Supplementary Information for

Advanced diesel from ethanol, a pathway to produce sustainable and high-quality drop-in biofuels

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S1. Supplemental information for cofeeding experiments

Table S1. Detailed mole flow in inlet and outlet of Guerbet coupling reactor for cofeed (Ethanol (70% mol) / Butanol (30%)) and control experiments (pure ethanol feed). WHSV values reported are in units of $g_{ethanol}\ h^{-1}\ g_{cat}^{-1}$.

	Cofeed 1		Control 1		Cofeed 2		Control 2		Cofeed 3		Control 3	
WHSV (h^{-1})	26.27		26.27		6.53		6.53		1.33		1.33	
Mass catalyst (g)	0.1005		0.1003		0.1002		0.1		0.7429		0.4047	
	C flow (μmol C/min)											
Compound	**inlet**	**outlet**	**inlet**	**outlet**	**inlet**	**outlet**	**inlet**	**outlet**	**inlet**	**outlet**	**inlet**	**outlet**
Methane				5.82		2.67		0.14		0.76		0.60
ethylene				0.16		0.07		0.04		0.44		0.26
ethane				0.12		0.07		0.03		0.28		0.08
propane		3.83		0.19		0.19		0.06		0.43		
propene				0.26		0.55		0.33		1.17		0.04
methanol								0.06		1.90		0.72
1-butene		3.27		0.81		0.10		0.33		0.80		
n-butane						0.24		0.01		0.10		
acetone								0.00		9.74		0.77
acetaldehyde		150.38		129.06		30.51		27.57		92.12		34.83
n-pentane		1.04				0.77						
diethyl ether		0.18		0.81		0.03		0.22				1.49
pentenes				1.21				0.86		0.14		
n-hexane		0.68		1.85		0.01		1.31				
ethanol	1910.51	1402.82	1918.15	1282.04	473.28	275.68	479.54	275.39	718.60	244.07	411.03	111.14
2-propanol				1.09		0.31		0.23		2.26		0.82
butyraldehyde		228.03		59.29		56.71		17.23		127.99		33.42
ethyl acetate		31.31		33.59		9.07		7.65		33.80		16.50
2-butanol				1.06		0.25		0.03				
2-butanone		2.02		3.71		0.87		0.49		11.40		1.24
1-butanol	1626.66	1427.11		268.31	401.28	329.95		72.88	612.70	368.37		73.33
cis-crotyl alcohol		0.73		1.26				0.48				
1,1-diethoxyethane		1.11		11.52		0.71		5.64				2.94
2-pentanone		9.86		4.48		3.50		1.34		34.88		7.15
2-pentanol				0.72				0.09		3.91		0.59
2-methyl-1-butanol		1.07				0.19				1.23		
2-ethylbutanal		7.66		3.78		0.20		0.45		11.48		3.65
ethyl butanoate		25.76		11.57		9.27		4.08		41.35		14.59
butyl acetate		22.98		4.90		7.52		1.41		34.09		13.18
hexanal		18.88		8.72		7.32		3.59		20.95		4.85
2-ethylbutan-1-ol		23.49		10.15		10.02		3.88		22.32		5.47
1,1-diethoxybutane		1.25		2.74		0.62		1.67				0.72
1-butoxy-1-ethoxyethane				4.50		1.49		2.52				
1-hexanol		98.20		37.82		35.88		15.39		51.09		11.04

