Production of sustainable and renewable biomass-derived monomer: conceptual process design and techno-economic analysis

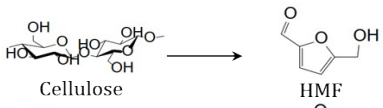
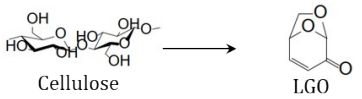
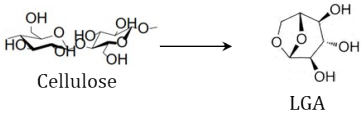
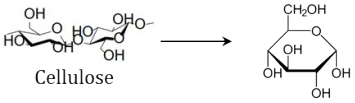
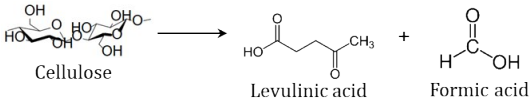
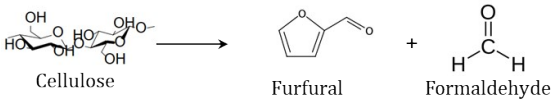
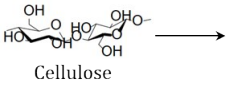
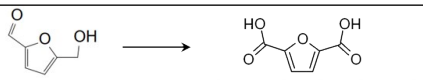
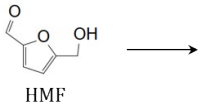
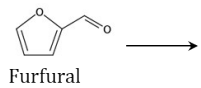
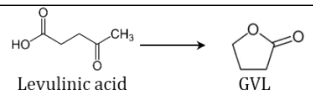
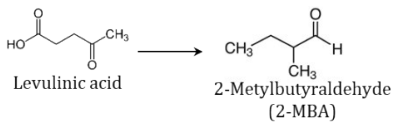
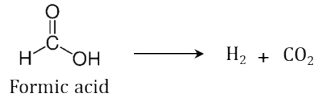
Hyunwoo Kim[1†], Julius Choi[2†], Junhyung Park[1], Wangyun Won[1*]

[1] Department of Chemical Engineering, Kyung Hee University, 1732 Deogyeong-daero, Giheung-gu, Yongin-si, Gyeonggi 17104, Republic of Korea
[2] Earth Energy Renewables, 6150 Mumford Rd, Bryan, TX 77807, USA
[*] Corresponding author (E-mail: wwon@khu.ac.kr)
[†] Equally contributed

Electronic Supplementary Information

Reaction condition and yield

Table S1. Specific reaction condition and yield per reactor (corresponding to Fig. 1 in flowsheet).

Reactor	Reaction	Yield (%)	Condition	Solvent
R-1		42.0	T: 483 K, P: 68.0 atm Catalyst: H_2SO_4	THF, water
		2.0		
		0.1		
		1.0		
		1.9		
		3.2		
		49.8		
R-3		93.7	T: 383 K, P: 40.0 atm Catalyst: 5% Pt/C	GVL, water
		6.3		
		100.0		
R-4		99.0	T: 493 K, P: 35.5 atm Catalyst: $RuSn_4/C$	GVL, water
		1.0		
		100.0		

Economic parameters and assumptions

Table S2. Major economic parameters and assumptions.

Cellulose price ($/ton) [a]	450.0
Sulfuric acid price ($/ton) [b]	110.0
Hydrogen price ($/ton) [b]	1367.5
Tetrahydrofuran price ($/ton) [c]	1532.0
Oxygen price ($/ton) [d]	40.0
$RuSn_4$/C catalyst ($/kg) [e]	539.3
Pt/C catalyst ($/kg) [g]	194.0
Activated carbon price ($/ton) [f]	1200.0
Gypsum disposal cost ($/ton) [b]	30.9
Cooling tower chemicals ($/ton) [b]	3671.4
Plant financing by equity (%) [b]	40.0
Plant life (years) [b]	30.0
Income tax rate (%) [b]	35.0
Discount rate (%)	10.0
Interest rate for debt financing (%) [b]	8.0
Term for debt financing (years) [b]	10.0
General plant depreciation (years) [b]	7.0
Working capital (% of fixed capital investment) [b]	5.0
On-stream percentage after startup (%) [b]	90.0
Startup time (years) [b]	0.5
Revenue and costs during startup	
Revenue (% of normal) [b]	50.0
Variable costs (% of normal) [b]	75.0
Fixed costs (% of normal) [b]	100.0
Construction period (years) [b]	3.0
First 12 months' expenditures (%) [b]	8.0
Next 12 months' expenditures (%) [b]	60.0
Last 12 months' expenditures (%) [b]	32.0

