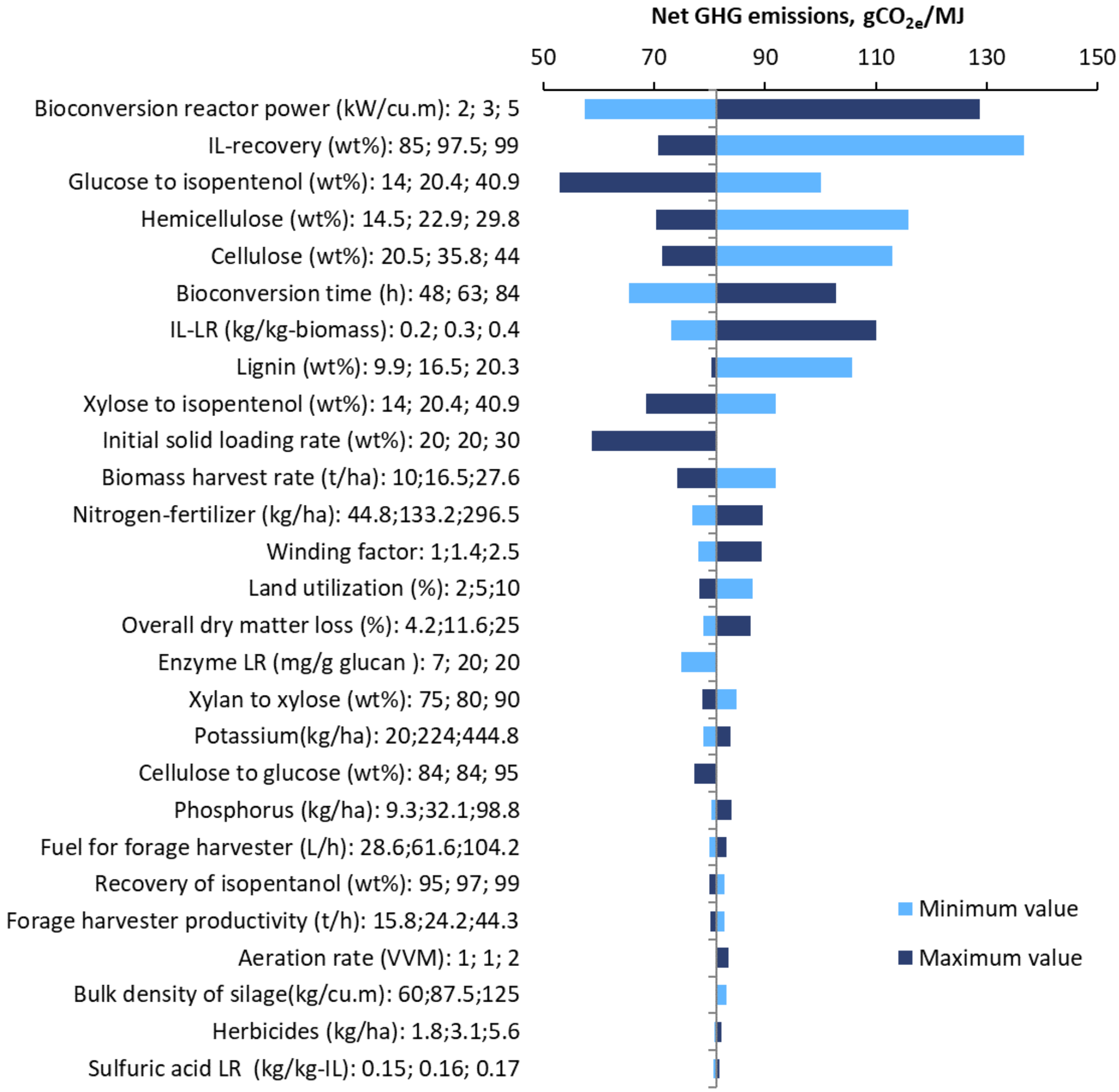


Figure S4. Most influential input parameters to GHG emissions associated with renewable isopentenol production

S4.3. Water consumption

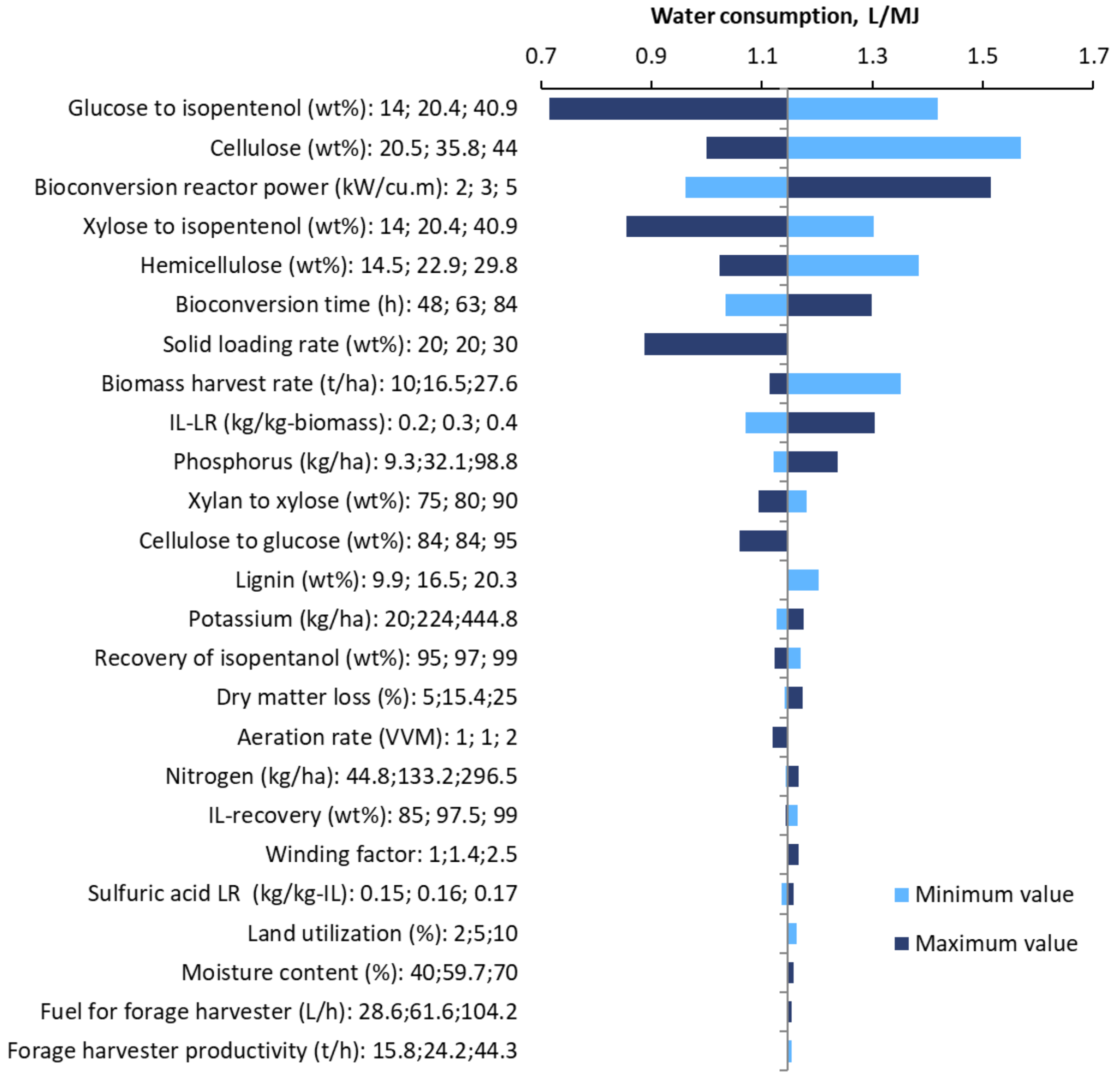


Figure S5. Most influential input parameters to water consumption for isopentenol production chain