4-heptanone		0.51		2.39		3.43		0.71		19.86		5.52
2-heptanol						0.29				0.94		
2-heptanone		1.87		0.85		1.15		0.32		9.92		2.30
2-ethylhexanal		2.98		1.10		1.62		0.67		5.79		1.35
2-ethylbutyl acetate										1.25		
butyl butanoate		18.35		1.49		7.24		0.72		35.40		4.12
ethyl hexanoate		4.56		2.59		2.61		1.17		9.72		3.54
3-octanone						0.18				1.00		
hexyl acetate		1.81		0.82		0.93		0.34		5.13		1.50
octanal		2.18		1.76		1.40		0.91		3.91		1.65
2-ethylhexan-1-ol		8.11		2.30		4.25		1.44		9.70		1.45
1,1-dibutoxyethane		1.61		1.15		1.06		0.62		1.06		0.68
1-octanol		10.62		7.02		5.61		3.99		8.56		2.45
4-nonanone		2.24		1.01		1.98		0.45		8.23		1.35
2-nonanone						0.39		0.08		2.38		1.19
2-Ethylbutyl butyrate						0.12				1.29		
butyl hexanoate		5.56		0.51		3.69		0.40		17.01		4.97
hexyl butanoate				0.70				0.38				
octyl acetate		0.40						0.13		1.09		
2-ethyloctan-1-ol						0.47		0.25		0.82		
decanal				0.60		0.49		0.42				
2-hexyl-1-octanol		0.98		0.70		1.10		0.68		2.08		0.16
1-decanol		1.47		1.11		0.68		1.26		1.41		0.18
4-undecanone						1.23		0.21		2.83		0.36
hexyl hexanoate		1.26				0.39		0.44		5.01		0.97
butyl decanoate						0.32						
decyl acetate								0.02				
butyl decanoate								0.03				
2-ethylhexyl ester butanoate										0.83		
2-undecanone										0.82		
2-butyl-1-octanol								0.03				
2-ethyl-1-decanol								0.35				
1-dodecanol								0.40		1.11		
2-tridecanone												1.13
Missing Carbon		10.96		0.53		47.88		16.90		55.72		36.74

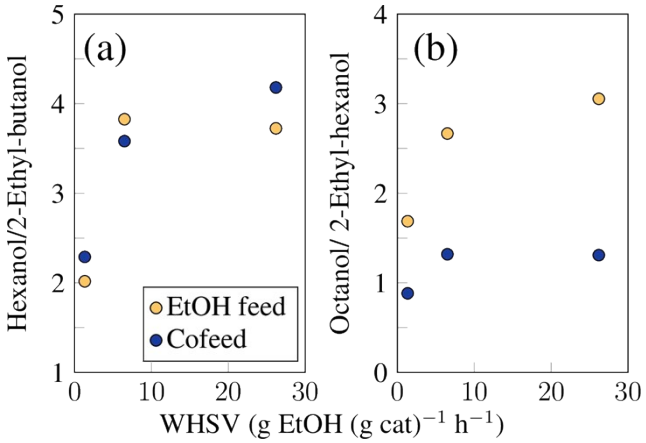

Figure S1. Mol ratio of (a) Hexanol to 2-Ethyl-butanol and (b) Octanol to 2-Ethyl-hexanol when cofeeding Ethanol (70% mol) / Butanol (30%) (blue circles) accompanied with control experiments with pure ethanol feed (yellow circles). T=325°C, P_{tot}=300 psig, Ethanol+Butanol:H_2= 4:1, 100-300 mg 0.1%Cu/Mg_3AlO.

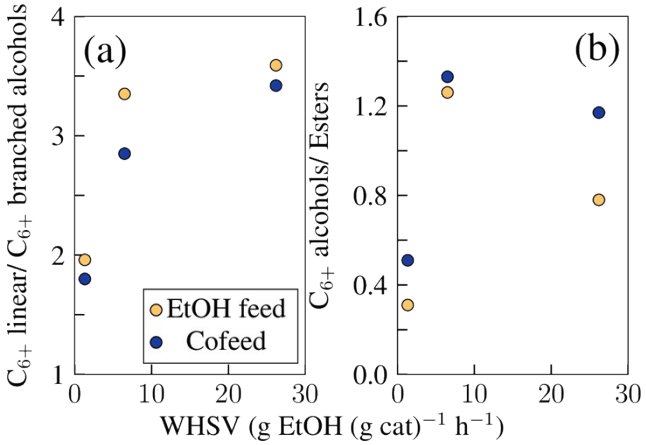

Figure S2. (a) C6+ Linear to branched alcohols ratio and (b) C6+ alcohols to ester ratio when cofeeding Ethanol (70% mol) / Butanol (30%) (blue circles) accompanied with control experiments with pure ethanol feed (yellow circles). T=325°C, Ptot=300 psig, Ethanol+Butanol:H2= 4:1, 100-300 mg 0.1%Cu/Mg3AlO.