[a] Taken from Abels et al.[1]
[b] Taken from Davis et al.[2]
[c] Taken from He et al.[3]
[d] Taken from Dorris et al.[4]
[e] Taken from Sen et al.[5]
[f] Taken from Motagamwala et al.[6]
[g] Taken from Han et al.[7]

Assumption:
■ 10% of the catalyst is refurbished every 6 months at a cost equivalent to 20% of its original value.[7]

Important stream information

Table S3. Process stream information (from flowsheet in Fig.1).

Stream number	1	2	3	4	5	8	9	14	16	18	20	26	30	36	38	41	43
Components mass flow (ton/hr)																	
H_2O	0.0	0.0	0.0	0.0	125.1	121.3	97.0	121.3	0.0	3.9	0.0	76.2	0.1	24.8	69.2	7.7	70.6
GVL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	121.2	0.0	0.0	74.4	0.0	1.8	71.4	8.0	74.4
H_2SO_4	0.0	1.3	0.0	0.0	1.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
THF	0.0	0.0	0.0	0.8	1091.2	1091.2	873.0	1091.2	1090.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Cellulose	37.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Glucose	0.0	0.0	0.0	0.0	0.4	0.0	0.0	0.0	0.0	0.4	0.0	0.1	0.0	0.0	0.1	0.0	0.1
HMF	0.0	0.0	0.0	0.0	12.3	0.0	0.0	0.0	0.0	12.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LA	0.0	0.0	0.0	0.0	0.5	0.0	0.0	0.0	0.0	0.5	0.0	1.9	0.0	0.0	1.8	0.2	1.7
FA	0.0	0.0	0.0	0.0	0.2	0.0	0.0	0.0	0.0	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Furfural	0.0	0.0	0.0	0.0	0.7	0.0	0.0	0.0	30.0	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Formaldehyde	0.0	0.0	0.0	0.0	30.1	30.1	24.1	30.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Humins	0.0	0.0	0.0	0.0	18.7	0.0	0.0	0.0	0.0	18.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LGA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LGO	0.0	0.0	0.0	0.0	0.6	0.0	0.0	0.0	0.0	0.6	0.0	5.1	0.0	0.1	4.9	0.5	5.1
2-MBA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO_2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O_2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	11.5	0.0	0.0	0.0	0.0	0.0	0.0
H_2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Lime	0.0	0.0	0.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FDCA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	14.6	13.9	0.0	0.7	0.1	0.7
AC (polymer)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.1	0.0	0.0	1.1	0.1	1.1
Total mass flow (ton/hr)	37.5	1.3	0.9	0.8	1281.1	1242.6	994.1	1242.6	1241.7	37.2	11.5	173.5	14.0	26.7	149.2	16.7	153.8
Temperature (K)	298.2	298.2	298.2	298.2	483.2	376.7	376.7	331.9	333.3	433.6	873.2	383.2	352.5	373.5	378.3	379.1	378.4
Pressure (atm)	1.0	1.0	1.0	1.0	68.0	3.0	3.0	1.0	68.0	3.0	20.0	40.0	1.0	1.0	1.0	35.0	1.0

