Electronic Supplementary Material to:

Economics and global warming potential of a commercial-scale delignifying biorefinery based on CELF pretreatment

Bruno Colling Klein [a,b], Brent Scheidemantle [b,c,d], Rebecca Hanes [b,e], Andrew W. Bartling [a,b], Nicholas Grundl [a,b], Robin Clark [a,f], Mary Biddy [a,b], Ling Tao [a,b], Cong Trinh [b,g], Adam Guss [b,h], Charles E. Wyman [b,c,d], Arthur J. Ragauskas [b,g,i], Erin G Webb [b,f], Brian H. Davison [b,h], Charles M. Cai [b,c,d]*

[a] Catalytic Carbon Transformation & Scale-up Center, National Renewable Energy Laboratory, Golden, CO 80401, USA

[b] Center for Bioenergy Innovation (CBI), Oak Ridge National Laboratory (ORNL), Oak Ridge, TN 37831, USA

[c] Department of Chemical and Environmental Engineering, Bourns College of Engineering, University of California, Riverside, 900 University Ave, Riverside, CA 92521, USA

[d] Center for Environmental Research and Technology, Bourns College of Engineering, University of California, Riverside, 1084 Columbia Avenue, Riverside, CA 92507, USA

[e] Strategic Energy Analysis Center, National Renewable Energy Laboratory, Golden, CO 80401, USA

[f] Environmental Sciences Division, Oak Ridge National Laboratory (ORNL), 1 Bethel Valley Road, Oak Ridge, Tennessee 37830, USA

[g] Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, TN, USA

[h] Biosciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN 37831, USA

[i] Department of Forestry, Wildlife, and Fisheries, Center for Renewable Carbon, The University of Tennessee Institute of Agriculture, Knoxville, TN 37996, USA

Biorefinery setup

Figure S1a depicts the overall integration between streams in biorefineries based on Cosolvent Enhanced Lignocellulosic Fractionation (CELF). Figure S1b shows a detailed flow diagram for CELF deconstruction of biomass with tetrahydrofuran (THF) and water as the solvents of choice, yielding three main streams:

- Cellulose-rich stream: recovered as the solid stream after solid-liquid separation of fractions after CELF deconstruction of biomass. Sent to conversion into isobutanol or ethanol via consolidated bioprocessing (CBP).
- Lignin-rich stream: water-insoluble (WIS) lignin precipitates from the aqueous solution after THF is removed with a distillation column for recycling purposes. This stream is sent directly to conversion via athermic oxygen removal (AOR) in supercritical methanol.
- Hemicellulose-rich stream: this stream contains several soluble organic compounds, mainly pentoses, water-soluble (WS) lignin, organic acids, and 1,4-butanediol (1,4-BDO). During CELF deconstruction of biomass, a small portion of THF (1%) is reversibly converted into 1,4-BDO. This byproduct of CELF reactions can be returned in full to the reactor and account for part of the organic solvent in the required THF:water ratio if the process configuration allows. In the biorefining context considered in this study, preparatory assessments deemed the recovery of 1,4-BDO from the main aqueous stream a highly costly alternative from an energy requirement standpoint due to the molecule's high boiling point (230 ^{o}C) and its low concentration in the process (~8 g/L). In this way, it has been chosen to design the biorefinery with 1,4-BDO being present in the hemicellulose-rich stream. Hemicellulose-derived sugars (pentoses) contained in this stream are initially converted to isobutyl acetate via a fed-batch, anaerobic fermentation using *Escherichia coli*. As other compounds in this stream remain untouched in this step, such as WS lignin, organic acids, and 1,4-BDO, spent medium from this operation is sent to muconic acid fermentation using *Pseudomonas putida*, as this microorganism can be engineered to biologically funnel aromatics [1] and diols [2] into muconic acid. This compound is then recovered from the fermentation broth and further converted into adipic acid.

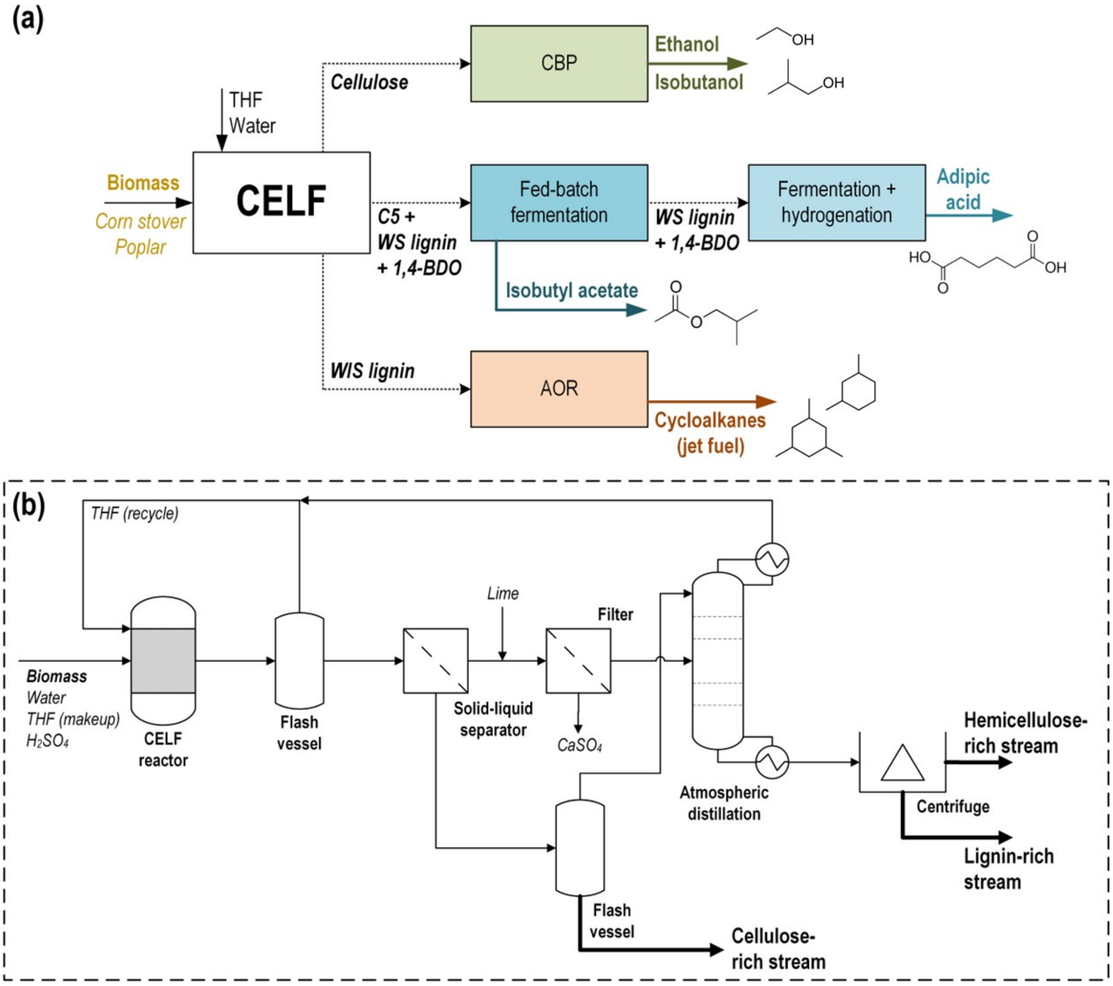

Figure S1. (a) Simplified block flow diagram for the proposed CELF-based biorefineries outlining the mass integration strategy. (b) Detailed flow diagram for the CELF deconstruction of lignocellulosic biomass.