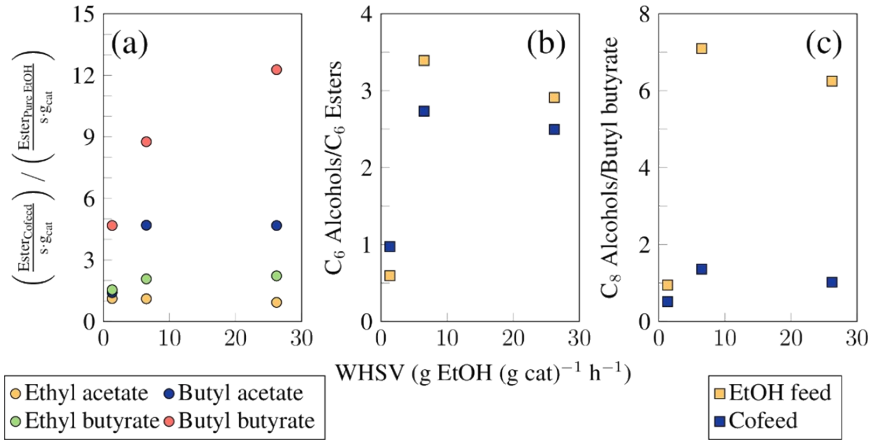

Figure S3. (a) Mol flow of esters in cofeed strategy / esters in control experiments, (b) mol ratio of C6 alcohols to C6 esters, and (c) mol ratio of C8 alcohols to butyl butyrate as a function of WHSV for cofeed strategy and control experiments.

S2. Supplemental information for hydrogenolysis experiments

Table S2. Composition used to evaluate the hydrogenolysis catalyst. Real G-66 data from a previous work[1]. Renormalized G-66 refers to the mol fractions produced when molecules with alkyl chains with more than eight carbons are neglected. Experimental G-66 represents the mol fraction of the simulated Guerbet stream produced in-house. In all the columns the overall alcohol and ester mol fraction was targeted to remain constant.

Compound	Real G-66 (%)	Renormalized G-66 (%)	Experimental G-66 (%)
1-Butanol	62.88	64.54	63.86
2-pentanol	1.74	1.79	2.08
1-hexanol	13.28	13.63	13.63
2-ethyl-1-butanol	4.67	4.79	4.99
2-heptanol	1.16	1.19	1.19
1-octanol	3.27	3.36	3.32
2-ethyl-1-hexanol	3.04	3.12	3.27
4-nonanol	0.69		
1-decanol	0.75		
2-undecanol	0.36		
1-dodecanol	0.36		
1-tetradecanol	0.09		
2-Pentadecanol	0.12		
2-Heptadecanol	0.00		
Isopropyl acetate	0.00		
ethyl butanoate	0.00		
Butyl acetate	0.00		
Isopropyl butyrate	0.09		
Butyl butanoate	1.95	2.23	2.20
Ethyl hexanoate	1.09	1.25	1.22
Hexyl acetate	0.70	0.80	0.86
Butyl hexanoate	1.62	1.85	1.83
Hexyl butanoate	0.19	0.21	0.22
Ethyl octanoate	0.00	0.00	0.00
Octyl acetate	0.12	0.14	0.16
Octyl butanoate	0.10	0.12	0.15
Butyl octanoate	0.05	0.06	0.07
Ethyl decanoate	0.73		
Decyl acetate	0.05		
Hexyl hexanoate	0.10	0.12	0.12
Hexyl octanoate	0.58	0.66	0.64
Ethyl dodecanoate	0.04		
Dodecyl acetate	0.04		
Octyl octanoate	0.12	0.13	0.19
Alcohol mol frac.	92.42	92.42	92.35
Ester mol frac.	7.58	7.58	7.65

Table S3. Mole concentration in the outlet of hydrogenolysis reactor for the model mixture Hexyl acetate – Butanol 95-5% mol, accompanied by the percentage of ethyl, butyl, and hexyl chains identified at the outlet of the reactor with respect to those that were fed. Data reported at WHSV=0 was obtained from Aspen Plus, while data at WHSV=$^{\infty}$ represents the mole concentration of all the species in the feed.