Heat integration

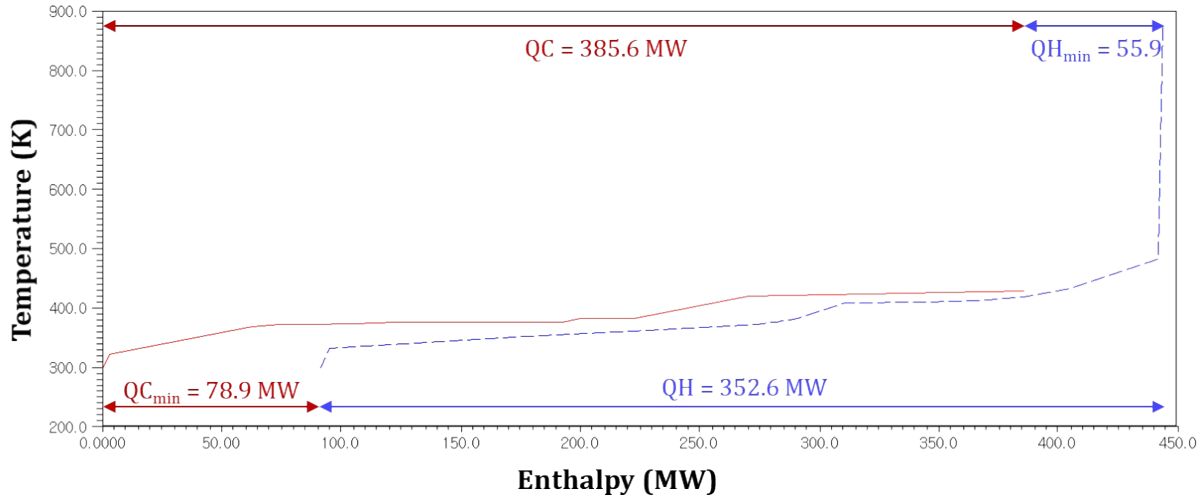


Fig. S1. Composite curve (obtained using Aspen Energy Analyzer) for the Strategy A. Minimum temperature difference (ΔT_{min}) is 10 K. QH_{min}: total minimum hot utility requirement, QC_{min}: total minimum cold utility requirement.

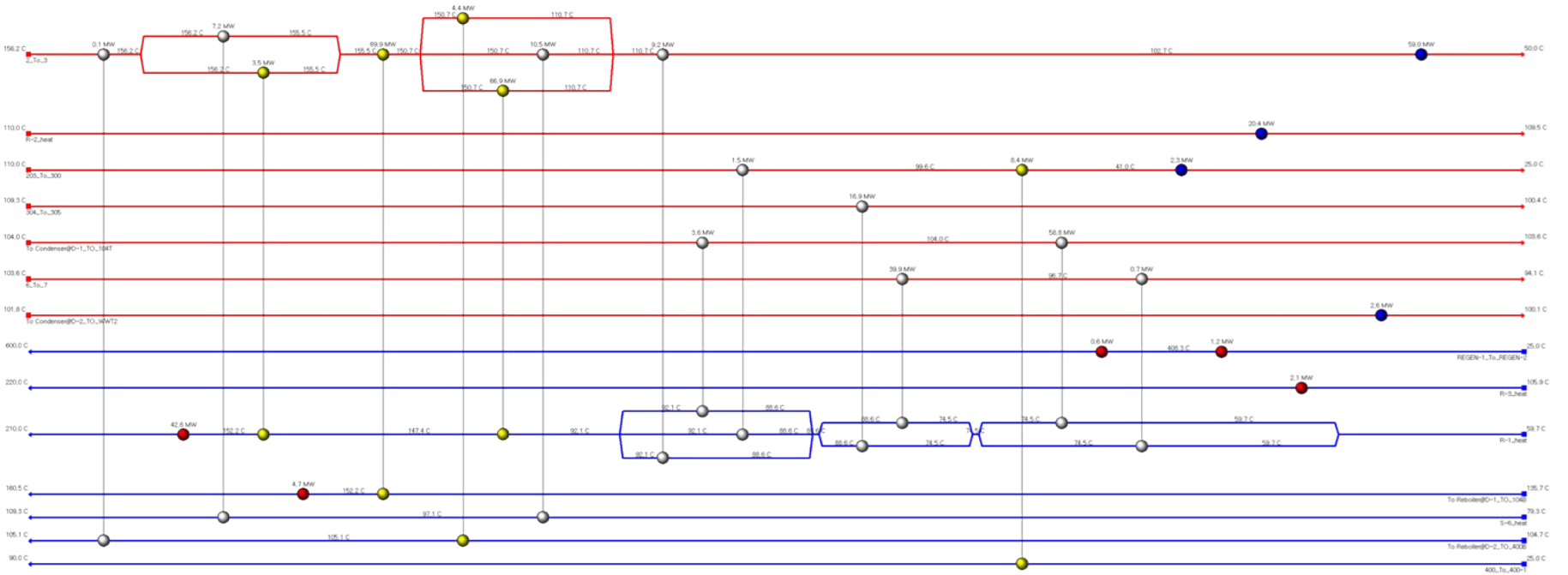


Fig. S2. Heat exchanger network.