S4.4. Water withdrawal

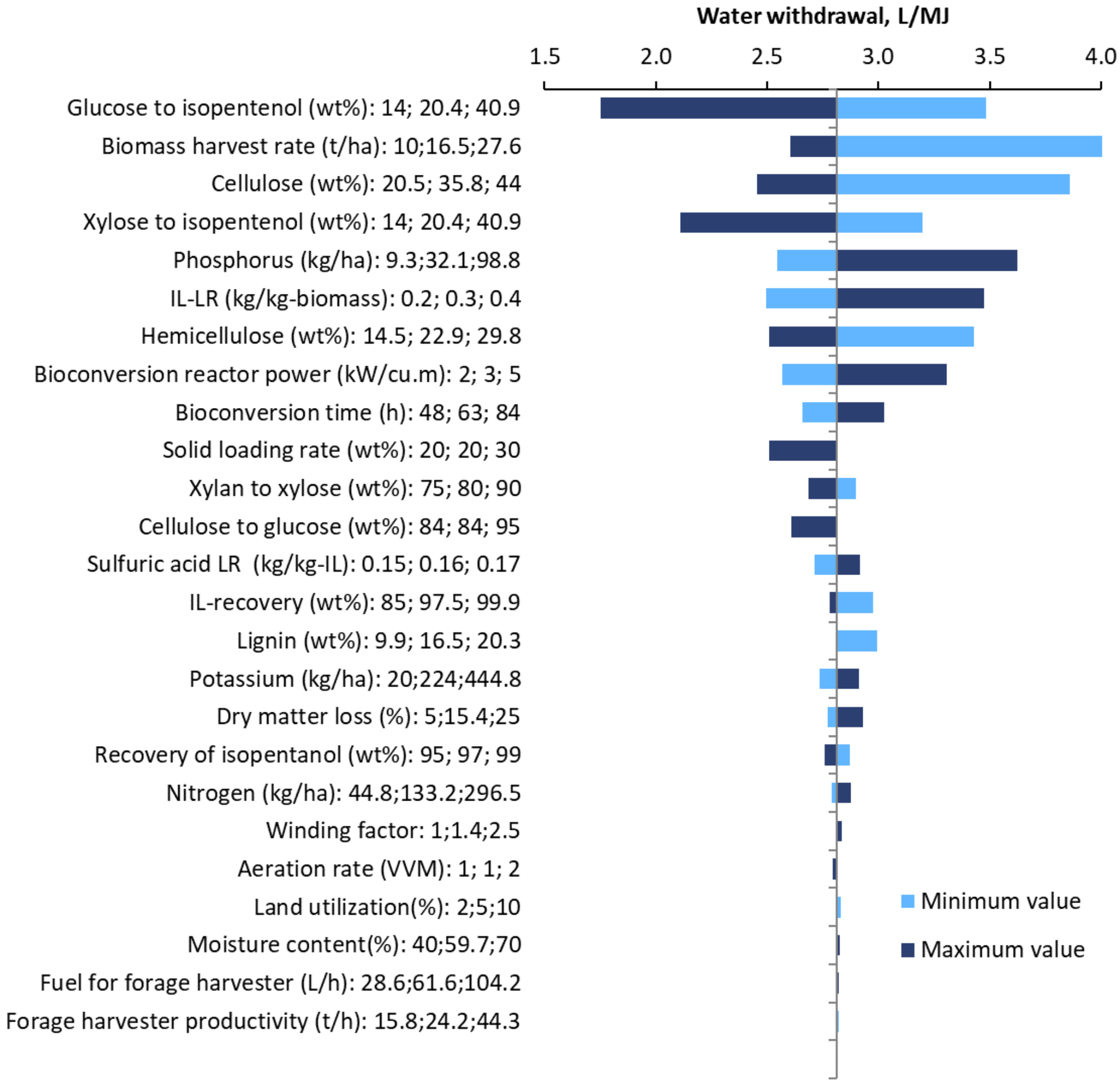
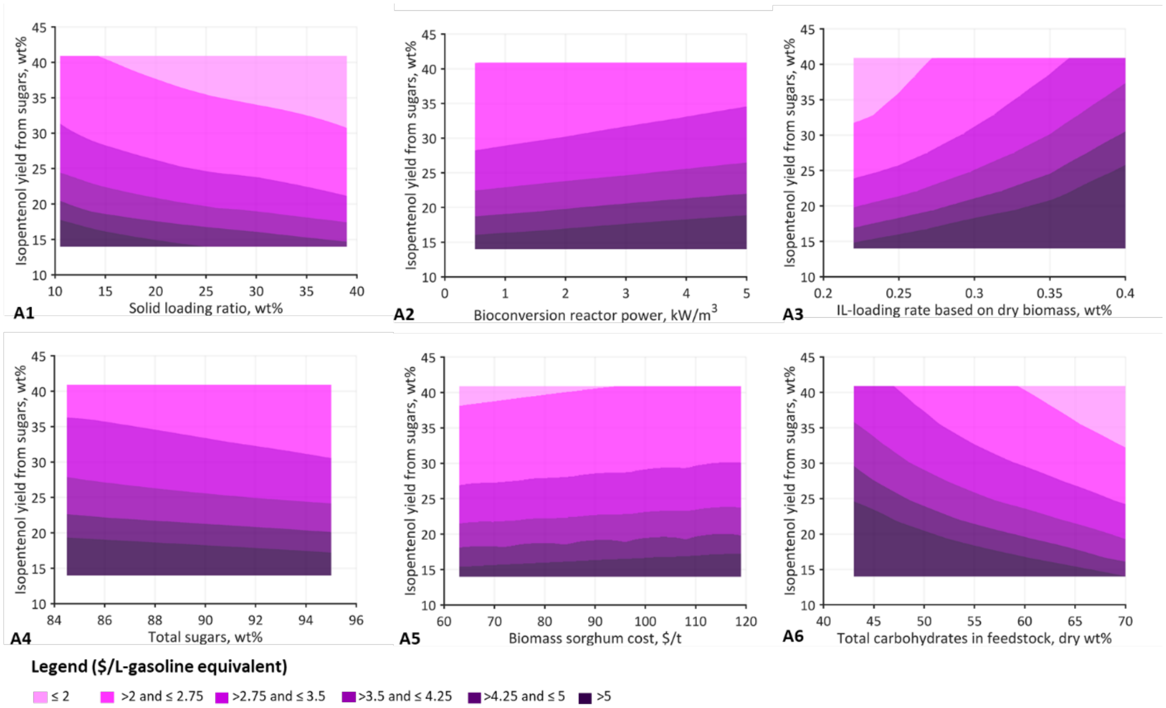


Figure S6. Most influential input parameters to water withdrawal for isopentenol production chain