WHSV (h^{-1})	$^{\infty}$ (Feed)	0.81	0.40	0.16	0.05	0 (ASPEN)
Compound	**(mM)**	**Mole concentration outlet reactor (mM)**				
acetaldehyde		9.17	0.01	0.01	10.89	1.59
ethanol		171.27	269.11	443.35	515.67	512.26
butyraldehyde		30.24	20.40	32.59	39.27	6.27
ethyl acetate		6.90	6.96	13.47	19.84	0.10
1-butanol	9973.90	9604.26	9718.54	9767.44	9777.09	9788.50
ethyl butanoate		5.04	2.54	5.44	3.37	3.10
butyl acetate		305.99	196.61	52.88	2.55	3.48
1-hexanol		482.34	460.94	479.58	483.80	516.31
butyl butanoate		13.14	23.50	40.85	40.50	45.98
hexyl acetate	524.94	19.08	22.85	2.77	0.08	0.16
butyl hexanoate		1.91	2.81	4.51	4.52	1.83
hexyl hexanoate		0.00	0.51	0.26	0.00	0.09
	Balance of Alkyl chains (%)					
Ethyl chain	-	101.9	100.8	103.1	101.3	-
Butyl chain	-	100.8	101.5	100	95.4	-
Hexyl chain	-	97.8	98.2	96.1	92.2	-

Table S4. Set of linearly independent reactions implemented in a thermodynamic equilibrium reactor in Aspen Plus for the hydrogenolysis of our model mixture.

item	Reaction
1	$ethyl\ acetate + H_2 \leftrightarrows$ ethanol + acetaldehyde
2	$butyl\ acetate + H_2 \leftrightarrows$ butanol + acetaldehyde
3	$hexyl\ acetate + H_2 \leftrightarrows$ hexanol + acetaldehyde
4	$ethyl\ butyrate + H_2 \leftrightarrows$ ethanol + butyraldehyde
5	$butyl\ butyrate + H_2 \leftrightarrows$ butanol + butyraldehyde
6	$hexyl\ \ butyrate + H_2 \leftrightarrows$ hexanol + butyraldehyde
7	$ethyl\ hexanoate + H_2 \leftrightarrows$ ethanol + hexanol
8	$butyl\ hexanoate + H_2 \leftrightarrows$ butanol + hexanol
9	$hexyl\ hexanoate + H_2 \leftrightarrows$ hexanol + hexanol
10	acetaldehyde $+ H_2 \leftrightarrows$ ethanol
11	$butylraldehyde + H_2 \leftrightarrows$ butanol
12	hexanal $+ H_2 \leftrightarrows$ hexanol