1,4-BDO: 1,4-butanediol; AOR: Athermic Oxygen Removal; C5: pentoses; CBP: consolidated bioprocessing; CELF: Co-solvent Enhanced Lignocellulosic Fractionation; THF: tetrahydrofuran; WS: water soluble; WIS: water insoluble.

Technical details

Table S1. Full biomass compositions (wt%).

Component	**Corn stover**	**Poplar**
Hexoses		
Glucan	*35.0%*	*50.4%*
Galactan	*1.4%*	*0.7%*
Mannan	*0.6%*	*2.9%*
Hemicellulose		
Xylan	*19.5%*	*15.3%*
Acetyl	*1.8%*	*2.0%*
Lignin	15.8%	21.8%
Organic extracts	14.6%	6.4%
Sucrose	0.8%	-
Ash	4.9%	0.5%
Protein	3.1%	-

Table S2. Detailed modeling parameters.

Parameter	**Value**		**Comments**
Biomass conditioning	**Poplar**	**Corn stover**	
Milling power requirement	28 kWh/dry tonne	22 kWh/dry tonne	[3]
CELF pretreatment			
Reaction temperature, pressure	160^{o}C, 200 psig	150 ^{o}C, 160 psig	[4-6]
Solids loading	20 wt%		
THF to water ratio	1:1		
H_2SO_4 loading	0.5%		
Biomass conversion			
Cellulose to oligomers	6.9%	5.9%	
Cellulose to glucose	7.2%	6.2%	
Xylan to xylose	90.8%	91.2%	
Xylan to furfural	1.5%	1.0%	
Galactan to olygomers	48.7%	48.7%	
Galactan to galactose	51.3%	51.3%	
Acetate solubilization	90.0%	90.0%	
Lignin solubilization	91.4%	76.6%	
Reversible conversion of THF to BDO	1.0%		
CBP	**Ethanol**	**Isobutanol**	
Solids loading			
Poplar	13%	8.5%	Assumption
Corn stover	20%	8.5%	
Titer			
Poplar	61 g/L	30 g/L	
Corn stover	75 g/L	23 g/L	
Component solubilization [a]			
Poplar	95%	90%	

Corn stover	95%	90%	
Component conversion [b]			
Poplar			
Glucose	***98%***	***98%***	
Xylose	***93.1%***	***92.7%***	
Arabinose	***88.2%***	***88.7%***	
Corn stover			
Glucose	***98%***	***98%***	
Xylose	***93.1%***	***92.7%***	
Arabinose	***88.2%***	***88.7%***	
AOR			
Component conversion			[7, 8]
$MeOH \rightarrow H_2 + CO$	6%		
Lignin → Cycloalkanes + MeOH	95%		
Reaction temperature, pressure	300 °C, 160 bar		
WHSV	5 h^{-1}		Assumptions for continuous operation
Methanol to lignin ratio	10 L/kg		
Fermentation to isobutyl acetate			
Base reaction [c]	Glucose + 0.07 NH_3 → 0.39 DCW + 0.62 IBA + 1.87 CO_2 + 1.24 H_2 + 0.78 H_2O		Estimates based on a separate spreadsheet for dedicated fed-batch fermentations
Glucose/xylose conversion	97%		
Productivity	0.79 g/L/h		
IBA recovery in LLE	96%		
Fermentation to muconic acid			
Volumetric productivity	1 g/L/h		Estimates based on [9]
Substrate utilization	98%		
Ratio of C diverted to product			
From aromatics and acids	100%		
From sugars and other organic molecules	54%		
Upgrading to adipic acid	Follows the concept presented in [9]		

[a] Glucose, xylose, arabinose, mannose, galactose, lignin, and acetate

[b] Ratio of C split: 95% to alcohol formation, 5% to cell biomass production

[c] As both five- and six-carbon sugars are converted in the fermentation operation, the reactions for xylose and arabinose can also be derived from the equation by multiplying all non-sugar compounds by a factor of 5/6

AOR: Athermic Oxygen Removal; BDO: 1,4-butanediol; CBP: Consolidated Bioprocessing; CELF: Co-solvent Enhanced Lignocellulosic Fractionation; DCW: dry cell weight; IBA: isobutyl acetate; LLE: liquid-liquid extraction; THF: tetrahydrofuran; WHSV: weight hour space velocity

Carbon recovery efficiency

Carbon recovery efficiency is calculated through the ratio between the carbon flow in carbon-based products synthesized in the biorefinery and the carbon flow of biobased inputs to the facility, as shown in Equation S1. Natural gas and methanol are not accounted for in the calculations in view of their use as energy carriers: while natural gas is used in the Cogeneration of Heat and Power (CHP) section of the biorefineries for energetic purposes, methanol is employed in the Athermic Oxygen Removal (AOR) of lignin both as a solvent and to generate hydrogen for the cleavage of lignin bonds into cycloalkanes.

$$\%Carbon\ recovery = \frac{Carbon\ flow\ products\ \left(\frac{kg}{h}\right)}{Carbon\ flow\ biobased\ inputs\ \left(\frac{kg}{h}\right)} \qquad \text{(S1)}$$

Table S3. Inputs and outputs considered for the calculation of the carbon recovery efficiency

Products	**Carbon content (kg C/kg compound)**
Ethanol	53.3%
Isobutanol	64.9%
Isobutyl acetate	62.1%
Adipic acid	49.3%
Cycloalkanes	85.7%

Biobased inputs	**Carbon content (kg C/kg compound)**
Poplar [a]	48.1%
Corn stover [a]	46.7%
1,4-butanediol (BDO) [b]	53.3%
Glucose	40.0%

[a] Calculated on dry basis.

[b] Originated from THF decomposition during CELF pretreatment of biomass. BDO is converted to muconic acid during aerobic fermentation to yield adipic acid after upgrading.

Economic parameters

Table S4. Main financial assumptions used in the techno-economic assessment (TEA), based on an nth-plant design basis.

Financial assumption	**Value**
Plant life	30 years
Cost year dollar	2016$
Capacity Factor	90%
Discount rate	10%
General plant depreciation	MACR
General plant recovery period	7 years
Steam plant depreciation	MACR
Steam plant recovery period	20 years
Federal tax rate	21%
Financing	40% equity
Loan terms	10-year loan at 8% APR
Construction period	3 years
First 12 months' expenditures	8%
Next 12 months' expenditures	60%
Last 12 months' expenditures	32%
Working capital	5% of fixed capital investment
Start-up time	6 months
Revenues during start-up	50%
Variable costs during start-up	75%

APR: annual percentage rate; MACR: modified accelerated cost recovery

Table S5. Detailed technical indicators of all assessed scenarios.

