Supplementary

S1. Process Specifications and Assumptions

S1.1. Feedstock composition

Composition of transgenic sugarcane-oilcane (Table S1) were consistent with previous literatures.[1, 2] Feedstock lipid content was varied from 5 to 15 % w w^{-1} in system analysis under uncertainties. The lipid content of oilcane increased at an expense of sucrose content, which was calculated by an energy balance approach from previous technoeconomic analyses using oilcane as feedstock.[1, 2]

Table S1. Chemical composition of transgenic sugarcane-oilcane at baseline assumption of lipid content (5 % w w^{-1}).

Components	Composition [% w w^{-1}]
Water	70.00
Glucose	0.91
Sucrose	10.35
Ash	0.60
Glucan (Cellulose)	7.12
Hemicellulose[a]	4.20
Lignin	3.81
Solids	1.50
Triolein[b]	1.20
Oleic acid[b]	0.15
Phosphatidylinositol[b]	0.15

[a] Hemicellulose fraction consists of 82.5%, 21.9%, 5.63% and 1.62 % w w^{-1} of xylan, acetate, arabinan, and galactan, respectively.
[b] Triolein, oleic acid, and phosphatidylinositol adds up to totally 5% w w^{-1} of vegetative lipid in dry oilcane.

S1.2. Hydrothermal pretreatment

Hydrothermal pretreatment of oilcane bagasse was operated at 210 °C for 5 min. The pretreatment conditions were optimized for oilcane bagasse to maximize the production of HMF and furfural without affecting yield of cellulosic sugars or degrading vegetative lipids.[3] Other specifications and designs of the pretreatment reactor system followed previous study.[2]

Pretreatment reactions and their conversion percentages (Table S2) were modified from Humbird et al based on bench-scale experimental data.[2-4]

Table S2. Hydrothermal pretreatment specifications.

	Baseline condition
Temperature [°C]	210
Reaction time [min]	5
Solids loading [% w w^{-1}]	50
Glucan to glucose conversion [% of glucan]	21.45
Glucan to HMF conversion [% of glucan]	14.40
Xylan to xylose conversion [% of xylan]	31.23
Xylan to furfural conversion [% of xylan]	51.10

S1.3. Nanofiltration systems

A unit operation for the nanofiltration system was modeled and designed using BioSTEAM. The nanofiltration system unit operation split chemical components of its input stream between two output streams (retentate and permeate) based on mass. Capital and operating costs of the unit were estimated based on previous literatures using membrane area and volumetric flow rate into the system.[5-7] Membrane purchase and replacement costs were calculated from the cost of a nanofiltration spiral-wound membrane (\$20.8 m^{-2}) and a membrane lifetime of 2.5 years in the baseline biorefinery.[5, 6] Costs of instruments and controls, tanks and frames, and miscellaneous facilities were scaled using membrane area.[5] Operating costs to clean and regenerate membrane were estimated based on volumetric flow rate into the nanofiltration system.[5] Expenses incurred by pumps were estimated individually using BioSTEAM's built-in methods.[8] Fractions of chemical components recovered in retentates of the 1st and 2nd nanofiltration systems (Table S3) were determined based on bench-scale experimental data.[3]

Table S3. Percentage of chemical components (% w w^{-1}) recovered in the retentate of the 1st and 2nd nanofiltration systems in the baseline oilcane biorefinery.

Chemicals	1st Nanofiltration system	2nd Nanofiltration system
HMF	40.72	47.55
Furfural	59.59	78.82
Glucose	98.39	100.00
Xylose	98.18	100.00
Arabinose	94.52	100.00
Acetic acid	84.28	77.54
Oligosaccharides	100.00	N/A[a]
Soluble lignin	100.00	N/A[a]

S1.4. Microbial lipid production

Pretreated biomass residues were enzymatically hydrolyzed by cellulase at 48 °C for 72 hr. Specifications and modeling of enzymatic saccharification were consistent with previous studies.[2] Enzymatic hydrolysis reactions were modified to obtain a glucan-to-glucose conversion of 93.47% based on bench-scale experimental data.[3] The enzymatic hydrolysate were combined with oilcane juice and concentrated retentate from the 1st nanofiltration system to produce microbial lipids using *R. toruloides* in aerated bioreactors. Designs, modelling and cost correlations of fermentation (Table S4) were consistent with Yoel et al.[9] The fermentation reactions of glucose and xylose included triolein production, cell growth and respiration. The batch time included loading, reaction, and cleaning time.