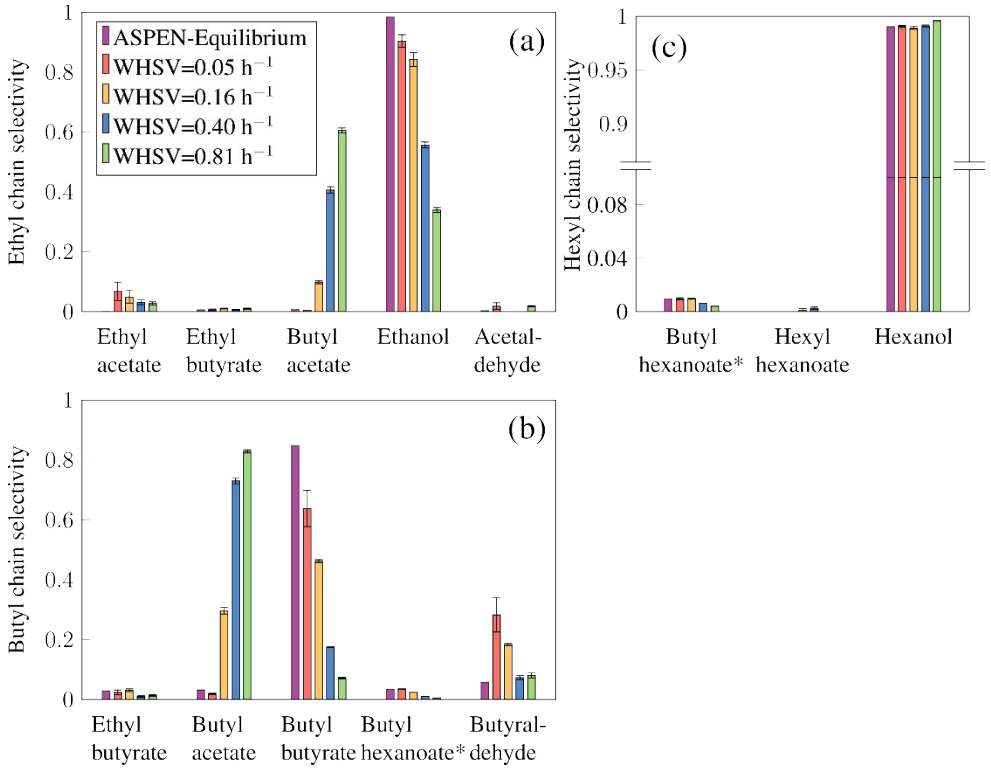

Figure S4. Alkyl chains selectivity at various WHSV for a blend of 5% hexyl acetate and 95% butanol, T=200°C, P_{tot}=420 psig, hexyl acetate:H_2= 1:480, 100-300 mg 10%wt. Cu/ZrO_2. The butyl hexanoate marked with *in figure (b) and (c) represents the sum of butyl hexanoate and hexyl butanoate given that both esters had similar retention times in our analytics and peak deconvolution was not possible to differentiate both species

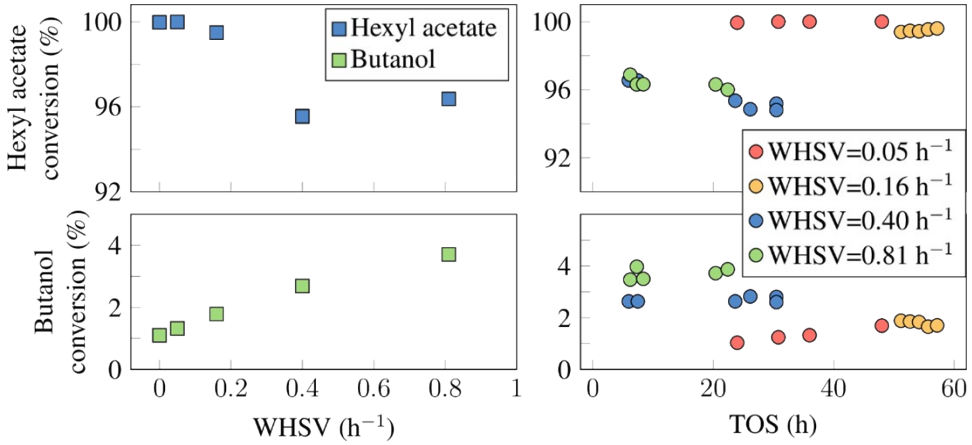

Figure S5. Hexyl acetate and Butanol conversion as a function of WHSV (left) and TOS (h) (right).

Table S5. Linearly independent reactions for the hydrogenolysis equilibrium reactor using a simulated Guerbet stream. *Item* starts from 13 because these reactions are a complement for Table S1.

item	Reaction
13	2-Pentanone $+ H_2 \leftrightarrows$ 2-Pentanol
14	2-Heptanone $+ H_2 \leftrightarrows$ 2-Heptanol
15	2-Ethyl-butanal $+ H_2 \leftrightarrows$ 2-Ethyl-butanol
16	2-Ethyl-hexanal $+ H_2 \leftrightarrows$ 2-Ethyl-hexanol
17	$Octanal + H_2 \leftrightarrows$ Octanol
18	$Ethyl\ octanoate + H_2 \leftrightarrows$ Ethanol + Octanal
19	$Butyl\ octanoate + H_2 \leftrightarrows$ Butanol + Octanal
20	$Hexyl\ octanoate + H_2 \leftrightarrows$ Hexanol + Octanal
21	$Octyl\ octanoate + H_2 \leftrightarrows$ Octanol + Octanal
22	$Octyl\ Acetate + H_2 \leftrightarrows$ Octanol + Acetaldehyde
23	$Octyl\ butyrate + H_2 \leftrightarrows$ Octanol + Butyraldehyde
24	$Octyl\ hexanoate + H_2 \leftrightarrows$ Octanol + hexanal

Table S6. Molar concentration distribution of all the species identified in our experiment for the Guerbet coupling stream Renormalized G-66 presented in table S2 run at WHSV=0.07 h^{-1}. Molar concentrations in the liquid phase for the feed, the experimental results after reaction and equilibrium concentrations predicted by Aspen are presented in mmol/L.