Feedstock	**Poplar**				**Stover**			
CBP alcohol	**Ethanol**		**Isobutanol**		**Ethanol**		**Isobutanol**	
Lignin fate	**Cycloalkanes**	**Combustion**	**Cycloalkanes**	**Combustion**	**Cycloalkanes**	**Combustion**	**Cycloalkanes**	**Combustion**
Products								
Ethanol (million gal/yr)	*51.9*	*51.9*	-	-	*37.8*	*37.8*	-	-
Isobutanol (million gal/yr)	-	-	*36.3*	*36.3*	-	-	*29.1*	*29.1*
Cycloalkanes (million gal/yr)	*18.2*	-	*18.2*	-	*11.0*	-	*11.0*	-
Isobutyl acetate (thousand t/yr)	*41.4*	*41.4*	*41.4*	*41.4*	*53.6*	*53.6*	*53.6*	*53.6*
Adipic acid (thousand t/yr)	*36.7*	*36.7*	*36.7*	*36.7*	*39.9*	*39.9*	*39.9*	*39.9*
Na_2SO_4 *(thousand t/yr)*	*37.5*	*38.5*	*38.0*	*39.0*	*39.9*	*41.3*	*42.0*	*43.2*
Surplus electricity (GWh/yr)	*0*	*0*	*34.6*	*0*	*0*	*0*	*0*	*0*
Fuel yield (GGE/dry ton feedstock)	75.9	46.7	70.1	40.8	51.8	34.2	49.7	32.1
Ethanol	*46.7*	*46.7*	-	-	*34.2*	*34.2*	-	-
Isobutanol	-	-	*40.8*	*40.8*	-	-	*32.1*	*32.1*
Cycloalkanes	*29.3*	-	*29.3*	-	*17.7*	-	*17.6*	-
Natural gas input (MMBTU/h)	574.0	0	1011.0	431.8	389.7	0	842.5	531.8
Electricity imports (GWh/yr)	81.4	112.7	0	6.5	96.4	101.2	3.9	19.8

GGE: gallon of gasoline equivalent; MMBTU: million British thermal unit

Table S6. Detailed economic indicators of all assessed scenarios.

Feedstock	**Poplar**				**Stover**			
CBP alcohol	**Ethanol**		**Isobutanol**		**Ethanol**		**Isobutanol**	
Lignin fate	**Cycloalkanes**	**Combustion**	**Cycloalkanes**	**Combustion**	**Cycloalkanes**	**Combustion**	**Cycloalkanes**	**Combustion**
CAPEX (MM$)								
Total Installed Costs [a]								
Biomass pretreatment (CELF)	*45.5*	*45.5*	*45.5*	*45.5*	*58.5*	*58.5*	*58.5*	*58.5*
Alcohol production	*39.0*	*39.0*	*49.3*	*49.3*	*29.8*	*29.8*	*48.2*	*48.2*
Isobutyl acetate production	*78.9*	*78.9*	*78.9*	*78.9*	*94.5*	*94.5*	*94.5*	*94.5*
Cycloalkanes production	*88.3*	-	*88.3*	-	*62.5*	-	*62.5*	-
Adipic acid production	*72.4*	*72.4*	*72.4*	*72.4*	*78.1*	*78.1*	*78.1*	*78.1*
Wastewater treatment	*59.6*	*56.6*	*68.1*	*65.0*	*53.7*	*49.8*	*69.3*	*65.5*
Cogeneration of heat and power	*74.5*	*61.7*	*95.6*	*83.9*	*67.5*	*57.1*	*88.7*	*82.8*
Utilities and storage	*14.9*	*13.5*	*16.8*	*15.0*	*14.6*	*13.7*	*16.4*	*15.3*
Other Direct Costs	*56.7*	*41.4*	*58.5*	*42.9*	*56.6*	*45.7*	*59.8*	*48.8*
Indirect Costs	*317.9*	*245.7*	*344.0*	*271.6*	*309.5*	*256.7*	*345.6*	*295.2*
Fixed Capital Investment (FCI)	**847.7**	**655.2**	**917.5**	**724.2**	**825.3**	**684.5**	**921.6**	**787.2**
IRR (%)	10.0%	10.1%	6.6%	5.8%	7.1%	7.6%	4.3%	3.7%
Alcohol MFSP ($/GGE) [b]	2.99	2.97	3.92	3.90	3.84	3.59	4.95	4.85
RIN credit to reach viability ($/gal) [c]	-	-	0.35	0.59	0.37	0.40	0.83	1.20
Carbon recovery efficiency (%)	52.5%	37.1%	49.3%	33.9%	46.2%	36.2%	44.9%	34.9%

[a] Feedstock processing and handling aspects are outside the scope of this work and are rolled into delivered feedstock costs at the throat of the biomass pretreatment section.

[b] Calculated without RIN credits.

[c] Combined gallons of alcohol (ethanol or isobutanol) and cycloalkanes (when lignin is converted in AOR).

Table S7. Detailed capital expenditures (CAPEX) of the scenario processing poplar to ethanol and producing cycloalkanes from lignin.

CELF PRETREATMENT	**Equipment Costs**						
EQUIPMENT TITLE	**NUM REQ**	**$**	**Year of Quote**	**Purch Cost in Base Yr**	**Scaling Exp**	**Inst Factor**	**Inst Cost in Proj year**
CELF reactor							
Pretreatment Reactor	1	$150,000	2013	$150,000	1.00	2.5	$21,484,664
Sulfuric Acid Pump	1	$8,000	2009	$8,000	0.80	2.3	$8,013
Hydrolyzate Solid-Liquid Separator	1	$35,000,000	2009	$10,500,000	0.70	1.7	$19,382,094
Oligomer Conversion Tank (reacidifiaction)	1	$203,000	2009	$203,000	0.70	2.0	$422,382
Evaporator							
Evaporator Feed Tank	1	$45,966	2011	$45,966	0.60	2.5	$39,389
Evaporator Feed Heater	1	$274,818	2011	$274,818	0.60	3.0	$161,468
Evaporator Flash Drum	1	$511,000	2009	$511,000	0.70	2.0	$356,520
Solvent Recovery Column							
THF Recovery Column Tower	1	$1,387,516	2007	$1,387,516	0.60	1.1	$2,706,157
THF Recovery Column Reboiler	1	$92,000	2010	$92,000	0.70	2.2	$196,068
THF Recovery Column Condenser	1	$85,000	2010	$85,000	0.70	2.2	$333,995
Tanks							
THF storage tank	1	$670,000	2009	$670,000	0.70	1.7	$309,844
Sulfuric Acid Storage Tank	1	$96,000	2010	$96,000	0.70	1.5	$102,952
						Area totals	**$45,503,547**

Table S7 (continued)