Table S4. Fermentation specifications in the baseline oilcane biorefinery.

	Baseline condition
Temperature [°C]	32
Batch time [hr]	92.4
Cleaning time [hr]	3
Maximum bioreactor volume [m^3]	500
Glucose to triolein yield [% maximum]	54.55
Xylose to triolein yield [% maximum]	54.55
Productivity (g L·hr^{-1})	0.31

Titer [g L^{-1}]	27.4

S1.5. Vegetative lipid recovery

Major fraction of vegetative lipids remained in the biomass residues after upstream processing (crushing, pretreatment and enzymatic hydrolysis). In the baseline biorefinery, 33.5% of vegetative lipids were obtained in juice, pretreatment liquor and hydrolysate and sent to wastewater treatment.[10] The 66.5% of vegetative lipids remaining in the biomass residues post-saccharification were extracted by hexane with a lipid extraction efficiency of 90%. A total of 60% of vegetative lipids in the oilcane stems were recovered and extracted to produce biodiesel.

S2. Capital and Operating Costs

Technoeconomic analysis (TEA) of the biorefinery was performed using method and parameters adopted by previous studies (Table S5).[1, 2] Raw material costs, labor cost, revenues and equipment costs are listed in Table S6 – S8.

Table S5. Main parameters of TEA for the baseline oilcane biorefinery.

Parameters	Value
Project lifetime [yr]	30
Annual operating days	330
Internal rate of return [%]	10
Construction duration [yr]	3
Depreciation schedule	MACRS 7-year
Income tax	21%

Table S6. Breakdown of variable operating cost and revenues for the baseline oilcane biorefinery.

	Input	Unit price [\$ MT^{-1}]	Costs [MM\$ yr^{-1}]	Reference
Raw materials	FGD lime	81.90	0.01	11, 12
	H3PO4	573.53	0.31	11, 12
	HCl	84.47	0.00	2, 12
	N2	779.37	0.11	13
	NaOH	390.00	0.00	14
	Boiler chemicals	5.36	0.00	15
	Catalyst	1489.70	0.01	2, 12
	Caustic	195.00	7.45	
	Cellulase	12.91	0.64	2, 12
	Cooling tower chemicals	2408.19	0.00	15
	Lime	8.35	0.01	11, 12
	Methanol	536.00	0.14	13
	Nanofiltration membrane	1.51E+11	1.38	6
	Oilcane	34.55	91.21	16
	Pure glycerine	1090.00	12.56	2, 12
Utilities	Propane [\$ kJ^{-1}]	0.00	0.55	8
	Electricity [\$ kWh^{-1}]	0.087	14.17	8
By-products and credits	Ash disposal	-31.80	-2.30	2
	Crude glycerol	202.93	5.60	2, 12
Variable operating cost (VOC)			125.23	/
Products	HMF	18020.67	229.43	17-19
	Biodiesel	1585.53	168.44	20
	Furfural	1898.38	18.91	12, 21

Table S7. Breakdown of fixed operating cost for the baseline oilcane biorefinery.

	Notes	Costs [MM\$ yr^{-1}]
Labor salary	-	2.50
Labor burden	90% of labor salary	2.25
Maintenance	3.0% of ISBL	10.20
Property insurance	0.7% of FCI	6.76
Fixed operating cost (FOC)		21.72

Table S8. Breakdown of capital costs for the baseline oilcane biorefinery.

	Notes	Costs [MM$]
ISBL installed equipment cost (ISBL)	-	340.07
OSBL installed equipment cost	-	204.34
Warehouse	4.0% of ISBL	13.60
Site development	9.0% of ISBL	30.61
Additional piping	4.5% of ISBL	15.30
Total direct cost (TDC)	-	603.92
Proratable costs	10.0% of TDC	60.39
Field expenses	10.0% of TDC	60.39
Construction	20.0% of TDC	120.78
Contingency	10.0% of TDC	60.39
Other indirect costs (start-up, permits, etc.)	10.0% of TDC	60.39
Total indirect cost	-	362.35
Fixed capital investment (FCI)	-	966.28
Working capital	5.0% of FCI	48.31
Total capital investment (TCI)	-	1014.59

S3. Life Cycle Assessment

Environmental impact of the biorefinery was estimated as one-hundred-year global warming potential (GWP_{100}) in the form of kg CO_2 eq. (carbon dioxide equivalent) by conducting a cradle-to-biorefinery-gate life cycle assessment (LCA). Life cycle inventory and allocation factors (energy and economic) are listed in Table S9 – 10.