S5. Selected most influential parameters to minimum selling price and GHG emissions: two-point sensitivity analysis

a. Minimum selling price



b. GHG emissions

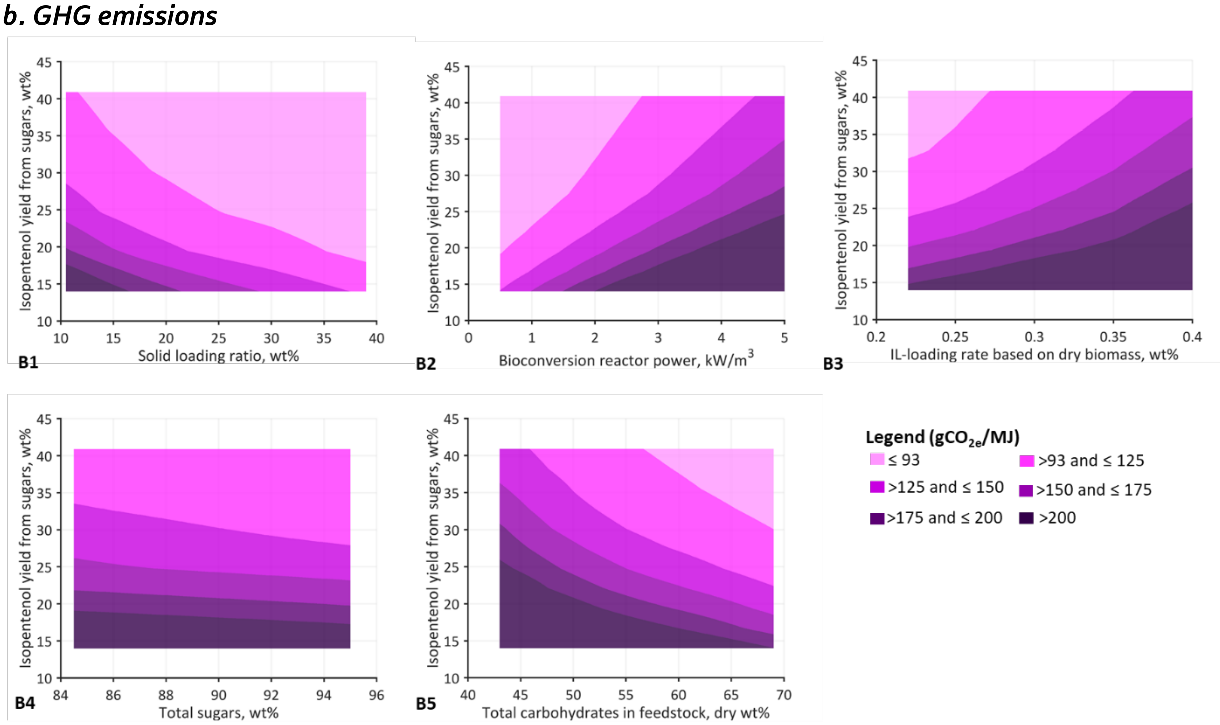
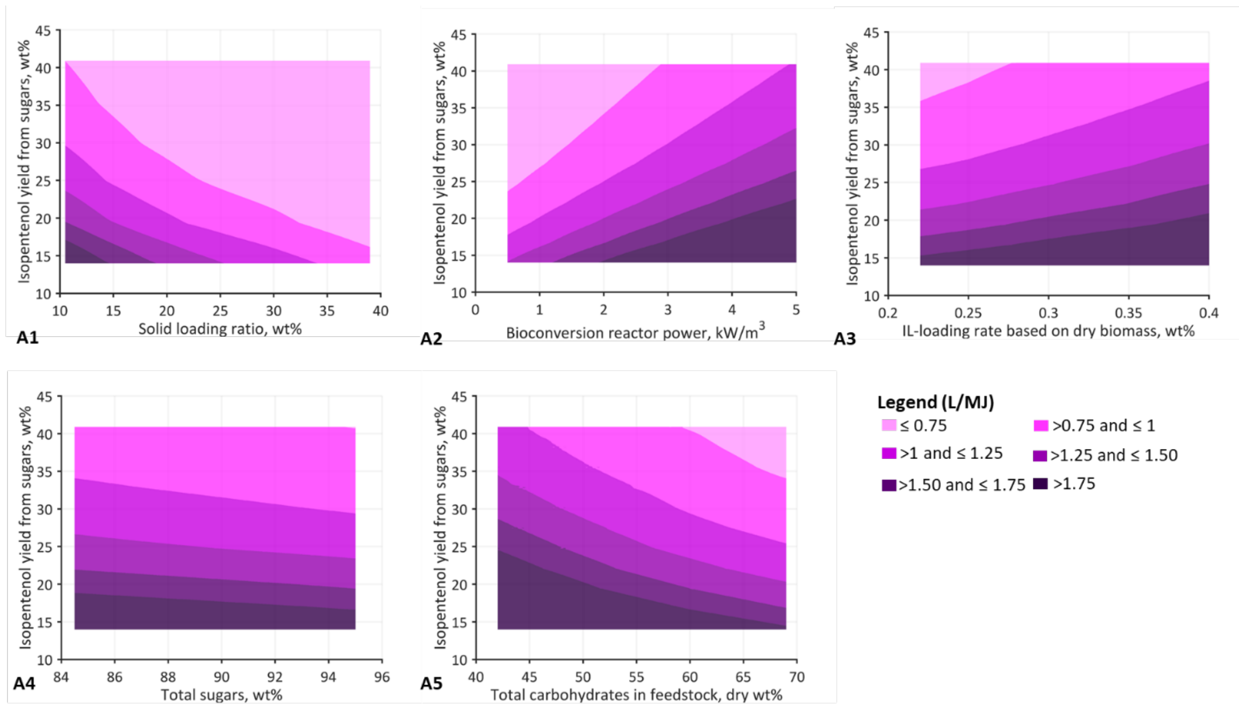


Figure S7. Heat maps with the selected influential parameters to the minimum selling price (A1 through A6) and GHG emissions (B1 through B5).