CONVERSION & UPGRADING	**Equipment Costs**						
EQUIPMENT TITLE	**NUM REQ**	**$**	**Year of Quote**	**Purch Cost in Base Yr**	**Scaling Exp**	**Inst Factor**	**Inst Cost in Proj year**
CBP to Ethanol							
Consolidated Bioprocessing (CBP)							
Fermenter Preheater	1	$23,900	2009	$23,900	0.70	1.8	$25,126
Ethanol Fermenter	1	$844,000	2009	$844,000	1.00	1.5	$18,396,418
Ethanol Fermenter Agitator	1	$52,500	2009	$52,500	1.00	1.5	$1,144,327
Fermenter Batch Cooler	1	$23,900	2009	$23,900	0.70	1.8	$43,811
Milling Equipment - Disc Refiner	8	$2,466,700	2013	$2,466,700	0.60	1.5	$2,788,948
Beer Transfer Pump	1	$26,800	2009	$26,800	0.80	2.3	$47,938
Beer Storage Tank	1	$636,000	2009	$636,000	0.70	1.8	$1,016,389
Beer Surge Tank Agitator	2	$68,300	2009	$68,300	0.50	1.5	$95,110
Seed Fermentation							
1st Seed Fermenter	2	$75,400	2009	$75,400	0.70	1.8	$140,869
2nd Seed Fermenter	2	$116,600	2009	$116,600	0.70	1.8	$217,842
3rd Seed Fermenter	2	$157,600	2009	$157,600	0.70	1.8	$294,442
4th Seed Fermenter	2	$352,000	2009	$352,000	0.70	2.0	$730,709
4th Seed Fermenter Coil	1	INCLUDED					
4th Seed Vessel Agitator	2	$26,000	2009	$26,000	0.50	1.5	$40,480
5th Seed Fermenter	2	$1,180,000	2009	$1,180,000	0.70	2.0	$2,449,534
5th Seed Fermenter Coil	1	INCLUDED					
5th Seed Vessel Agitator	2	$43,000	2009	$43,000	0.50	1.5	$66,947
Seed Transfer Pump	2	$24,300	2009	$24,300	0.80	2.3	$39,892
Seed Hold Tank	1	$439,000	2009	$439,000	0.70	1.8	$618,766
Seed Hold Tank Agitator	1	$31,800	2009	$31,800	0.50	1.5	$40,483
Seed Hold Transfer Pump	1	$8,200	2009	$8,200	0.80	2.3	$13,462
Ethanol Recovery							
Preheater	1	$274,818	2011	$274,818	0.60	3.0	$1,078,429
1st Column Condenser	1	$9,900	2016	$9,900	0.44	2.5	$28,423
1st Column Condenser Acc	1	$12,900	2016	$12,900	0.44	2.5	$37,037
1st Column Reboiler	1	$120,700	2016	$120,700	0.79	2.5	$384,812
1st Column Reflux Pump	1	$4,600	2016	$4,600	0.79	2.5	$16,013
1st Column Tower	1	$222,500	2016	$222,500	0.68	2.5	$721,188
2nd Column Condenser	1	$60,900	2016	$60,900	0.44	2.5	$181,579
2nd Column Condenser Acc	1	$16,300	2016	$16,300	0.44	2.5	$48,600
2nd Column Reboiler	1	$24,900	2016	$24,900	0.79	2.5	$76,272
2nd Column Reflux Pump	1	$6,700	2016	$6,700	0.79	2.5	$22,588
2nd Column Tower	1	$358,500	2016	$358,500	0.68	2.5	$1,029,883
Molecular Sieve Package (9 pieces)	1	$2,601,000	2009	$2,601,000	0.60	1.8	$4,442,496
Pump	1	$26,800	2009	$26,800	0.80	2.3	$90,563
Vent Scrubber	1	$215,000	2009	$215,000	0.60	2.4	$493,151
Solids Removal							
Lignin Wet Cake Conveyor	1	$70,000	2009	$70,000	0.80	1.7	$30,827
Lignin Wet Cake Screw	1	$20,000	2009	$20,000	0.80	1.7	$8,808
Pressure Filter Pressing Compr	1	$75,200	2009	$75,200	0.60	1.6	$104,266
Pressure Filter Drying Compr	2	$405,000	2009	$405,000	0.60	1.6	$557,672
Filtrate Tank Discharge Pump	1	$13,040	2010	$13,040	0.80	2.3	$6,766
Feed Pump	1	$18,173	2010	$18,173	0.80	2.3	$9,430
Manifold Flush Pump	1	$17,057	2010	$17,057	0.80	2.3	$8,850
Cloth Wash Pump	1	$29,154	2010	$29,154	0.80	2.3	$15,127
Filtrate Discharge Pump	1	$13,040	2010	$13,040	0.80	2.3	$6,766
Pressure Filter	2	$3,294,700	2010	$3,294,700	0.80	1.7	$1,263,572
Filtrate Tank	1	$103,000	2010	$103,000	0.70	2.0	$55,864
Feed Tank	1	$174,800	2010	$174,800	0.70	2.0	$94,806
Recycled Water Tank	1	$1,520	2010	$1,520	0.70	3.0	$1,237
Pressing Air Compressor Receiver	1	$8,000	2010	$8,000	0.70	3.1	$6,725
Drying Air Compressor Receiver	2	$17,000	2010	$17,000	0.70	3.1	$14,291
						Area totals	**$39,047,536**

Table S7 (continued)

CONVERSION & UPGRADING	**Equipment Costs**						
EQUIPMENT TITLE	**NUM REQ**	**$**	**Year of Quote**	**Purch Cost in Base Yr**	**Scaling Exp**	**Inst Factor**	**Inst Cost in Proj year**
Fed-batch Fermentation to Isobutyl Acetate							
Sugar Concentration	1	$6,370,000	2013	$6,370,000	0.70	2.0	$10,208,077
Concentrated Sugar Storage Tank	1	$168,000	2011	$168,000	0.70	1.8	$383,934
1st Seed Fermenter	1	$37,700	2009	$37,700	0.70	1.8	$114,421
2nd Seed Fermenter	1	$58,300	2009	$58,300	0.70	1.8	$176,943
3rd Seed Fermenter	1	$78,800	2009	$78,800	0.70	1.8	$239,161
4th Seed Fermenter	1	$176,000	2009	$176,000	0.70	2.0	$593,520
4th Seed Vessel Agitator	1	$13,000	2009	$13,000	0.50	1.5	$28,623
Isobutyl Acetate Production Fermenter	1	$590,000	2009	$590,000	0.70	2.0	$6,973,976
Isobutyl Acetate Production Fermenter Agitator	1	$21,500	2009	$21,500	0.50	1.5	$115,956
Seed Transfer Pump	1	$12,150	2009	$12,150	0.80	2.3	$10,173
Seed Hold Tank	1	$439,000	2009	$439,000	0.70	1.8	$343,307
Seed Hold Tank Agitator	1	$31,800	2009	$31,800	0.50	1.5	$26,578
Seed Hold Transfer Pump	1	$8,200	2009	$8,200	0.80	2.3	$6,866
Beer Storage Tank	1	$636,000	2009	$636,000	0.70	1.8	$54,763
Beer Surge Tank Agitator	1	$44,150	2009	$44,150	0.50	1.5	$7,632
Beer Transfer Pump	1	$26,800	2009	$26,800	0.80	2.3	$1,702
Ultrafiltration Membrane Separator	1	$2,048,000	2011	$2,048,000	1.00	2.5	$56,824,395
Isobutyl Acetate Recovery Column Tower	1	$286,000	2015	$286,000	1.00	3.3	$208,937
Isobutyl Acetate Recovery Column Condenser	1	$16,400	2015	$16,400	1.00	4.8	$8,300
Isobutyl Acetate Recovery Column Condenser Acc	1	$32,600	2015	$32,600	1.00	5.1	$17,535
Isobutyl Acetate Recovery Column Reboiler	1	$318,800	2015	$318,800	1.00	2.3	$63,169
Isobutyl Acetate Recovery Column Reflux pump	1	$13,100	2015	$13,100	1.00	5.5	$7,610
Centrifuge For Cell Removal	1	$327,680	2011	$327,680	0.60	2.3	$2,452,971
						Area totals	**$78,868,551**