Project cost

Table S4. The calculation method of major equipment cost.

Subsystem	Equipment type	Equipment ID	Equipment cost ($)	Installed cost ($)	Calculation method
HMF production	Reactor	R-1[a]/R-2[b]	12,207,273	94,972,442	Scaled on area[a] Scaled on flow[b]
	Distillation column	D-1	926,907	2,224,577	APEA[c]
	Adsorption bed	A-1	4,619,000	8,314,201	Scaled on area[d]
	Compressor	CP-1	8,375,702	11,725,983	Scaled on electricity[a]
FDCA production	Reactor	R-3	4,577,793	10,071,144	Scaled on area[a]
FDCA separation	Separator	S-2/S-3/S-4	1,334,726	2,182,072	Scaled on flow[a]
Solvent recovery	Reactor	R-4	87,500	148,750	APEA[c]
	Distillation column	D-2	259,300	622,320	APEA[c]

[a] The cost is scaled based on the size and cost data provided in the NREL reports.[2]
[b] The cost is scaled based on the size and cost data provided in the technical report.[8]
[c] The cost is estimated by Aspen Process Economic Analyzer.
[d] The cost is scaled based on the size and cost data provided in the NREL reports.[9]

Table S5. Project cost worksheet.

Subsystems			Installed cost
HMF production			$ 121,546,372
FDCA production			$ 10,268,484
FDCA separation			$ 2,903,232
Solvent recovery			$ 1,202,400
Wastewater treatment			$ 9,695,442
Storage			$ 3,506,387
Utilities			$ 5,032,961
Total installed equipment cost			**$ 154,155,278**
Warehouse	4.0%	of ISBL†	$ 5,436,820
Site development	9.0%	of ISBL†	$ 12,232,844
Additional piping	4.5%	of ISBL†	$ 6,116,422
Total direct cost (TDC)			$ **177,941,363**
Prorateable expenses	10.0%	of TDC	$ 17,794,136
Field expenses	10.0%	of TDC	$ 17,794,136
Home office & construction fee	20.0%	of TDC	$ 35,588,273
Project contingency	10.0%	of TDC	$ 17,794,136
Other costs (start-up, permits, etc.)	10.0%	of TDC	$ 17,794,136
Total indirect cost			**$ 106,764,818**
Fixed capital investment (FCI)			**$ 284,706,181**
Land			$ 831,603
Working capital	5.0%	of FCI	$ 14,235,309
Total capital investment (TCI)			**$ 299,773,093**

† Inside battery limits (ISBL): HMF production, FDCA production, FDCA separation, and Solvent recovery.

Pioneer plant analysis

Table S6. Pioneer plant analysis parameters and equations.

Parameter	Definition	Range	Value
Plant performance [a]		0–89	25
NEWSTEPS	number of new process steps based on block	≥ 0	4
BALEQS	percentage of heat and mass balance equations based on actual prior plant data	0–100	0
WASTE	factor for waste handling encountered during development	0-5	1
SOLIDS	factor for presence of solid feedstock or products	0 or 1	1
Cost growth [b]		>0	0.46
PCTNEW	estimate (%) of unproven technology incorporated in commercial use	0–100	66
IMPURITIES	factor for impurities present in process	0-5	3
COMPLEXITY	block count of all process steps in plant	≥ 1	8
INCLUSIVENESS	percentage of three factors: pre-startup personnel costs, pre-startup inventory cost, and land purchase	0–100	100
PROJECT DEFINITION	levels of site-specific information and engineering included in estimate	2–8	8

[a] *Plant performance* = 85.77 – 9.69 × NEWSTEPS + 0.33 × BALEQS – 4.12 × WASTE - 17.91 × SOLIDS.

[b] *Cost growth* = 1.1219 – 0.00297 × PCTNEW – 0.02125 × IMPURITIES – 0.01137 × COMPLEXITY + 0.00111 × INCLUSIVENESS – 0.06361 × PROJECT DEFINITION.

Table S7. Assumptions and equations for pioneer plant analysis.