S6. Selected most influential parameters to water footprints

a. Water consumption



b. Water withdrawal

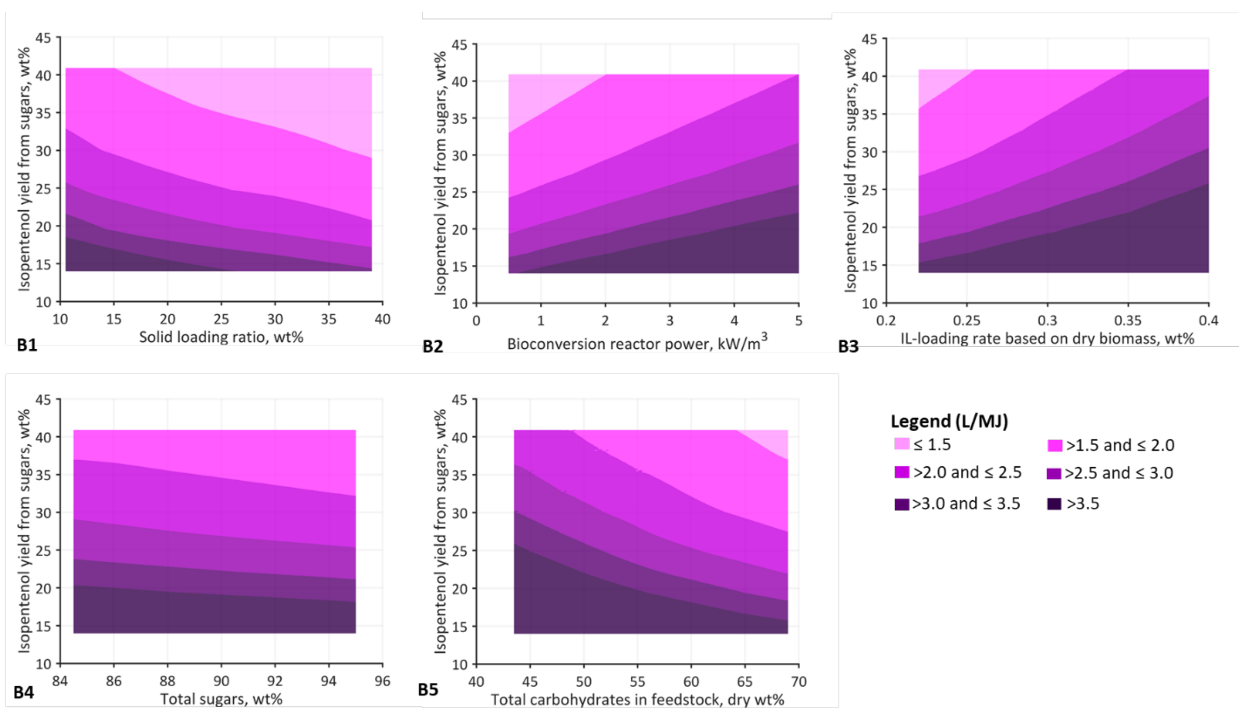


Figure S8. Heat maps with the selected influential parameters to water consumption (A1 trough A5) and water withdrawal (B1 through B5).

S7. Probability distributions of the minimum selling price, GHG emissions, water consumption and water withdrawals for each life-cycle stage of the entire isopentenol production chain

S7.1 Uncertainty associated with minimum selling price

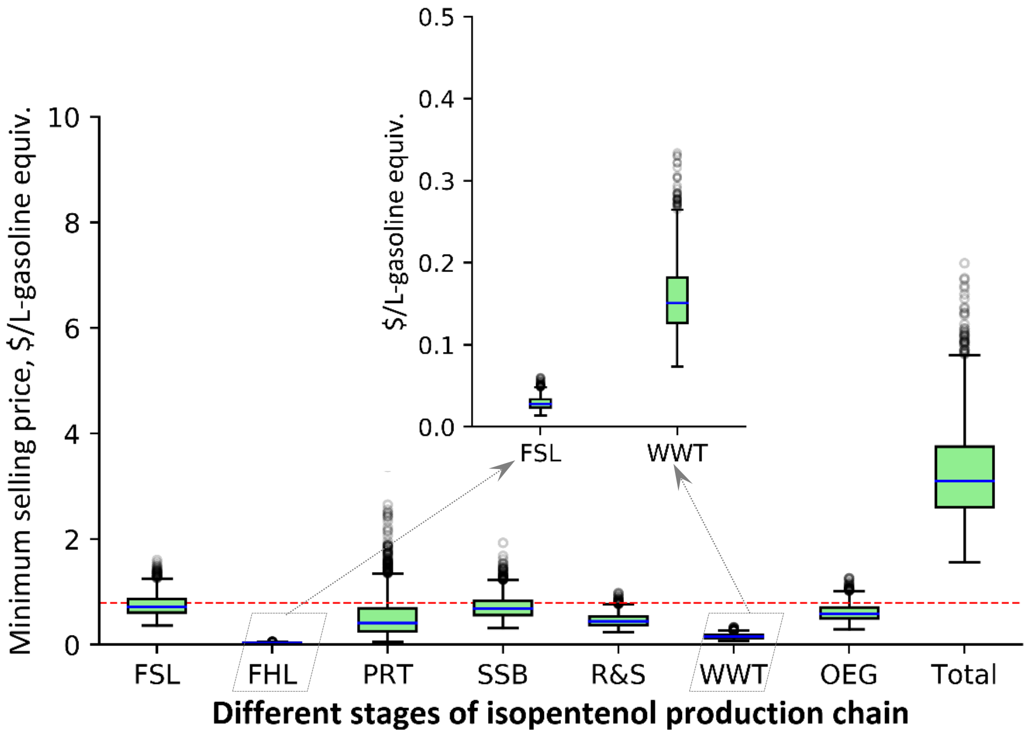


Figure S9. Uncertainty associated with the minimum selling price of isopentenol. In this figure, ***FSL:*** *Feedstock supply logistics;* ***FHL****: Feedstock handling;* ***PRT****: Pretreatment;* ***SSB****: Simultaneous saccharification and bioconversion;* ***R&S****: Recovery and separation;* ***WWT****: Wastewater treatment;* ***OEG:*** *Onsite energy generation. The horizontal dashed line (- - - - -) refers to the targeted selling price of $0.79/L-gasoline equivalent ($3/gge).*