CONVERSION & UPGRADING	**Equipment Costs**						
EQUIPMENT TITLE	**NUM REQ**	**$**	**Year of Quote**	**Purch Cost in Base Yr**	**Scaling Exp**	**Inst Factor**	**Inst Cost in Proj year**
AOR to Cycloalkanes (Jet Fuel)							
Lignin Preparation							
Lignin Wet Cake Conveyor	1	$70,000	2009	$70,000	0.80	1.7	$88,374
Lignin Wet Cake Screw	1	$20,000	2009	$20,000	0.80	1.7	$25,250
Pressure Filter Pressing Compr	1	$75,200	2009	$75,200	0.60	1.6	$26,277
Pressure Filter Drying Compr	2	$405,000	2009	$405,000	0.60	1.6	$140,542
Filtrate Tank Discharge Pump	1	$13,040	2010	$13,040	0.80	2.3	$19,397
Feed Pump	1	$18,173	2010	$18,173	0.80	2.3	$27,032
Manifold Flush Pump	1	$17,057	2010	$17,057	0.80	2.3	$25,372
Cloth Wash Pump	1	$29,154	2010	$29,154	0.80	2.3	$43,366
Filtrate Discharge Pump	1	$13,040	2010	$13,040	0.80	2.3	$19,397
Pressure Filter	2	$3,294,700	2010	$3,294,700	0.80	1.7	$3,622,341
Filtrate Tank	1	$103,000	2010	$103,000	0.70	2.0	$140,393
Feed Tank	1	$174,800	2010	$174,800	0.70	2.0	$238,260
Recycled Water Tank	1	$1,520	2010	$1,520	0.70	3.0	$3,108
Pressing Air Compressor Receiver	1	$8,000	2010	$8,000	0.70	3.1	$16,902
Drying Air Compressor Receiver	2	$17,000	2010	$17,000	0.70	3.1	$35,916
Milling Equipment - Disc Refiner	8	$2,466,700	2013	$2,466,700	0.60	1.5	$1,364,334
Continuous Supercritical Reactor (AOR)							
AOR Feed Tank	1	$45,966	2011	$45,966	0.60	2.5	$62,857
AOR Reactor Pump	1	$802,861	2014	$802,861	0.80	1.4	$684,340
AOR Fixed Bed Reactor	1	$6,513,387	2011	$6,513,387	0.70	2.0	$77,020,110
Methanol Recovery Column Condenser	1	$152,200	2016	$152,200	0.44	2.5	$229,183
Methanol Recovery Column Condenser Acc	1	$14,500	2016	$14,500	0.44	2.5	$21,834
Methanol Recovery Column Reboiler	1	$77,800	2016	$77,800	0.79	2.5	$107,725
Methanol Recovery Column Reflux Pump	1	$5,900	2016	$5,900	0.79	2.5	$9,187
Methanol Recovery Column Tower	1	$408,700	2016	$408,700	0.68	2.5	$1,267,894
Cycloalkane Recovery Column Condenser	1	$91,300	2016	$91,300	0.44	2.5	$240,187
Cycloalkane Recovery Column Condenser Acc	1	$22,800	2016	$22,800	0.44	2.5	$59,981
Cycloalkane Recovery Column Reboiler	1	$200,400	2016	$200,400	0.79	2.5	$541,356
Cycloalkane Recovery Column Reflux Pump	1	$9,200	2016	$9,200	0.79	2.5	$150,827
Cycloalkane Recovery Column Tower	1	$1,107,300	2016	$1,107,300	0.68	2.5	$2,027,444
						Area totals	**$88,259,187**

Table S7 (continued)

CONVERSION & UPGRADING	**Equipment Costs**						
EQUIPMENT TITLE	**NUM REQ**	**$**	**Year of Quote**	**Purch Cost in Base Yr**	**Scaling Exp**	**Inst Factor**	**Inst Cost in Proj year**
Fermentation and Upgrading to Adipic Acid							
Muconate Fermentation							
Sugar Concentration	1	$6,370,000	2013	$6,370,000	0.70	2.0	$6,326,540
Concentrated Sugar Storage Tank	1	$168,000	2011	$168,000	0.70	1.8	$241,135
1st Aerobic Seed	1	$46,000	2009	$46,000	1.00	1.80	$257,824
1st Seed Vessel Agitator	1	$3,420	2009	$3,420	1.00	1.50	$15,974
2nd Aerobic Seed	1	$57,500	2009	$57,500	1.00	1.80	$322,280
2nd Seed Vessel Agitator	1	$11,000	2009	$11,000	1.00	1.50	$51,378
Bubble Column Seed Fermenter	1	$274,100	2014	$274,100	1.00	2.30	$1,778,358
Seed Circulation Cooler	1	$8,400	2014	$8,400	1.00	2.20	$52,130
Bubble Column Production Fermenter	1	$1,691,400	2014	$1,691,400	1.00	2.30	$29,263,422
Production Circulation Cooler	1	$48,100	2014	$48,100	1.00	2.20	$796,010
Production Circulation Pump	1	$11,500	2014	$11,500	1.00	2.30	$198,965
Fermentation Air Compressor	1	$1,318,600	2014	$1,318,600	1.00	1.60	$965,802
Fermentation Air Receiver	1	$104,600	2014	$104,600	1.00	2.00	$95,767
Fermentation Surge Tank	1	$45,966	2011	$45,966	0.60	2.50	$43,900
Ultrafiltration Membrane Separator	1	$2,048,000	2011	$2,048,000	0.60	2.50	$4,735,366
Recovery and Upgrading to Adipic Acid							
Carbon Filter	1	$345,234	2011	$345,234	0.60	2.50	$798,247
CCM Crystallizer	2 (series)	$7,104,192	2011	$7,104,192	0.60	2.50	$3,977,613
CCM Centrifuge	1	$327,680	2011	$327,680	0.60	2.30	$377,432
CCM Drier	2 (parallel)	$555,008	2011	$555,008	0.60	2.60	$767,457
Dissolution Tank	1	$1,317,325	2011	$1,317,325	0.70	1.80	$337,228
Dissolution Tank agitator	1	$63,000	2009	$63,000	1.00	1.50	$98,085
Filtration Centrifuge (Salt Removal)	1	$327,680	2011	$327,680	0.60	2.30	$27,874
HDO Feed Tank	1	$45,966	2011	$45,966	0.60	2.50	$22,951
HDO Reactor Pump	1	$802,861	2014	$802,861	0.80	1.40	$178,595
HDO Feed Effluent Economizer	1	$353,600	2011	$353,600	0.70	2.66	$144,121
HDO Fixed Bed Reactor	1	$6,513,387	2011	$6,513,387	0.70	2.00	$10,818,487
Hydrogenation Intercooler (Bed 1)	1	$2,353,181	2007	$2,353,181	0.65	2.21	$480,336
Hydrogenation Intercooler (Bed 2)	1	$2,353,181	2007	$2,353,181	0.65	2.21	$659,401
H2 Makeup Compressor	1	$1,621,200	2011	$1,621,200	0.60	1.09	$1,185,438
H2 Makeup Compressor (Spare)	1	$1,621,200	2011	$1,621,200	0.60	1.08	$1,176,045
HHPS	1	$436,000	2013	$436,000	1.00	1.50	$119,027
HDO Hot Gas Cooler	1	$321,600	2011	$321,600	0.70	1.66	$17,178
CHPS	1	$328,500	2011	$328,500	0.70	2.59	$11,843
AA Evaporator Feed Tank	1	$45,966	2011	$45,966	0.60	2.50	$32,322
AA Evaporator Feed Heater	1	$274,818	2011	$274,818	0.60	3.00	$128,568
AA Evaporator Flash Drum	1	$511,000	2009	$511,000	0.70	2.00	$283,070
AA Condenser Drum	1	$487,000	2010	$487,000	0.60	2.80	$447,069
AA Crystallizer	2 (series)	$7,104,192	2011	$7,104,192	0.60	2.50	$4,042,752
AA Centrifuge Separator	1	$327,680	2011	$327,680	0.60	2.30	$380,919
AA Drier	2 (parallel)	$555,008	2011	$555,008	0.60	2.60	$775,462
						Area totals	**$72,432,373**

Table S7 (continued)