Assumptions
1. The parameter of plant performance increases 20 % every year until it reaches full capacity (100 %).
2. If plant capacity fails to reach 40 % after year 1, it is hard to achieve design capacity without a significant capital investment.
Equations
1. Total capital investment (pioneer plant) = Total capital investment (*n*th plant)/Cost growth
2. Variable operating cost (pioneer plant) = Variable operating cost (nth plant) × Plant performance
3. Annual product sales (pioneer plant) = Annual product sales (*n*th plant) × Plant performance

Discounted cash flow

Table S8. Discounted cash flow calculations.

Year	-2	-1	0	1	2	3	4	5	6	7	8
Fixed capital investment	9,110,598	68,329,483	36,442,391								
Land	831,603										
Working capital			14,235,309								
Loan payment				25,457,770	25,457,770	25,457,770	25,457,770	25,457,770	25,457,770	25,457,770	25,457,770
Loan interest payment	1,093,272	9,292,810	13,665,897	13,665,897	12,722,547	11,703,729	10,603,406	9,415,057	8,131,639	6,745,549	5,248,571
Loan principal	13,665,897	116,160,122	170,823,709	159,031,835	146,296,612	132,542,571	117,688,207	101,645,494	84,319,363	65,607,142	45,397,944
Activated carbon sales				45,941,007	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676
FDCA sales				126,732,644	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859
Total annual sales				172,673,651	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535
Annual manufacturing cost											
Feedstock				92,166,720	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960
Other variable costs				50,672,098	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969
Fixed operating costs				8,428,864	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864
Total product cost				151,267,683	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794
Annual depreciation											
General plant writedown				14.29%	24.49%	17.49%	12.49%	8.93%	8.92%	8.93%	4.46%
Depreciation charge				40,684,513	69,724,544	49,795,111	35,559,802	25,424,262	25,395,791	25,424,262	12,697,896
Remaining value				244,021,668	174,297,124	124,502,013	88,942,211	63,517,949	38,122,158	12,697,896	0
Net revenue				-32,944,441	-41,444,349	-20,496,099	-5,160,467	6,163,423	7,475,310	8,832,930	23,056,274
Losses forward					-32,944,441	-74,388,791	-94,884,889	-100,045,356	-93,881,933	-86,406,623	-77,573,693
Taxable income				-32,944,441	-74,388,791	-94,884,889	-100,045,356	-93,881,933	-86,406,623	-77,573,693	-54,517,419
Income tax				0	0	0	0	0	0	0	0
Annual cash income				-4,051,801	15,544,971	15,544,971	15,544,971	15,544,971	15,544,971	15,544,971	15,544,971
Discount factor	1.210	1.100	1.000	0.909	0.826	0.751	0.683	0.621	0.564	0.513	0.467
Annual present value				-3,683,456	12,847,084	11,679,167	10,617,425	9,652,204	8,774,731	7,977,028	7,251,844
Total capital investment + interest	13,352,922	85,384,522	64,343,597								
Net present worth			0								

Year	9	10	11	12	13	14	15	16	17	18	19
Fixed capital investment											
Land											
Working capital											
Loan payment	25,457,770	25,457,770	0	0	0	0	0	0	0	0	0
Loan interest payment	3,631,835	1,885,761	0	0	0	0	0	0	0	0	0
Loan principal	23,572,009	0	0	0	0	0	0	0	0	0	0
Activated carbon sales	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676
FDCA sales	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859
Total annual sales	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535
Annual manufacturing cost											
Feedstock	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960
Other variable costs	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969
Fixed operating costs	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864
Total product cost	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794
Annual depreciation											
General plant writedown											
Depreciation charge											
Remaining value											
Net revenue	37,370,906	39,116,980	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741
Losses forward	-54,517,419	-17,146,513	0	0	0	0	0	0	0	0	0
Taxable income	-17,146,513	21,970,468	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741
Income tax	0	7,689,664	14,350,959	14,350,959	14,350,959	14,350,959	14,350,959	14,350,959	14,350,959	14,350,959	14,350,959
Annual cash income	15,544,971	7,855,308	26,651,782	26,651,782	26,651,782	26,651,782	26,651,782	26,651,782	26,651,782	26,651,782	26,651,782
Discount factor	0.424	0.386	0.350	0.319	0.290	0.263	0.239	0.218	0.198	0.180	0.164
Annual present value	6,592,585	3,028,561	9,341,287	8,492,079	7,720,072	7,018,247	6,380,225	5,800,204	5,272,913	4,793,557	4,357,779
Total capital investment + interest											
Net present worth											