Table S9. Life cycle inventory for the baseline oilcane biorefinery.

	Material	Flow [kg yr^{-1}]	Characterization factor [kg CO_2 eq. kg^{-1} input]
Input	FGD lime	1.34E+05	0.52
	H3PO4	5.37E+05	1.00
	HCl	2.81E+03	1.96
	NaOH	3.16E+02	2.01
	Boiler chemicals	4.37E+03	1.56
	Catalyst	7.92E+03	0.73
	Caustic	3.82E+07	1.01
	Cellulase	4.92E+07	0.40
	Cooling tower chemicals	7.44E-13	0.26
	Lime	1.07E+06	0.05
	Methanol	2.54E+05	0.45
	Nanofiltration membrane[a]	9.13E-03	2.54E+06
	Oilcane	2.64E+09	0.04
	Pure glycerine	1.15E+07	1.67
	Electricity [kWh yr^{-1}]	1.63E+08	0.39 [kg CO_2 eq. kWh^{-}

			1]
Output	HMF	1.27E+07	-
	Biodiesel	1.06E+08	-
	Furfural	9.96E+06	-
	Crude glycerol	2.76E+07	-

[a] The characterization factor for nanofiltration membrane is based on the production and maintenance for a thin-film composite membrane.[22, 23]

Table S10. Energy and economic allocation factors for the baseline oilcane biorefinery.

Allocation method	HMF	Biodiesel	Furfural	Crude glycerol
Energy	0.06	0.82	0.05	0.07
Economic	0.54	0.40	0.04	0.01

S4. Parameter distributions

Table S11. Distribution of parameters included in uncertainty analysis.

#	Parameter	Baseline	Shape	Lower	Upper	Reference
1	HMF retention in 1st nanofiltration [%]	40.72	Uniform	-50%	+0%	3
2	HMF retention in 2nd nanofiltration [%]	47.55	Uniform	-50%	+0%	3
3	Furfural retention in 1st nanofiltration [%]	59.59	Uniform	-50%	+0%	3
4	Furfural retention in 2nd nanofiltration [%]	78.82	Uniform	-25%	+25%	3
5	Nanofiltration membrane lifetime [yr]	2.50	Uniform	0.5	5	6
6	Nanofiltration membrane cost [$\$$ m^{-2}]	20.80	Uniform	-25%	+25%	6
7	Microbial lipid yield from glucose [% maximum]	54.55	Uniform	-25%	+25%	9, 24
8	Microbial lipid yield from xylose [% maximum]	54.55	Uniform	-25%	+25%	9, 24
9	Microbial lipid yield productivity (g L·hr^{-1})	0.31	Uniform	-25%	+25%	9, 24
10	Microbial lipid titer [g L^{-1}]	27.40	Uniform	-25%	+25%	9, 24
11	Feedstock lipid content [%]	5.00	Uniform	5	15	2
12	Vegetative lipid recovery after processing (pretreatment & saccharification) [%]	70.00	Uniform	-25%	+25%	10, 25
13	Oilcane price [$\$$ kg^{-1}]	3.46	Uniform	-25%	+25%	16
14	Furfural price [$\$$ kg^{-1}]	1.90	Uniform	-25%	+25%	21
15	HMF price [$\$$ kg^{-1}]	18.02	Uniform	-25%	+25%	17, 19
16	Biodiesel price [$\$$ kg^{-1}]	1.59	Uniform	-25%	+25%	20
17	Crude glycerol price [$\$$ kg^{-1}]	0.20	Uniform	-25%	+25%	2, 12
18	Caustic price [$\$$ kg^{-1}]	0.20	Uniform	-25%	+25%	14
19	Glycerine price [$\$$ kg^{-1}]	1.09	Uniform	-25%	+25%	26
20	Natural gas price [$\$$ kg^{-1}]	0.20	Uniform	-25%	+25%	27
21	Electricity price [$\$$ kWh^{-1}]	0.087	Uniform	-25%	+25%	28
22	Pretreatment reactor system cost[a] [MM$\$$]	19.67	Uniform	-25%	+25%	4