WASTEWATER TREATMENT	**Equipment Costs**						
EQUIPMENT TITLE	**NUM REQ**	**$**	**Year of Quote**	**Purch Cost in Base Yr**	**Scaling Exp**	**Inst Factor**	**Inst Cost in Proj year**
Anaerobic Digestion (AD) System							
Anaerobic System	4	$25,800,000	2012	$25,800,000	0.60	1.1	$20,512,669
Biogas Emergency Flare	4	INCLUDED	2012				
Aeration Basin	3	$4,908,054	2012	$4,908,054	0.60	2.1	$9,454,996
Pump - Submersible, Anaerobic Feed	2	INCLUDED	2012				
Pump - Centrifugal, Aeration Basin Feed	4	INCLUDED	2012				
Aeration Grid	1	INCLUDED	2012				
Caustic Feed System	4	$20,000	2012	$20,000	0.60	3.0	$42,976
Blowers	9	$2,070,000	2012	$2,070,000	0.60	2.0	$2,965,376
Surface Aerators	3	$150,000	2012	$150,000	0.60	2.7	$372,721
Membrane Bioreactor	1	$4,898,500	2012	$4,898,500	1.00	1.6	$7,497,959
Pump, Centrifugal , MBR, RAS	6	INCLUDED	2012				
Gravity Belt Thickeners	3	$750,000	2012	$750,000	0.60	1.6	$854,157
Centrifuge	1	$686,800	2012	$686,800	0.60	2.7	$1,323,311
Pump, Centrifugal, Centrifuge Feed	2	INCLUDED	2012				
Pump, Submersible, Centrate	2	INCLUDED	2012				
Dewatering Polymer Addition	2	INCLUDED	2012				
Conveyor	1	$7,000	2012	$7,000	0.60	2.9	$14,340
Reverse Osmosis	7	$2,450,000	2012	$2,450,000	1.00	1.8	$4,001,661
Evaporator	1	$5,000,000	2012	$5,000,000	0.60	1.6	$7,491,651
Ammonia Addition System	4	$195,200	2012	$195,200	0.60	1.5	$215,318
Sodium Sulfate Recovery							
Evaporator Feed Tank	1	$45,966	2011	$45,966	0.60	2.5	$255,872
Evaporator Feed Heater	1	$274,818	2011	$274,818	0.60	3.0	$241,453
Evaporator Flash Drum	1	$511,000	2009	$511,000	0.70	2.0	$3,163,561
Centrifuge	1	$327,680	2011	$327,680	0.60	2.3	$422,357
Dryer	1	$555,008	2011	$555,008	0.60	2.6	$785,346
						Area totals	**$59,615,726**

Table S7 (continued)

COGENERATION OF HEAT AND POWER	**Equipment Costs**						
EQUIPMENT TITLE	**NUM REQ**	**$**	**Year of Quote**	**Purch Cost in Base Yr**	**Scaling Exp**	**Inst Factor**	**Inst Cost in Proj year**
Burner Combustion Air Preheater	1	INCLUDED					
BFW Preheater	1	INCLUDED					
Pretreatment/BFW heat recovery	1	$41,000	2009	$41,000	0.70	2.2	$37,627
Air Intake Fan		INCLUDED					
Boiler	1	$28,550,000	2010	$28,550,000	0.60	1.8	$58,845,939
Turbine/Generator	1	$9,500,000	2010	$9,500,000	0.60	1.8	$14,332,829
Hot Process Water Softener System	1	$78,000	2010	$78,000	0.60	1.8	$160,634
Amine Addition Pkg.	1	$40,000	2010	$40,000	0.00	1.8	$70,810
Ammonia Addition Pkg	1	INCLUDED					
Phosphate Addition Pkg.	1	INCLUDED					
Condensate Pump	2	INCLUDED					
Turbine Condensate Pump	2	INCLUDED					
Deaerator Feed Pump	2	INCLUDED					
BFW Pump	5	INCLUDED					
Blowdown Pump	2	INCLUDED					
Amine Transfer Pump	1	INCLUDED					
Condensate Collection Tank	1	INCLUDED					
Condensate Surge Drum	1	INCLUDED					
Deaerator	1	$305,000	2010	$305,000	0.60	3.0	$1,046,868
Blowdown Flash Drum	1	INCLUDED					
Amine Drum	1	INCLUDED					
						Area totals	**$74,494,707**

UTILITIES AND STORAGE	**Equipment Costs**						
EQUIPMENT TITLE	**NUM REQ**	**$**	**Year of Quote**	**Purch Cost in Base Yr**	**Scaling Exp**	**Inst Factor**	**Inst Cost in Proj year**
Utilities System							
Cooling Tower System	1	$1,375,000	2010	$1,375,000	0.60	1.5	$2,221,224
Plant Air Compressor	1	$28,000	2010	$28,000	0.60	1.6	$44,060
Chilled Water Package	1	$1,275,750	2010	$1,275,750	0.60	1.6	$2,726,071
CIP System	1	$421,000	2009	$421,000	0.60	1.8	$1,297,008
Cooling Water Pump	3	$283,671	2010	$283,671	0.80	3.1	$908,382
Make-up Water Pump	1	$6,864	2010	$6,864	0.80	3.1	$75,178
Process Water Circulating Pump	1	$15,292	2010	$15,292	0.80	3.1	$63,888
Instrument Air Dryer	1	$15,000	2009	$15,000	0.60	1.8	$28,024
Plant Air Receiver	1	$16,000	2009	$16,000	0.60	3.1	$51,482
Process Water Tank No. 1	1	$250,000	2009	$250,000	0.70	1.7	$640,561
Storage							
Ammonia Storage Tank	2	$196,000	2010	$196,000	0.70	2.0	$478,711
CSL Storage Tank	1	$70,000	2009	$70,000	0.70	2.6	$20,169
CSL Storage Tank Agitator	1	$21,200	2009	$21,200	0.50	1.5	$6,678
CSL Pump	1	$3,000	2009	$3,000	0.80	3.1	$749
DAP Bulk Bag Unloader	1	$30,000	2009	$30,000	0.60	1.7	$54,582
DAP Bulk Bag Holder	1	INCLUDED					
DAP Make-up Tank	1	$102,000	2009	$102,000	0.70	1.8	$39,662
DAP Make-up Tank Agitator	1	$9,800	2009	$9,800	0.50	1.5	$15,652
DAP Pump	1	$3,000	2009	$3,000	0.80	3.1	$10,055
Sulfuric Acid Pump	1	$7,493	2010	$7,493	0.80	2.3	$40,584
Sulfuric Acid Storage Tank	1	$96,000	2010	$96,000	0.70	1.5	$304,042
Caustic Storage Tank	1	$96,000	2011	$96,000	0.70	1.5	$201,820
Firewater Storage Tank	1	$803,000	2009	$803,000	0.70	1.7	$1,416,890
Firewater Pump	1	$15,000	2009	$15,000	0.80	3.1	$48,264
Ethanol Storage	1	$670,000	2009	$670,000	0.70	1.7	$1,730,001
Isobutyl Acetate Storage	1	$670,000	2009	$670,000	0.70	1.7	$689,508
Cycloalkane Storage	1	$670,000	2009	$670,000	0.70	1.7	$904,222
Adipic Acid Storage	1	$690,900	2007	$690,900	0.65	1.850	$462,853
Sodium Sulfate Storage	1	$690,900	2007	$690,900	0.65	1.850	$469,189
						Area totals	**$14,949,507**