S7.2 Uncertainty associated with GHG emissions

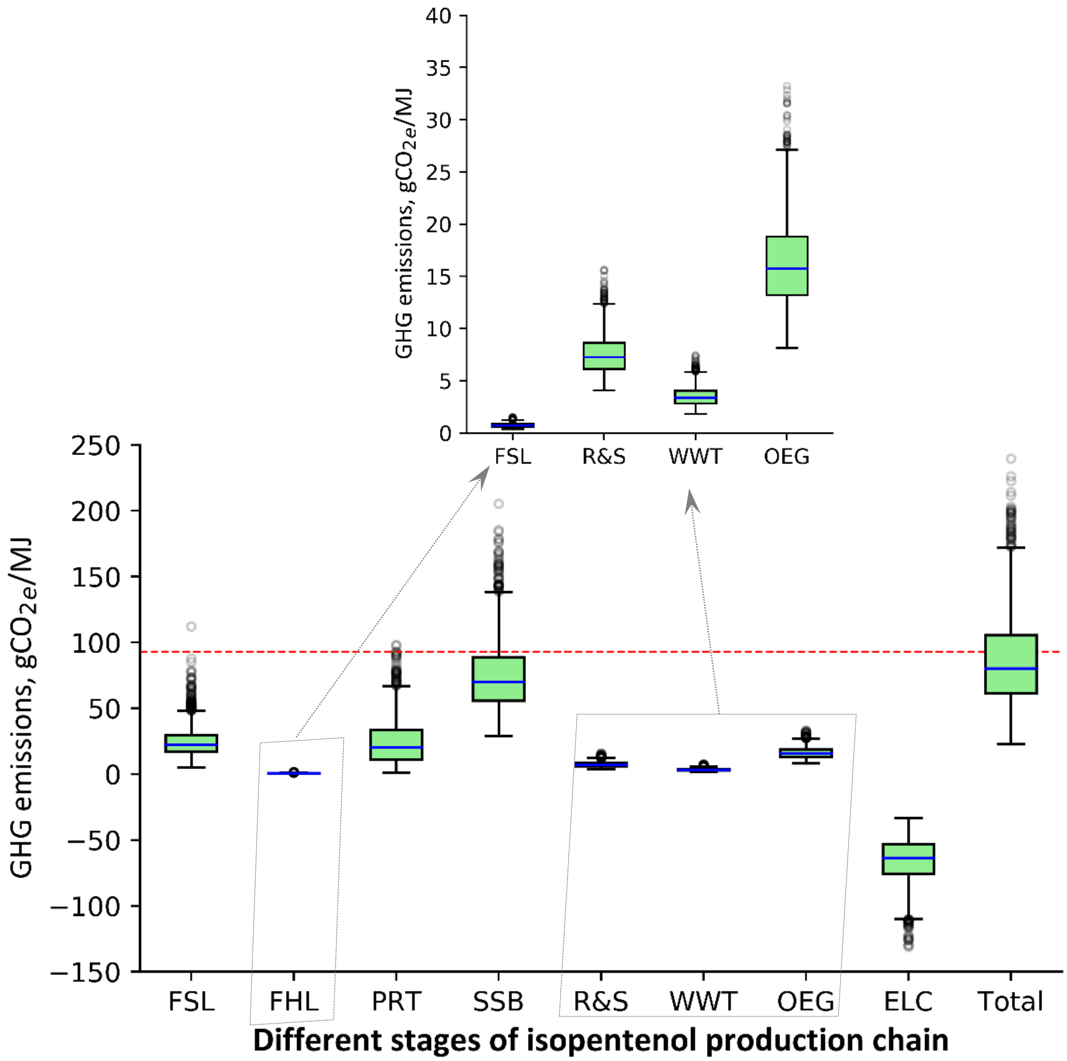


Figure S10. Uncertainty associated with GHG emissions. In this figure, ***FSL:*** *Feedstock supply logistics;* ***FHL****: Feedstock handling;* ***PRT****: Pretreatment;* ***SSB****: Simultaneous saccharification and bioconversion;* ***R&S****: Recovery and separation;* ***WWT****: Wastewater treatment;* ***OEG:*** *Onsite energy generation;* ***ELC****: onsite electricity credits; and* ***Total****: Net GHG emissions. The horizontal dashed line (- - - - -) refers to the GHG emissions from gasoline of 93 gCO_{2e}/MJ.*

S7.3 Uncertainty associated with water consumption

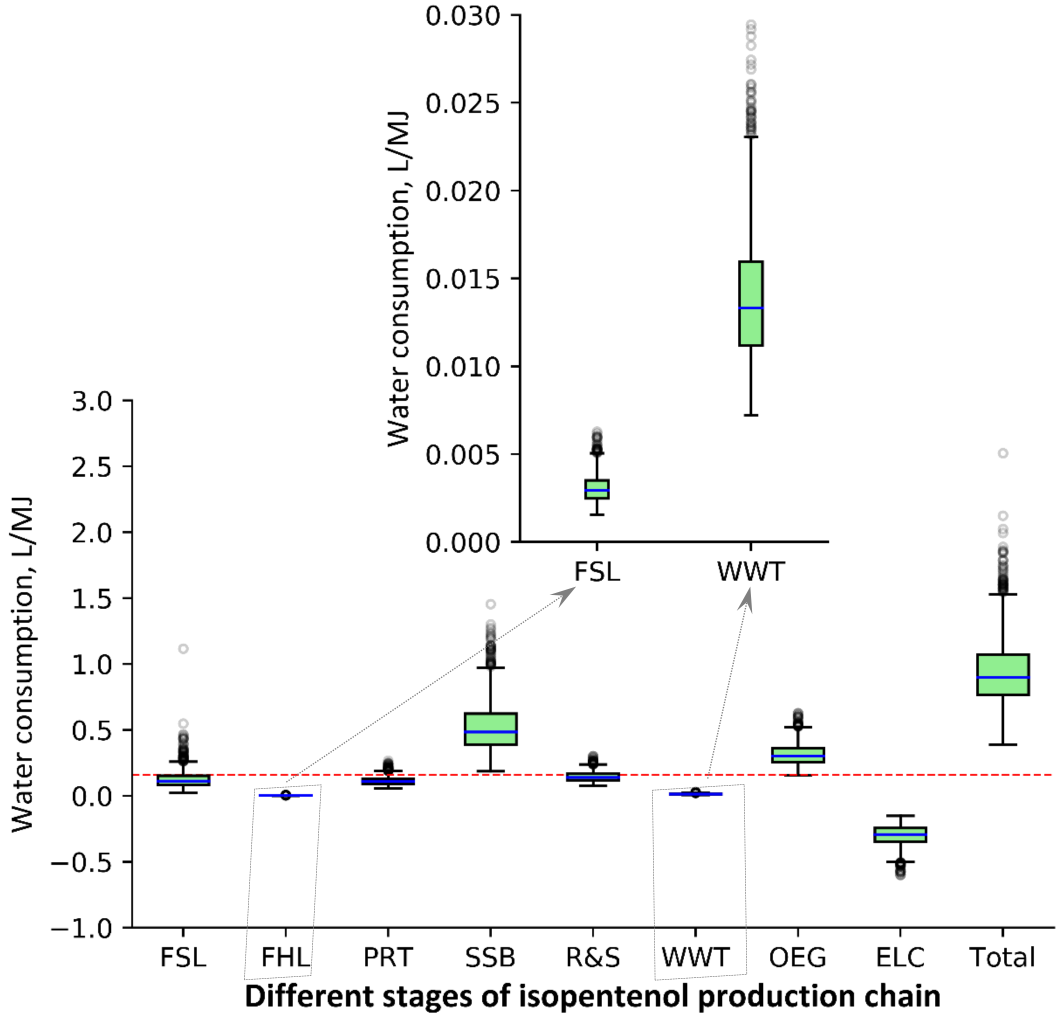


Figure S11. Uncertainty associated with water consumption. In this figure, ***FSL:*** *Feedstock supply logistics;* ***FHL****: Feedstock handling;* ***PRT****: Pretreatment;* ***SSB****: Simultaneous saccharification and bioconversion;* ***R&S****: Recovery and separation;* ***WWT****: Wastewater treatment;* ***OEG:*** *Onsite energy generation;* ***Direct****: Direct water consumption at biorefinery;* ***ELC****: onsite electricity credits; and* ***Total****: Net water consumption. The horizontal dashed line (- - - - -) refers to water consumption for gasoline of 0.16 L/MJ.*