Year	20	21	22	23	24	25	26	27	28	29	30
Fixed capital investment											
Land											-831,603
Working capital											-14,235,309
Loan payment	0	0	0	0	0	0	0	0	0	0	0
Loan interest payment	0	0	0	0	0	0	0	0	0	0	0
Loan principal	0	0	0	0	0	0	0	0	0	0	0
Activated carbon sales	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676	61,254,676
FDCA sales	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859	168,976,859
Total annual sales	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535	230,231,535
Annual manufacturing cost											
Feedstock	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960	122,888,960
Other variable costs	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969	57,910,969
Fixed operating costs	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864	8,428,864
Total product cost	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794	189,228,794
Annual depreciation											
General plant writedown											
Depreciation charge											
Remaining value											
Net revenue	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741
Losses forward	0	0	0	0	0	0	0	0	0	0	0
Taxable income	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741	41,002,741
Income tax	14,350,959	14,350,959	14,350,959	14,350,959	14,350,959	14,350,959	14,350,959	14,350,959	14,350,959	14,350,959	14,350,959
Annual cash income	26,651,782	26,651,782	26,651,782	26,651,782	26,651,782	26,651,782	26,651,782	26,651,782	26,651,782	26,651,782	26,651,782
Discount factor	0.149	0.135	0.123	0.112	0.102	0.092	0.084	0.076	0.069	0.063	0.057
Annual present value	3,961,618	3,601,470	3,274,064	2,976,422	2,705,838	2,459,853	2,236,230	2,032,936	1,848,124	1,680,113	1,527,375
Total capital investment + interest											-863,463
Net present worth											

Life-cycle assessment

Table S9. Input and output database for the LCA.

Materials	Name of data set	Database
Acetic acid	Acetic acid, without water, in 98% solution state {GLO} | market for | Cut-off, U	Ecoinvent 3.6
Ash	Dummy_Disposal, fly ash, to unspecified landfill/kg/RNA	USLCI
Average incineration residue	Average incineration residue {RoW} | market for | Cut-off, U	Ecoinvent 3.6
Biomass	Wood chips, wet, measured as dry mass {RoW} | market for | Cut-off, U	Ecoinvent 3.6
Chemical factory	Chemical factory, organics {GLO} | market for | Cut-off, U	Ecoinvent 3.6
CO_2	Carbon dioxide, biogenic	Ecoinvent 3.6
Electricity	Electricity, medium voltage {RER} | market for | Cut-off, U	Ecoinvent 3.6
Gypsum	Waste gypsum {RoW} | market for waste gypsum| APOS, S	Ecoinvent 3.6
H_2	Hydrogen, liquid {RoW} | market for | Cut-off, U	Ecoinvent 3.6
H_2O	Water/m3	Ecoinvent 3.6
H_2O	Water, cooling, unspecified natural origin, RER	Ecoinvent 3.6
H_2O	Water, completely softened, from decarbonized water, at user {GLO} | market for | Cut-off, U	Ecoinvent 3.6
Hazardous waste	Hazardous waste, for underground deposit {GLO} | market for | Cut-off, U	Ecoinvent 3.6
Hydrocarbons	Hydrocarbons, aromatic	Ecoinvent 3.6
Heavy oil	Heavy fuel oil {RoW} | market for | Cut-off, U	Ecoinvent 3.6
Heat	Heat, district or industrial, natural gas {GLO} | market for | Cut-off, U	Ecoinvent 3.6
Heat	Heat, district or industrial, natural gas {RER} | market group for | Cut-off, U	Ecoinvent 3.6
Heat	Heat, district or industrial, other than natural gas {RER} | market group for | Cut-off, U	Ecoinvent 3.6
Lime	Lime, hydrate, packed {GLO} | market for | Cut-off, U	Ecoinvent 3.6
N_2	Nitrogen, liquid {RER} | market for | Cut-off, U	Ecoinvent 3.6
NaCl	Sodium chloride, brine solution {GLO} | market for | Cut-off, U	Ecoinvent 3.6
NaOH	Sodium hydroxide, without water, in 50% solution state {GLO} | market for | Cut-off, U	Ecoinvent 3.6
NMVOC	NMVOC, non-methane volatile organic compounds, unspecified origin	Ecoinvent 3.6
Particulates	Particulates, < 2.5 um	Ecoinvent 3.6
Particulates	Particulates, >10 um	Ecoinvent 3.6
Particulates	Particulates, > 2.5 um, and < 10 um	Ecoinvent 3.6
O_2	Oxygen, liquid {RoW} | market for | Cut-off, U	Ecoinvent 3.6
Steam	Steam, in chemical industry {GLO} | market for | Cut-off, U	Ecoinvent 3.6
Sulfuric acid	Sulfuric acid {GLO} | market for | Cut-off, U	Ecoinvent 3.6
Tetrahydrofuran	Tetrahydrofuran {GLO} | market for | Cut-off, U	Ecoinvent 3.6
Xylene	Xylene {GLO} | market for | Cut-off, U	Ecoinvent 3.6