	Mole concentration (mM)		
Compound	**Feed**	**Experiment (WHSV=0.07 h^{-1})**	**Equilibrium (ASPEN)**
Ethanol	0.00	239.16	198.07
Butanol	5824.53	6376.23	6271.45
Hexanol	1243.16	1625.34	1658.94
Octanol	302.81	386.49	420.13
2-ethyl-butanol	455.13	439.07	445.11
2-ethyl-hexanol	298.25	282.55	292.33
2-pentanol	189.71	170.42	181.31
2-heptanol	108.54	91.10	34.65
Acetaldehyde	0.00	7.41	0.62
Butyraldehyde	0.00	17.19	4.02
Hexanal	0.00	0.37	1.56
Octanal	0.00	0.00	0.13
2-ethyl-butanal	0.00	0.00	1.56
2-Ethyl-hexanal	0.00	0.00	0.37
2-pentanone	0.00	9.83	4.87
2-heptanone	0.00	5.09	71.87
Butyl butyrate	200.66	13.97	14.64
Butyl acetate	0.00	0.00	0.66
Ethyl acetate	0.00	0.00	0.01
Ethyl butyrate	0.00	1.79	0.59
Hexyl acetate	78.44	0.00	0.15
Ethyl hexanoate	111.27	0.00	0.09
Hexyl butyrate	20.07	7.58	2.95
Butyl hexanoate	166.91	0.00	2.95
Hexyl hexanoate	10.94	0.00	0.76
Ethyl octanoate	0.00	0.00	0.25
Butyl octanoate	6.38	2.75	0.73
Hexyl octanoate	58.37	0.89	0.19
Octyl octanoate	17.33	0.54	0.05
Octyl acetate	14.59	0.00	0.05
Octyl butyrate	13.68	0.00	0.73
Octyl hexanoate	0.00	0.00	0.19

S3. Supplemental information for etherification experiments

Table S7. Set of reactions used in the etherification reactor model. Conversion for each reaction was determined based on the experimental results obtained. Chemical species labeling: letter indicates species type, and number carbon length. A: alcohol, O: olefins, E:Ethers, and W: water. If more than one ether of length "X" is produced it is indicated with a second number (e.g., E12-1, and E12-2). Secondary alcohols are shown by adding the particle 2N to the name (e.g., A9-2N).

Item	Reaction	Conversion
1	2A4->E8+W	0.159
2	A4 + A6-2 --> E10 + W	0.115
3	A4 + A6 --> E10-1+ W	0.258
4	A4 + A8-2 --> E12 + W	0.153
5	A4 + A8 --> E12-3 + W	0.195
6	A4--> O4 + W	0.013
7	A4-2N --> O4 + W	1
8	A5-2 -->O5 + W	0.491
9	A6 + A6-2 --> E12-1 + W	0.03
10	2 A6 --> E12-2+ W	0.372
11	A6 + A8 --> E14 + W	0.373
12	A6 + A8-2 --> E14-1+ W	0.272
13	2 A6 --> E12-2 + W	0.028
14	A6-2 + A8 --> E14-2 + W	0.035
15	A6-2 --> O6+ W	0.385
16	A7-2N --> O7 + W	1
17	A8-2 --> O8 + W	0.432
18	2 A8 --> E16-3 + W	0.04
19	A8 --> O8 + W	0.107
20	A8-2N --> O8 + W	0.432
21	A8-2N --> O8 + W	0.432
22	A9-2N --> O9 + W	1