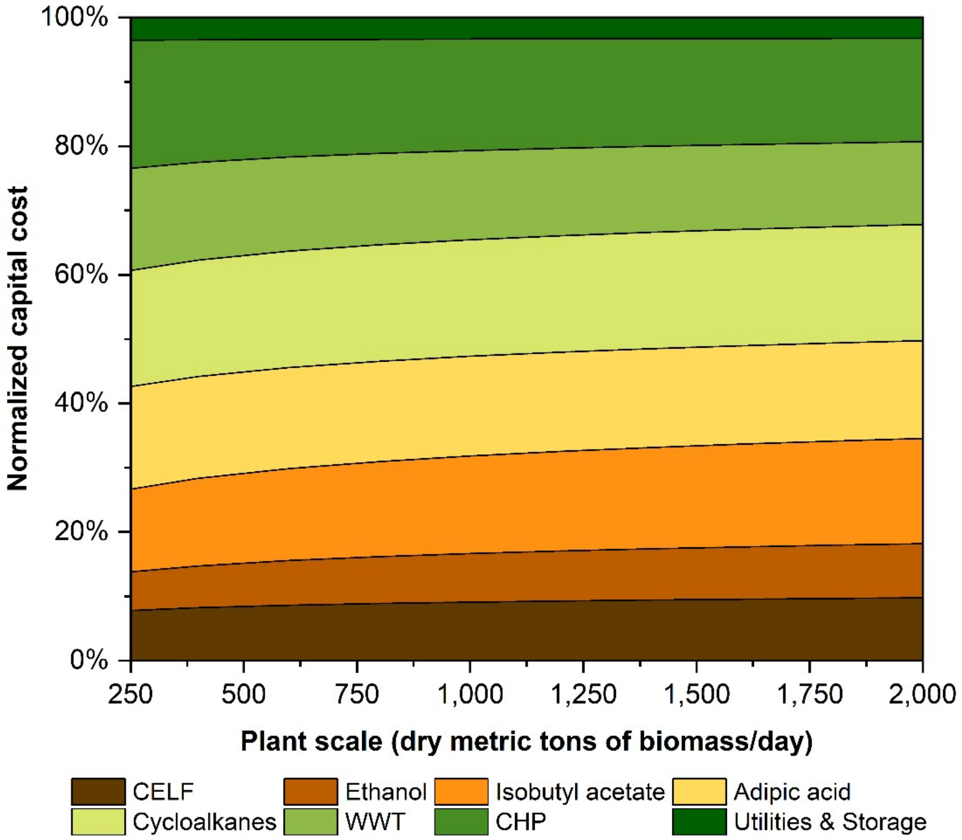

Figure S2. Breakdown of capital cost in a poplar/ethanol biorefinery with processing of lignin to cycloalkanes via AOR for different plant scales.

LCA methodology

Goal and Scope

The goal of this LCA is to quantify the environmental impacts of a CELF-based biorefinery and how those impacts are affected by feedstock selection, the primary alcohol product, and whether jet fuel is produced as a co-product. The scope of this LCA is farm-to-biorefinery-gate. Hereinafter, the assessed scenarios will be referred to by the numeric identification in Table S8.

Table S8. Numeric identification of scenarios for LCA discussion

Scenario	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Feedstock	Poplar	Poplar	Stover	Stover	Poplar	Poplar	Stover	Stover
Alcohol	iBuOH	iBuOH	iBuOH	iBuOH	EtOH	EtOH	EtOH	EtOH
Lignin fate	Jet	Burn	Jet	Burn	Jet	Burn	Jet	Burn

Allocation Methods

Allocation based on product mass and on product economic value is applied to divide total biorefinery impacts among the various co-products. In Scenario 1, the biorefinery also produces excess electricity for sale to the grid; emissions credits from this excess electricity are quantified using system expansion or displacement. The product mass-based allocation factors for the eight scenarios are given in Table S9. The product economic value-based allocation factors are given in Table S10, and the product prices used to calculate these factors are given in Table S11.

Table S9. Mass-based allocation factors.

Scenario	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Isobutanol	0.384	0.485	0.342	0.396	-	-	-	-
Ethanol	-	-	-	-	0.466	0.569	0.398	0.456
Jet fuel (cycloalkanes)	0.212	-	0.140	-	0.184	-	0.130	-
Adipic acid	0.128	0.161	0.153	0.176	0.111	0.135	0.141	0.161
Isobutyl acetate	0.144	0.182	0.205	0.237	0.125	0.153	0.189	0.217
Sodium sulfate	0.132	0.171	0.160	0.191	0.114	0.142	0.141	0.167

Table S10. Economic value-based allocation factors.

Scenario	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Isobutanol	0.334	0.413	0.288	0.328	-	-	-	-
Ethanol	-	-	-	-	0.326	0.404	0.260	0.298
Jet fuel (cycloalkanes)	0.192	-	0.123	-	0.194	-	0.128	-
Adipic acid	0.262	0.324	0.303	0.345	0.266	0.329	0.315	0.361
Isobutyl acetate	0.189	0.234	0.260	0.296	0.192	0.238	0.271	0.310
Sodium sulfate	0.022	0.028	0.026	0.031	0.022	0.029	0.026	0.031

Table S11. Product prices used to calculate economic value allocation factors.

	Product Prices (USD/kg)
Isobutanol	0.8
Ethanol	0.55075
Jet fuel (cycloalkanes)	0.83
Adipic acid	1.886
Isobutyl acetate	1.206
Sodium sulfate	0.156

Inventory Analysis

The biorefinery inputs normalized to the production of 1 GGE alcohol product are given in Table S12 for scenarios 1 – 4 and in Table S13 for scenarios 5 – 8. The corn stover feedstock is assumed to have 12% moisture by mass, and the poplar feedstock 20% moisture by mass. Glucose is assumed to be sourced from corn wet milling, as is the corn steep liquor and ethanol. Methanol is assumed to be synthesized from natural gas to obtain a lower purchase price.

Two biorefinery inputs, the C_{16} solvent and the polymer used in wastewater treatment, were excluded from the LCA system boundary due to a lack of reasonable proxy data. As both inputs were in small quantities (< 0.01 kg/GGE), this is expected to have no impact on the LCA conclusions.

Finally, Table S14 presents the GWP per GGE attributable to each biorefinery input for isobutanol (scenario 1) and ethanol (scenario 5).

Table S12. Biorefinery inputs per GGE of alcohol product, scenarios 1-4. Input units are in kg unless specified otherwise.

	Scenario	**1**	**2**	**3**	**4**
Feedstock	Poplar, bone dry	22.244	22.250	0	0
	Corn stover, bone dry	0	0	30.115	30.115
CELF	Sulfuric acid, 100%	0.335	0.335	0.427	0.427
	Water, ultrapure	0.025	0.025	0.032	0.032
	Tetrahydrofuran	0.447	0.447	0.552	0.552
	Lime	0.266	0.266	0.339	0.339
CBP to alcohol	Glucose	1.137	1.137	0.986	0.986
	Ammonia	0.115	0.115	0.102	0.102
Fermentation to isobutyl acetate	Ammonia	0.080	0.080	0.127	0.127
Adipic acid	Glucose	0.071	0.071	0.087	0.087
	Ammonia	0.013	0.013	0.024	0.024
	Diammonium phosphate	0.046	0.046	0.105	0.105
	Corn steep liquor	0.015	0.015	0.019	0.019
	Sulfuric acid, 100%	1.127	1.127	1.506	1.506
	Water, ultrapure	0.085	0.085	0.113	0.113
	Sodium hydroxide	0.231	0.231	0.308	0.308
	Ethanol	5.53E-03	5.54E-03	7.18E-03	7.18E-03
	Hydrogen	0.061	0.061	0.079	0.079
AOR to jet fuel	Methanol	0.910	0.000	0.675	0.000
Wastewater treatment	Sulfuric acid, 100%	2.62E-02	2.62E-02	6.44E-02	6.44E-02
	Water, ultrapure	1.97E-03	1.97E-03	4.85E-03	4.85E-03
	Ammonia	1.42E-02	1.09E-02	2.14E-02	1.60E-02
	Sodium hydroxide	7.27E-03	7.29E-03	1.09E-02	1.09E-02
Boiler	Boiler chemicals	2.90E-05	2.37E-05	3.22E-05	2.91E-05
	Lime	4.89E-03	4.45E-03	2.81E-02	2.72E-02
	Ammonia	0.218	0.209	0.409	0.398
	Natural gas (MMBTU)	0.270	0.115	0.277	0.175
Utilities	Cooling tower chemicals	1.19E-03	9.21E-04	1.29E-03	1.12E-03
	Makeup water	86.724	71.314	96.587	88.897
	Electricity (kWh)	0.000	0.218	0.164	0.824

Table S13. Biorefinery inputs per GGE of alcohol product, scenarios 5 – 8. Input units are in kg unless specified otherwise.