S7.3 Uncertainty associated with water withdrawals

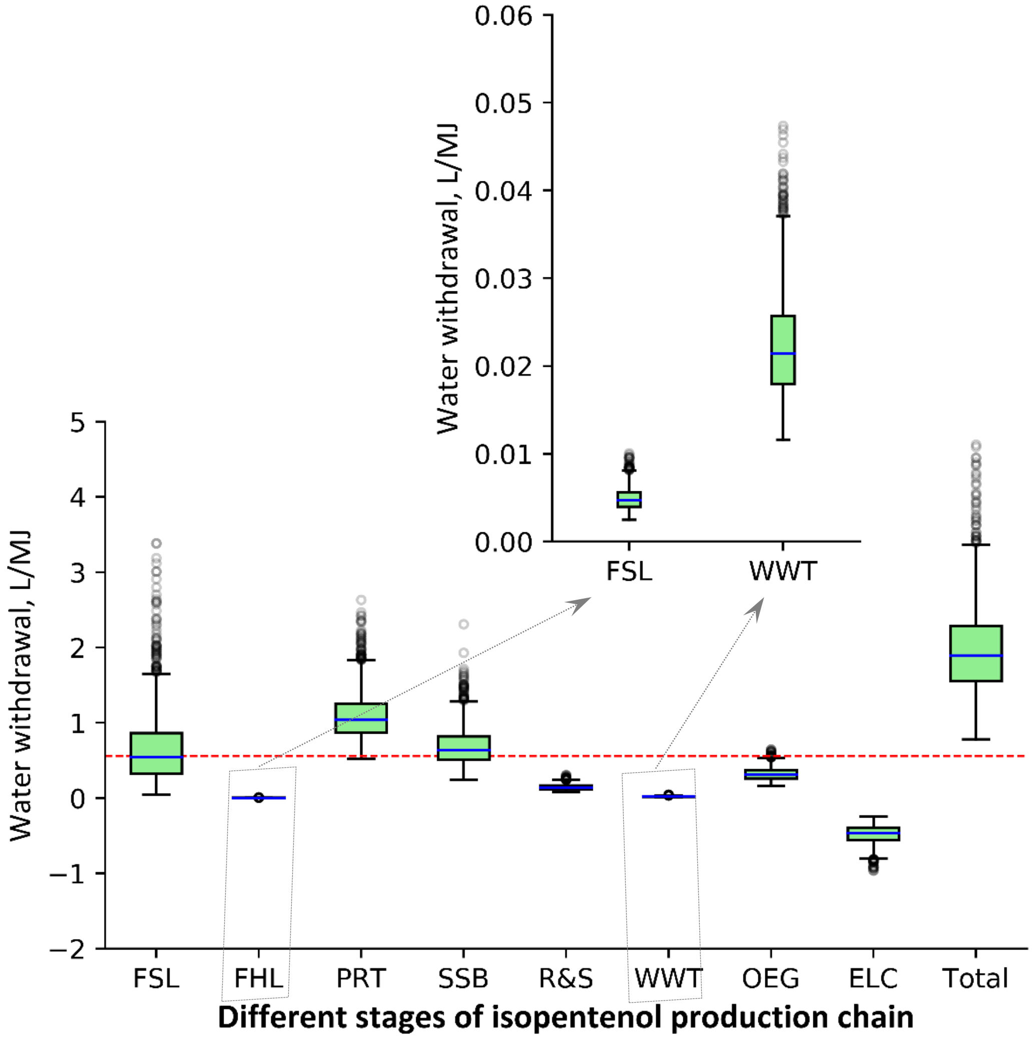


Figure S12. Uncertainty associated with water withdrawals. In this figure, ***FSL:*** *Feedstock supply logistics;* ***FHL****: Feedstock handling;* ***PRT****: Pretreatment;* ***SSB****: Simultaneous saccharification and bioconversion;* ***R&S****: Recovery and separation;* ***WWT****: Wastewater treatment;* ***OEG:*** *Onsite energy generation;* ***ELC****: onsite electricity credits; and* ***Total****: Net water withdrawal. The horizontal dashed line (- - - - -) refers to water withdrawal for gasoline of 0.56 L/MJ.*

S8. Optimal process conditions and isopentenol selling price

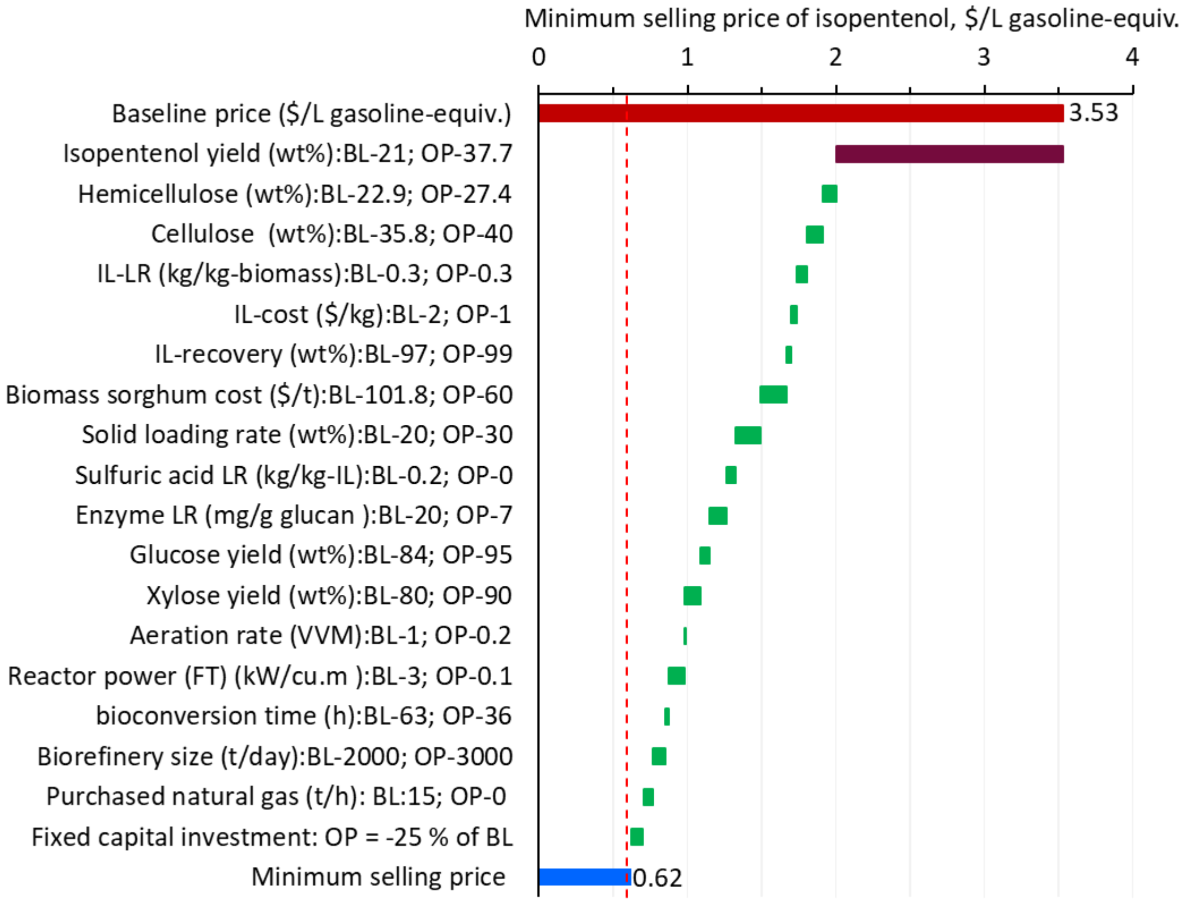


Figure S13. Pathways to achieve optimal selling price of isopentenol. In this figure 'BL' refers to the baseline and 'OP' refers to the optimal.

References

(1) Billa, E.; Koullas, D. P.; Monties, B.; Koukios, E. G. Structure and Composition of Sweet Sorghum Stalk Components. *Ind. Crops Prod.* **1997**, *6* (3), 297–302.

(2) Borden, D. Effect of Harvest Dates on Biomass Accumulation and Composition in Bioenergy Sorghum Effect of Harvest Dates on Biomass Accumulation and Composition in Bioenergy Sorghum. MS Thesis, Texas A & M University, Texas, USA, **2011**; https://oaktrust.library.tamu.edu/handle/1969.1/ETD-TAMU-2011-12-10401 (accessed July 18, 2019).

(3) Langholtz, M. H.; Stokes, B. J.; Eaton, L. M. 2016 Billion-Ton Report: Advancing Domestic Resources for a Thriving Bioeconomy, Volume 1: Economic Availability of Feedstock. U.S. Department of Energy, *Washington, DC*, **2016**; https://www.srs.fs.usda.gov/pubs/books/2016/book_2016_abt_001.pdf (accessed July 18, 2019).

(4) Baral, N. R.; Quiroz-Arita, C.; Bradley, T. H. Uncertainties in Corn Stover Feedstock Supply Logistics Cost and Life-Cycle Greenhouse Gas Emissions for Butanol Production. *Appl. Energy* **2017**, 208, 1343-1356.

(5) Roni, M. S.; Thompson, D.; Hartley, D.; Searcy, E.; Nguyen, Q. Optimal Blending Management of Biomass Resources Used for Biochemical Conversion. *Biofuels Bioprod. Biorefin.* **2018**, 12(4), 624-648.