S4. Supplemental information for the technoeconomic analysis

Table S8. Parameters and assumptions in the discounted cash flow analysis

	Parameter value	Source
General parameters		
Reference capacity	504 Ton/day	[2]
Reference year	2021	
Financial variables		
Equity	40%	
Loan interest	8%	
Loan term (years)	10	
Operation period (years)	30	[2]
Depreciation period (years)	7	
Construction period (years)	3	
Discount rate	10%	
Income tax	21%	
Working capital (% of FCI)	5%	
Direct costs		
OSBL (% of ISBL)	40%	
Warehouse (% of ISBL)	4%	[2]
Site development (% of ISBL)	9%	
Additional piping (% of ISBL)	4.5%	
Indirect costs		
Proratable expenses (% TDC)	10%	
Field development (% TDC)	10%	
Office & construction fee (% TDC)	20%	[2]
Contingency (% TDC)	40%	
Other cost (%TDC)	10%	
Materials		
Ethanol ($/kg)	0.999	[2]
H_2 ($/kg)	1.43	[3]
Catalyst Guerbet ($/Kg)	27.76	[4]
Catalyst Hydrogenolysis ($/Kg)	28.72	[4]
Catalyst Etherification ($/Kg)	18.5	[5]
Catalyst Oligomerization ($/Kg)	6	[6]
Utilities		
Refrigerant ($/kJ)	2.24×10^{-7}	
Water ($/kJ)	2.24×10^{-7}	
Low pressure steam ($/kJ)	2.00×10^{-6}	
Medium pressure steam ($/kJ)	2.32×10^{-6}	[1]
Hot oil ($/kJ)	3.69×10^{-6}	
Fired heat ($/kJ)	4.48×10^{-6}	
Electricity ($/kJ)	1.68×10^{-5}	
Waste management		
Waste treatment($/kg-organic)	0.35	[7]
Labor		
Shifts	5	
Manager	1 ($193.000)	
Engineers	3($92.000)	
Maintenance supervision	3 ($75.000)	[2]
Maintenance technicians	15 ($53.000)	
Shift supervisors	5 ($63.000)	
Shift operators	25($52.000)	

Table S9. Details of the process equipment cost and design parameters for the different areas. P: pressure of operation. T: temperature of operation. ΔP: pressure drop. N: number of plates.

	Equipment	Cost	P [Bar]	T [°C]	Duty	ΔP [Bar]	N	Reflux	Feed stage
Guerbet coupling area	Guerbet reactor	$1.41	25	325					
	Hydrogenolysis reactor	$3.85	25		0				
	Compressor 1	$5.15				1			
	Compressor 2	$1.41				3			
	Compressor 3	$1.52				5			
	Pump 1	$0.44				25			
	Pump 2	$0.54				25			
	Pump 3	$0.53				25			
	Pump 4	$0.39				22			
	Pump 5	$0.05				7			
	Pump 6	$0.35				17			
	Flash vessel 1	$0.56	24	25					
	Flash vessel 2	$0.18	1	35					
	Flash vessel 3	$0.08	3	35					
	Flash vessel 4	$0.08	8	35					
	Column 1-Guerbet	$4.63	1				20	1	10
	Column 2-Guerbet	$3.57	1				30	1	10
	Column 3-Guerbet	$4.25	1				60	1	10
	Column 4-Guerbet	$9.11	1				60	1.7	10
	Column 5-Guerbet	$1.71	1				31	1	10
Etherification area	Etherification reactor	$0.24	7		0				
	Pump 1	$0.13	6						
	Pump 2	$0.04	6						
	Flash vessel	$0.12	1	78					
	Column 1-Etherification	$3.39	5				35	2	10
	Column 2-Etherification	$1.08	1				20	2	10
	Column 3-Etherification	$4.79	1				60	6	15
	Column 4-Etherification	$7.93	3				40	4	9
	Column 5-Etherification	$0.61	1				20	2	10
	Column 6-Etherification	$1.84	1				20	2	10
	Column 7-Etherification	$1.10	1				20	2	10
Olig.	Oligomerization reactor	$0.41	40	230					
	Pump 1	$0.50				40			
	Pump 2	$0.49				38			
	Column 1-Oligomerization	$0.82	2				25	2	10
Sep.	Column 1-Final fractionation	$0.62	1				20	2	10
	Column 3-Final fractionation	$0.52	1				20	1.5	10
	Column 3-Final fractionation	$2.04	1				40	3	10

Table S10. Results for Guerbet coupling with 30% conversion using a cofeed strategy. The table shows the carbon stoichiometry of the reaction, i.e., it shows that at 30% conversion 73.73 mols of ethanol and 26.27 mols of butanol, yield a blend consisting of parafins (P), olefins (O), alcohols (A), aldehydes (AL), ketones (K), esters (ES) and some other minor components.