[a] Pretreatment reactor system cost is based on a system processing 92 MT hr^{-1} of biomass.[4]

S5. Monte Carlo Simulation Results

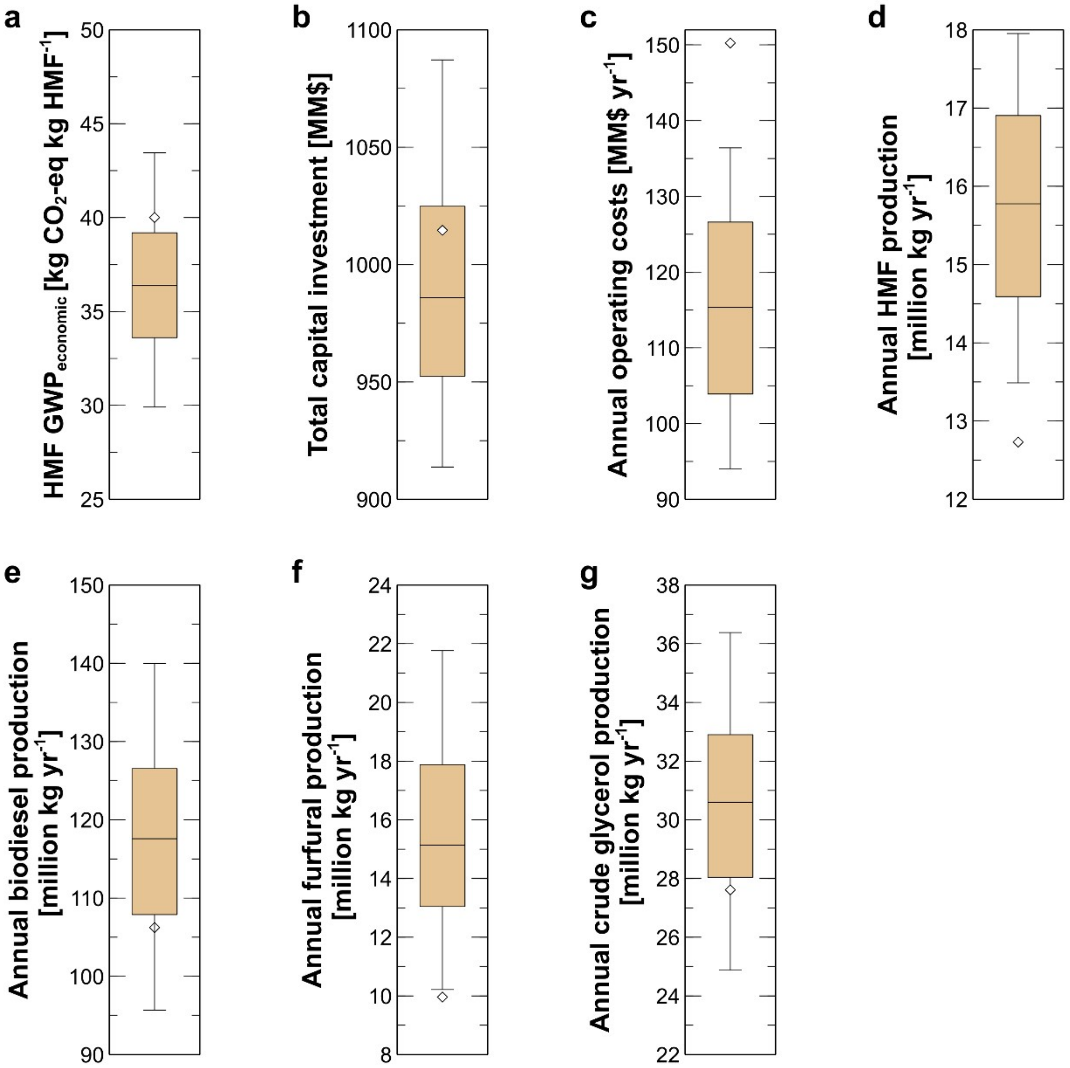

Figure S1. Box and whisker plots of a) economic-allocated GWP_{100} of HMF, b) TCI, c) AOC, annual production of d) HMF, e) biodiesel, and f) furfural, and g) crude glycerol. Whiskers, boxes, and middle line are 5th/95th, 25th/75th, and 50th percentiles, respectively, from the Monte Carlo simulation results. Diamond markers represent values from baseline biorefinery.