Table S10. The results of environmental impact for the biomass-derived FDCA production.

Impact category	Unit	Biomass	H2SO4	THF	Heavy oil	NaCl	Lime	H2	O2	Heat	Electricity	Gypsum	H2O	Ash
Climate change	kg CO2 eq	0.096	0.013	0.156	0.006	0.003	0.027	0.001	0.675	0.038	0.580	0.001	0.000	0.000
Ozone depletion	kg CFC-11 eq	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Terrestrial acidification	kg SO2 eq	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.003	0.000	0.002	0.000	0.000	0.000
Freshwater eutrophication	kg P eq	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Marine eutrophication	kg N eq	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Human toxicity	kg 1,4-DB eq	0.013	0.030	0.055	0.001	0.004	0.001	0.000	0.221	0.001	0.206	0.001	0.000	0.000
Photochemical oxidant formation	kg NMVOC	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.001	0.000	0.000	0.000
Particulate matter formation	kg PM10 eq	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.001	0.000	0.000	0.000
Terrestrial ecotoxicity	kg 1,4-DB eq	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Freshwater ecotoxicity	kg 1,4-DB eq	0.000	0.001	0.002	0.000	0.000	0.000	0.000	0.008	0.000	0.007	0.000	0.000	0.000
Marine ecotoxicity	kg 1,4-DB eq	0.000	0.001	0.001	0.000	0.000	0.000	0.000	0.007	0.000	0.007	0.000	0.000	0.000
Ionising radiation	kBq U235 eq	0.007	0.002	0.010	0.003	0.000	0.001	0.000	0.066	0.000	0.080	0.000	0.000	0.000
Agricultural land occupation	m2a	7.015	0.001	0.008	0.000	0.000	0.001	0.000	0.009	0.000	0.013	0.000	0.000	0.000
Urban land occupation	m2a	0.032	0.000	0.001	0.000	0.000	0.000	0.000	0.004	0.000	0.004	0.000	0.000	0.000
Natural land transformation	m2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Water depletion	m3	0.000	0.002	0.007	0.000	0.000	0.000	0.000	0.015	0.000	0.004	0.000	0.000	0.000
Metal depletion	kg Fe eq	0.004	0.005	0.006	0.000	0.001	0.000	0.000	0.005	0.000	0.005	0.000	0.000	0.000
Fossil depletion	kg oil eq	0.033	0.012	0.055	0.017	0.001	0.003	0.001	0.168	0.015	0.145	0.000	0.000	0.000

Table S11 The results of environmental impact for the petroleum-derived TPA production.