	Scenario	**5**	**6**	**7**	**8**
Feedstock	Poplar, bone dry	19.477	19.477	0	0
	Corn stover, bone dry	0	0	29.269	29.269
CELF	Sulfuric acid, 100%	0.294	0.294	0.415	0.415
	Water, ultrapure	0.022	0.022	0.031	0.031
	Tetrahydrofuran	0.391	0.392	0.536	0.536
	Lime	0.233	0.233	0.329	0.329
CBP to alcohol	Glucose	0.992	0.992	0.958	0.958
	Ammonia	0.103	0.103	0.102	0.102
Fermentation to isobutyl acetate	Ammonia	0.070	0.070	0.124	0.124
Adipic acid	Glucose	0.062	0.062	0.084	0.084
	Ammonia	0.012	0.012	0.023	0.023
	Diammonium phosphate	0.040	0.040	0.102	0.102
	Corn steep liquor	0.013	0.013	0.019	0.019
	Sulfuric acid, 100%	0.987	0.986	1.464	1.462
	Water, ultrapure	0.074	0.074	0.110	0.110
	Sodium hydroxide	0.203	0.202	0.300	0.299
	Ethanol	4.85E-03	4.86E-03	6.97E-03	6.98E-03
	Hydrogen	0.053	0.053	0.076	0.076
AOR to jet fuel	Methanol	0.797	0.000	0.657	0.000
Wastewater treatment	Sulfuric acid, 100%	2.29E-02	2.29E-02	6.26E-02	6.26E-02
	Water, ultrapure	1.73E-03	1.73E-03	4.71E-03	4.71E-03
	Ammonia	2.33E-02	1.96E-02	6.01E-02	5.10E-02
	Sodium hydroxide	5.33E-03	4.84E-03	8.79E-03	7.94E-03
Boiler	Boiler chemicals	1.74E-05	1.28E-05	2.10E-05	1.62E-05
	Lime	4.36E-03	3.98E-03	2.73E-02	2.65E-02
	Ammonia	0.188	0.180	0.393	0.381
	Natural gas (MMBTU)	0.134	0.000	0.124	0.000
Utilities	Cooling tower chemicals	5.46E-04	4.17E-04	6.76E-04	5.76E-04
	Makeup water	44.925	38.345	58.159	54.470
	Electricity (kWh)	2.402	3.325	3.885	4.081

Table S14. GWP per GGE attributable to each biorefinery input for isobutanol (scenario 1) and ethanol (scenario 5).

	Isobutanol	**Ethanol**
Process-level emissions	**13.62**	**11.49**
Feedstock (poplar)	**-15.11**	**-16.06**
Sulfuric acid	7.80E-02	8.29E-02
Water, ultrapure (for sulfuric acid dilution)	3.62E-05	3.85E-05
Tetrahydrofuran	1.20	1.27
Lime	8.12E-02	8.63E-02
Glucose	**0.25**	**0.03**
Ammonia	0.40	0.39
Diammonium phosphate	5.73E-02	6.08E-02
Corn steep liquor	5.16E-05	5.48E-05
Sodium hydroxide	6.29E-02	6.65E-02
Ethanol	1.37E-03	1.46E-03
Hydrogen	4.14E-02	4.40E-02
Methanol	0.26	0.27
Boiler water chemicals	1.77E-05	1.28E-05
Cooling tower chemicals	9.82E-04	5.45E-04
Natural gas	**2.34**	**1.41**
Electricity	**-0.35**	**0.88**

Table S15. GWP attributable to each product in CELF-based biorefineries producing isobutanol (baseline data for Figure 7, main text).

Scenario	**Coproduct**	***Production, kg/GGE main product***	**Baseline**	**CELF-Based biorefinery**
			GWP, kg CO_2eq/GGE main product	***GWP, kg CO_2eq/GGE main product***
1	Isobutanol	3.73	11.15	2.93
	Cycloalkanes	2.07	1.12	1.62
	Adipic acid	1.24	30.18	0.98
	Isobutyl acetate	1.40	6.01	1.10
	Sodium sulfate	1.29	0.74	1.01
	TOTAL	**-**	**49.19**	**7.65**
2	Isobutanol	3.73	11.15	0.92
	Cycloalkanes	0.00	0.00	0.00
	Adipic acid	1.24	30.20	0.31
	Isobutyl acetate	1.40	6.01	0.35
	Sodium sulfate	1.32	0.76	0.33
	TOTAL	**-**	**48.12**	**1.90**
3	Isobutanol	3.73	11.15	4.05
	Cycloalkanes	1.53	0.83	1.66
	Adipic acid	1.66	40.46	1.81
	Isobutyl acetate	2.23	9.58	2.43
	Sodium sulfate	1.75	1.01	1.90
	TOTAL	**-**	**63.03**	**11.86**
4	Isobutanol	3.73	11.15	3.29
	Cycloalkanes	0.00	0.00	0.00
	Adipic acid	1.66	40.46	1.47
	Isobutyl acetate	2.23	9.58	1.97
	Sodium sulfate	1.80	1.04	1.59
	TOTAL	**-**	**62.23**	**8.32**

Table S16. GWP attributable to each product in CELF-based biorefineries producing ethanol (baseline data for Figure 7, main text).

Scenario	**Coproduct**	***Production, kg/GGE main product***	**Baseline**	**CELF-Based biorefinery**
			GWP, kg CO_2eq/GGE main product	***GWP, kg CO_2eq/GGE main product***
5	Ethanol	4.57	-19.10	0.04
	Cycloalkanes	1.81	0.98	0.01
	Adipic acid	1.09	26.43	0.01
	Isobutyl acetate	1.23	5.26	0.01
	Sodium sulfate	1.11	0.64	0.01
	TOTAL	**-**	**14.21**	**0.08**
6	Ethanol	4.57	-19.10	-2.83
	Cycloalkanes	0.00	0.00	0.00
	Adipic acid	1.09	26.41	-0.67
	Isobutyl acetate	1.23	5.26	-0.76
	Sodium sulfate	1.14	0.66	-0.71
	TOTAL	**-**	**13.23**	**-4.98**
7	Ethanol	4.57	-19.10	2.45
	Cycloalkanes	1.49	0.81	0.80
	Adipic acid	1.62	39.32	0.87
	Isobutyl acetate	2.17	9.31	1.17
	Sodium sulfate	1.62	0.93	0.87
	TOTAL	**-**	**31.26**	**6.16**
8	Ethanol	4.57	-19.10	0.21
	Cycloalkanes	0.00	0.00	0.00
	Adipic acid	1.62	39.30	0.08
	Isobutyl acetate	2.17	9.31	0.10
	Sodium sulfate	1.67	0.96	0.08
	TOTAL	**-**	**30.46**	**0.47**

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