(6) An, H.; Searcy, S. W. Economic and Energy Evaluation of a Logistics System Based on Biomass Modules. *Biomass Bioenergy* **2012**, *46*, 190–202.

(7) Turhollow, A. The Economics of Energy Crop Production. *Biomass Bioenergy* **1994**, *6* (3), 229–241.

(8) U.S. Department of Agriculture. Usual Planting and Harvesting Dates for U.S. Field Crops. U.S. Department of Agriculture, *Washington, DC*, **1997;** https://swat.tamu.edu/media/90113/crops-typicalplanting-harvestingdates-by-states.pdf (accessed July 18, 2019).

(9) Thompson, J. L.; Tyner, W. E. Corn Stover for Bioenergy Production: Cost Estimates and Farmer Supply Response. *Biomass Bioenergy* **2014**, *62*, 166–173.

(10) Hess, J. R.; Kenney, K. L.; Ovard, L. P.; Searcy, E. M; Wright, C. T. *Commodity-scale production of an infrastructure-compatible bulk solid from herbaceous lignocellulosic biomass.* Idaho National Laboratory (INL), Idaho Falls, Idaho, USA, **2009**; https://bioenergy.inl.gov/Reports/Uniform%20Format%20Bioenergy%20Feedstock.pdf (accessed July 18, 2019).

(11) Sokhansanj, S.; Kumar, A.; Turhollow, A. F. Development and Implementation of Integrated Biomass Supply Analysis and Logistics Model (IBSAL). *Biomass Bioenergy* **2006**, *30* (10), 838–847.

(12) Gutesa, S. Using GIS and Intelligent Transportation Tools for Biomass Supply Chain Modeling and Cost Assessment. MS Thesis, Iowa State University, Ames, Iowa, USA, **2013**; https://lib.dr.iastate.edu/cgi/viewcontent.cgi?article=4393&context=etd (accessed July 18, 2019).

(13) Williams, J.; Brammer, J.; Llewelyn, R.; Bergtold, J. An Economic Analysis of Harvesting Biomass from Sorghums and Corn. *J. ASFMRA* **2016**, 1–28; 10.2307/90016042.

(14) Rooney, W. L.; Blumenthal, J.; Bean, B.; Mullet, J. E. Designing Sorghum as a Dedicated Bioenergy Feedstock. *Biofuels Bioprod. Biorefin.* **2007**, *1* (2), 147–157.

(15) Linton, J. A.; Miller, J. C.; Little, R. D.; Petrolia, D. R.; Coble, K. H. Economic Feasibility of Producing Sweet Sorghum as an Ethanol Feedstock in the Southeastern United States. *Biomass bioenergy* **2011**, *35* (7), 3050–3057.

(16) Zegada-Lizarazu, W.; Monti, A. Are We Ready to Cultivate Sweet Sorghum as a Bioenergy Feedstock? A Review on Field Management Practices. *Biomass Bioenergy* **2012**, *40*, 1–12.

(17) Hoskinson, R. L.; Karlen, D. L.; Birrell, S. J.; Radtke, C. W.; Wilhelm, W. W. Engineering, Nutrient Removal, and Feedstock Conversion Evaluations of Four Corn Stover Harvest Scenarios. *Biomass Bioenergy* **2007**, *31* (2), 126–136.

(18) Johnson, J. M. F.; Wilhelm, W. W.; Karlen, D. L.; Archer, D. W.; Wienhold, B.; Lightle, D. T.; Laird, D.; Baker, J.; Ochsner, T. E.; Novak, J. M. Nutrient Removal as a Function of Corn Stover Cutting Height and Cob Harvest. *BioEnergy Res.* **2010**, *3* (4), 342–352.

(19) Kaliyan, N.; Morey, R. V.; Tiffany, D. G. Economic and Environmental Analysis for Corn Stover and Switchgrass Supply Logistics. *BioEnergy Res.* **2015**, *8* (3), 1433–1448.

(20) Morey, R. V.; Kaliyan, N.; Tiffany, D. G.; Schmidt, D. R. A Corn Stover Supply Logistics System. *Appl. Eng. Agric.* **2010**, *26* (3), 455–461.

(21) Tao, L.; Tan, E. C. D.; McCormick, R.; Zhang, M.; Aden, A.; He, X.; Zigler, B. T. Techno-economic Analysis and Life-cycle Assessment of Cellulosic Isobutanol and Comparison with Cellulosic Ethanol and N-butanol. *Biofuels Bioprod. Biorefin.* **2014**, *8* (1), 30–48.

(22) Bennett, A. S.; Anex, R. P. Farm-Gate Production Costs of Sweet Sorghum as a Bioethanol Feedstock. *Trans. ASABE* **2008**, *51* (2), 603–613.

(23) Amosson, S.; Girase, J.; Bean, B.; Rooney, W.; Becker, J. Economic Analysis of Biomass Sorghum for Biofuels Production in the Texas High Plains. Texas A&M AgriLife Research and Extension Center, Amarillo, Texas, USA, **2011**; http://amarillo.tamu.edu/files/2011/05/Biomass-Sorghum.pdf (accessed July 18, 2019).

(24) Bowling, R. G.; McKinley, T. L.; Rawls, E. L. Tennessee Forage Budgets. University of Tennessee, Knoxville, TN, USA, **2006**, https://extension.tennessee.edu/publications/Documents/PB1658.pdf (accessed July 18, 2019).

(25) University of California. 2016 Sample Costs to Produce and Harvest. University of California Cooperative Extension Agriculture and Natural Resources, Agricultural Issues Center, CA, USA, **2016**, https://coststudyfiles.ucdavis.edu/uploads/cs_public/cb/2c/cb2c22b4-04b7-45fb-a29b-7a5babe95776/2016sorghumgrainsjvfinaldraftmar23.pdf (accessed July 18, 2019).

(26) Baral, N.R.; Putnam, D.; Dahlberg, J.; Scown, C.D. Biomass Sorghum Supply Systems for Advanced Biofuel Production. Genomic Sciences Program Annual Principal Investigator (PI) Meeting, U.S. Department of Energy, Washington, DC, 2019; https://genomicscience.energy.gov/pubs/2019abstracts/abstracts/Keasling_Baral.pdf (accessed April 15, 2019).

(27) Murray, S. C.; Rooney, W. L.; Mitchell, S. E.; Sharma, A.; Klein, P. E.; Mullet, J. E.; Kresovich, S. Genetic Improvement of Sorghum as a Biofuel Feedstock: II. QTL for Stem and Leaf Structural Carbohydrates. *Crop Sci.* **2008**, *48* (6), 2180-2193.

(28) Zhao, Y. L.; Dolat, A.; Steinberger, Y.; Wang, X.; Osman, A.; Xie, G. H. Biomass Yield and Changes in Chemical Composition of Sweet Sorghum Cultivars Grown for Biofuel. *F. Crop. Res.* **2009**, *111* (1), 55–64.

(29) Li, B.Z.; Balan, V.; Yuan, Y.J.; Dale, B. E. Process Optimization to Convert Forage and Sweet Sorghum Bagasse to Ethanol Based on Ammonia Fiber Expansion (AFEX) Pretreatment. *Bioresour. Technol.* **2010**, *101* (4), 1285–1292.

(30) Theerarattananoon, K.; Wu, X.; Staggenborg, S.; Propheter, J.; Madl, R.; Wang, D. Evaluation and Characterization of Sorghum Biomass as Feedstock for Sugar Production. *Trans. ASABE* **2010**, *53* (2), 509–525.