Impact category	Unit	Acetic acid	Chemical factory	N2	NaOH	Steam	H2O	Xylene	Electricity	Heat; NG	Heat; other than NG	Incineration residue	Waste
Climate change	kg CO2 eq	0.086	0.067	0.012	0.002	0.202	0.000	1.113	0.208	0.026	0.082	0.002	0.000
Ozone depletion	kg CFC-11 eq	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Terrestrial acidification	kg SO2 eq	0.000	0.001	0.000	0.000	0.001	0.000	0.003	0.001	0.000	0.000	0.000	0.000
Freshwater eutrophication	kg P eq	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Marine eutrophication	kg N eq	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Human toxicity	kg 1,4-DB eq	0.036	0.191	0.008	0.001	0.022	0.000	0.020	0.131	0.000	0.018	0.008	0.000
Photochemical oxidant formation	kg NMVOC	0.000	0.000	0.000	0.000	0.000	0.000	0.003	0.000	0.000	0.000	0.000	0.000
Particulate matter formation	kg PM10 eq	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000
Terrestrial ecotoxicity	kg 1,4-DB eq	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Freshwater ecotoxicity	kg 1,4-DB eq	0.001	0.004	0.000	0.000	0.001	0.000	0.001	0.004	0.000	0.000	0.001	0.000
Marine ecotoxicity	kg 1,4-DB eq	0.001	0.004	0.000	0.000	0.001	0.000	0.001	0.004	0.000	0.000	0.001	0.000
Ionising radiation	kBq U235 eq	0.011	0.006	0.006	0.000	0.006	0.000	0.003	0.109	0.000	0.002	0.000	0.000
Agricultural land occupation	m2a	0.003	0.016	0.001	0.000	0.002	0.000	0.001	0.022	0.000	0.030	0.000	0.000
Urban land occupation	m2a	0.001	0.002	0.000	0.000	0.001	0.000	0.002	0.001	0.000	0.001	0.000	0.000
Natural land transformation	m2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Water depletion	m3	0.002	0.001	0.001	0.000	0.000	0.000	0.019	0.003	0.000	0.001	0.000	0.000
Metal depletion	kg Fe eq	0.005	0.048	0.000	0.000	0.001	0.000	0.003	0.003	0.000	0.000	0.000	0.000
Fossil depletion	kg oil eq	0.054	0.016	0.003	0.001	0.061	0.000	0.948	0.054	0.010	0.020	0.000	0.000

References

1. Abels C, Thimm K, Wulfhorst H, Spiess AC, Wessling M. Membrane-based recovery of glucose from enzymatic hydrolysis of ionic liquid pretreated cellulose. Bioresource Technology 2013;149:58-64.
2. Davis R, Tao L, Scarlata C, Tan ECD, Ross J, Lukas J, Sexton D. Process design and economics for the conversion of lignocellulosic biomass to hydrocarbons. National Renewable Energy Laboratory Report 2015;NREL/TP-5100-62498.
3. He J, Huang K, Barnett KJ, Krishna SH, Alonso DM, Brentzel ZJ, Burt SP, Walker T, Banholzer WF, Maravelias CT, Hermans I, Dumesic JA, Huber GW. New catalytic strategies for α,ω-dios production from lignocellulosic biomass. Faraday Discussion 2017;202:247-267.
4. Dorris CC, Lu E, Park S, Toro FH. High-purity oxygen production using mixed ionic-electronic conducting sorbent, Working paper, University of Pennsylvania, 2016.
5. Sen SM, Alonso DM, Wettstein SG, Gürbüz EI, Henao CA, Dumesic JA, Maravelias CT. A sulfuric acid management strategy for the production of liquid hydrocarbon fuels via catalytic conversion of biomass-derived levulinic acid. Energy and Environmental Science 2012;5:9690-9697.
6. Motagamwala AH, Won W, Senner C, Alonso DM, Maravelias CT, Dumesic JA. Toward biomass-derived renewable plastics: production of 2,5-furandicarboxylic acid from fructose. Science Advances 2018;4:eaap9722.
7. Han J, Sen SM, Alonso DM, Dumesic JA, Maravelias CT. A strategy for the simultaneous catalytic conversion of hemicellulose and cellulose from lignocellulosic biomass to liquid transportation fuels. Green Chemistry 2014;16:653-661.
8. Huber GW, He J. Catalytic processes for production of α,ω-diols from lignocellulosic biomass. University of Wisconsin, Madison, WI (United States).
9. Humbird D, Davis R, Tao L, Kinchin C, Hsu D, Aden A, Schoen P, Lukas J, Olthof B, Worley M, Sexton D, Dudgeon D. Process design and economics for biochemical conversion of lignocellulosic biomass to ethanol. National Renewable Energy Laboratory Report 2011;NREL/TP-5100-47764.