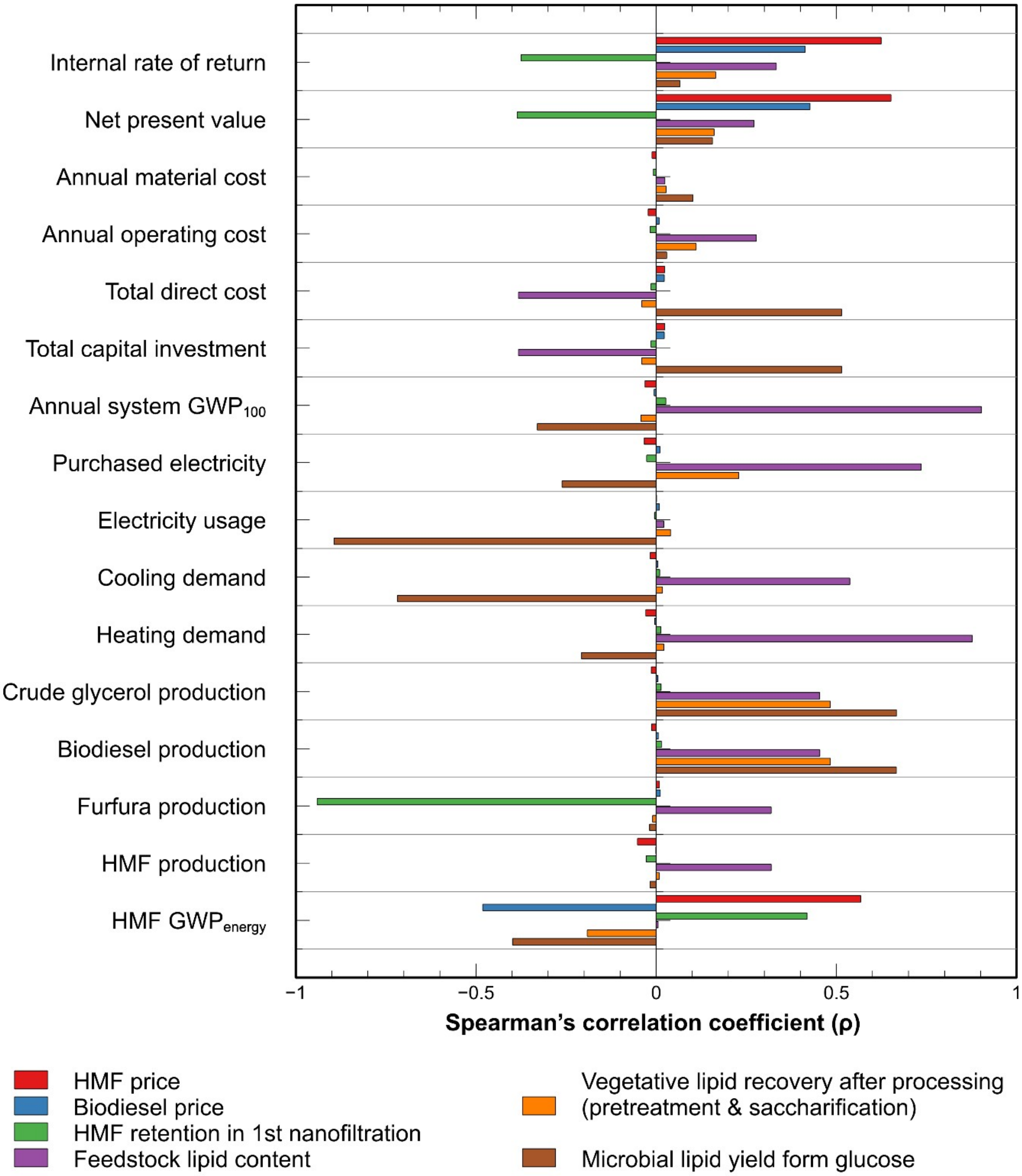

Figure S2. Spearman's ρ values between six parameters significantly affecting maximum feedstock purchasing price (MFPP) of feedstock and HMF GWP$_{100}$ using economic allocation, capital and operating costs, utility usage, annual production, and annual system GWP$_{100}$ of the biorefinery.

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