(31) Wu, L.; Arakane, M.; Ike, M.; Wada, M.; Takai, T.; Gau, M.; Tokuyasu, K. Low Temperature Alkali Pretreatment for Improving Enzymatic Digestibility of Sweet Sorghum Bagasse for Ethanol Production. *Bioresour. Technol.* **2011**, *102* (7), 4793–4799.

(32) Corredor, D. Y.; Salazar, J. M.; Hohn, K. L.; Bean, S.; Bean, B.; Wang, D. Evaluation and Characterization of Forage Sorghum as Feedstock for Fermentable Sugar Production. *Appl. Biochem. Biotechnol.* **2009**, *158* (1), 164-179.

(33) Koradiya, M.; Duggirala, S.; Tipre, D.; Dave, S. Pretreatment Optimization of Sorghum Pioneer Biomass for Bioethanol Production and Its Scale-Up. *Bioresour. Technol.* **2016**, *199*, 142–147.

(34) Qureshi, N.; Liu, S.; Hughes, S.; Palmquist, D.; Dien, B.; Saha, B. Cellulosic Butanol (ABE) Biofuel Production from Sweet Sorghum Bagasse (SSB): Impact of Hot Water Pretreatment and Solid Loadings on Fermentation Employing Clostridium Beijerinckii P260. *BioEnergy Res.* **2016**, *9* (4), 1167–1179.

(35) Humbird, D.; Davis, R.; Tao, L.; Kinchin, C.; Hsu, D.; Aden, A.; Schoen, P.; Lukas, J.; Olthof, B.; Worley, M. *Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol: Dilute-Acid Pretreatment and Enzymatic Hydrolysis of*

Corn Stover; National Renewable Energy Laboratory (NREL), Golden, CO., 2011.

(36) Xu, F.; Sun, J.; Konda, N. M.; Shi, J.; Dutta, T.; Scown, C. D.; Simmons, B. A.; Singh, S. Transforming Biomass Conversion with Ionic Liquids: Process Intensification and the Development of a High-Gravity, One-Pot Process for the Production of Cellulosic Ethanol. *Energy Environ. Sci.* **2016**, *9* (3), 1042–1049.

(37) Sun, J.; Konda, N. M.; Parthasarathi, R.; Dutta, T.; Valiev, M.; Xu, F.; Simmons, B. A.; Singh, S. One-Pot Integrated Biofuel Production Using Low-Cost Biocompatible Protic Ionic Liquids. *Green Chem.* **2017**, *19* (13), 3152–3163.

(38) Neupane, B.; Konda, N. M.; Singh, S.; Simmons, B. A.; Scown, C. D. Life-Cycle Greenhouse Gas and Water Intensity of Cellulosic Biofuel Production Using Cholinium Lysinate Ionic Liquid Pretreatment. *ACS Sustain. Chem. Eng.* **2017**, *5* (11), 10176–10185.

(39) Aden, A.; Ruth, M.; Ibsen, K.; Jechura, J.; Neeves, K.; Sheehan, J.; Wallace, B.; Montague, L.; Slayton, A.; Lukas, J. *Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehydrolysis and Enzymatic Hydrolysis for Corn Stover*; National Renewable Energy Lab., Golden, CO.(US), 2002.

(40) Davis, R.; Tao, L.; Tan, E. C. D.; Biddy, M. J.; Beckham, G. T.; Scarlata, C.; Jacobson, J.; Cafferty, K.; Ross, J.; Lukas, J. *Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbons: Dilute-Acid and Enzymatic Deconstruction of Biomass to Sugars and Biological Conversion of Sugars to Hydrocarbons*; National Renewable Energy Laboratory (NREL), Golden, CO., 2013.

(41) Hiremath, A.; Kannabiran, M.; Rangaswamy, V. 1, 3-Propanediol Production from Crude Glycerol from Jatropha Biodiesel Process. *N. Biotechnol.* **2011**, *28* (1), 19–23.

(42) Chen, X.; Zhang, D.-J.; Qi, W.-T.; Gao, S.-J.; Xiu, Z.-L.; Xu, P. Microbial Fed-Batch Production of 1, 3-Propanediol by Klebsiella Pneumoniae under Micro-Aerobic Conditions. *Appl. Microbiol. Biotechnol.* **2003**, *63* (2), 143–146.

(43) Mendez-Perez, D.; Alonso-Gutierrez, J.; Hu, Q.; Molinas, M.; Baidoo, E. E. K.; Wang, G.; Chan, L. J. G.; Adams, P. D.; Petzold, C. J.; Keasling, J. D.; Lee, T.S. Production of Jet Fuel Precursor Monoterpenoids from Engineered Escherichia Coli. *Biotechnol. Bioeng.* **2017**, 114(8), 1703-1712.

(44) Fernández-Sandoval, M. T.; Galíndez-Mayer, J.; Moss-Acosta, C. L.; Gosset, G.; Martinez, A. Volumetric Oxygen Transfer Coefficient as a Means of Improving Volumetric Ethanol Productivity and a Criterion for Scaling up Ethanol Production with Escherichia Coli. *J. Chem. Technol. Biotechnol.* **2017**, *92* (5), 981–989.

(45) Huang, Y.; Li, Z.; Shimizu, K.; Ye, Q. Co-Production of 3-Hydroxypropionic Acid and 1, 3-Propanediol by Klebseilla Pneumoniae Expressing AldH under Microaerobic Conditions. *Bioresour. Technol.* **2013**, *128*, 505–512.

(46) Meyer, H.; Minas, W.; Schmidhalter, D. Industrial-Scale Fermentation. *Ind. Biotechnol.* **2016**, 1–53.

(47) Hannon, J.; Bakker, A.; Lynd, L.; Wyman, C. Comparing the Scale-up of Anaerobic and Aerobic Processes. In *Annual Meeting of the American Institute of Chemical Engineers: Salt Lake City*; 2007.

(48) Kang, A.; Meadows, C. W.; Canu, N.; Keasling, J. D.; Lee, T. S. High-Throughput Enzyme Screening Platform for the IPP-Bypass Mevalonate Pathway for Isopentenol Production. *Metab. Eng.* **2017**, *41*, 125–134.

(49) Kang, A.; Mendez-Perez, D.; Goh, E.-B.; Baidoo, E.; Wang, G.; Beller, H.; Keasling, J.; Lee, T.S. Optimization of the IPP-bypass mevalonate pathway and fed-batch fermentation for the production of isoprenol in *Escherichia coli*. 2019. Metabol Eng. Under Review.

(50) Kang, A.; George, K. W.; Wang, G.; Baidoo, E.; Keasling, J. D.; Lee, T. S. Isopentenyl Diphosphate (IPP)-Bypass Mevalonate Pathways for Isopentenol Production. *Metab. Eng.* **2016**, *34*, 25–35.

(51) Brandt-Talbot, A.; Gschwend, F. J. V; Fennell, P. S.; Lammens, T. M.; Tan, B.; Weale, J.; Hallett, J. P. An Economically Viable Ionic Liquid for the Fractionation of Lignocellulosic Biomass. *Green Chem.* **2017,** 19(13), 3078-3102.

(52) O'Brien, D. J.; Roth, L. H.; McAloon, A. J. Ethanol Production by Continuous Fermentation-Pervaporation: A Preliminary Economic Analysis. *J. Memb. Sci.* **2000**, *166* (1), 105–111.