Component	Symbol	Carbon stoichiometry
Ethanol	A2	-73.73
Butanol	A4	-26.27
ethane	P2	0.03
n-propane	P3	0.09
n-butane	P4	0.01
n-pentane	P5	0.15
n-hexane	P6	0.00
ethylene	O2	0.03
propene	O3	0.25
1-butene	O4	0.14
1-pentene	O5	0.15
2-propanol	A3	0.52
2-butanol	A4-2	0.11
2-methyl-1-butanol	A5-2N	0.09
2-ethylbutan-1-ol	A6-2	4.50
1-hexanol	A6	16.13
2-heptanol	A7-2N	0.13
2-ethylhexan-1-ol	A8-2	1.91
1-octanol	A8	2.52
2-ethyloctan-1-ol	A10-2	0.21
1-decanol	A10	0.31
2-hexyl-1-octanol	A12-2	0.50
acetaldehyde	AL2	13.72
butyraldehyde	AL4	25.50
2-ethyl-2-butenal	AL6-2	0.09
hexanal	AL6	3.29
2-ethylhexanal	AL8-2	0.73
octanal	AL8	0.63
decanal	AL10	0.22
2-butanone	K4	0.39
2-pentanone	K5	1.57
2-heptanone	K7	2.06
3-octanone	K8	0.08
2-nonanone	K9	1.07
4-undecanone	K11	0.55
ethyl acetate	ES4	4.08
ethyl butanoate	ES6	4.17
butyl acetate	ES6-2	3.38
butyl butanoate	ES8	3.26
ethyl hexanoate	ES8-2	1.18
acetic acid, hexyl ester	ES8-3	0.42
butyl hexanonate	ES10	1.66
butanoic acid, 2-ethyl, butyl ester	ES10-2	0.14
hexyl hexanoate	ES12	0.62
butyl decanoate	ES14	0.14
diethyl ether	E4	0.01
1-propoxy-1-ethanol	B5	0.64
1,1-diethoxybutane	B8	0.28
1-butoxy-1-ethoxyethane	B8-2	0.67
1,1-dibutoxyethane	B10	0.48
COx	CO2	1.20

S5. Supplemental information for lifecycle analysis

The inventory for the upgrading process is shown in table S11 and the composition of the energy mix in this study in table S12. The upgrading process is modelled in detail. Other processes such as biomass cultivation, and ethanol production are modeled based on processes on GREET. Figure S6 shows the boundaries of the system as well as the foreground and background processes.

Table S11. Inventory for the upgrading process

Inputs	Feedstock	Ethanol	21034.7	Kg/h
		Hydrogen	1164.0	Kg/h
	Catalyts	0.1%Cu/Mg_3AlO	0.4	Kg/h
		Cu/ZrO_2	73.0	kg/h
		Zeolite	6.2	kg/h
	Energy	Natural gas	241594646.0	kJ/h
		Electricity	9798416.6	kJ/h
Outputs	Products	Diesel	486647074.2	kJ/h
		Gasoline	23203594.5	kJ/h
	Emissions to water	Organic components to water	344.1	kg/hr
		Water	6081.6	kg/hr
	Emissions to air	CO2	4160.1	kg/hr
		Water	12971.0	kg/hr

Table S12. US energy mix used in this study.

Source	Percentage
Oil fired power generation	0.2736
Coal fired power generation	23.8358
Natural gas fired power generation	36.47.33
Nuclear power generation	19.5598
Biomass power generation	0.32
Hydroelectric power generation	6.5338
Geothermal electricity production	0.3989
Wind power generation	9.4761
Solar power plant	2.6834
Electricity from biogenic waste, and other sources	0.4413

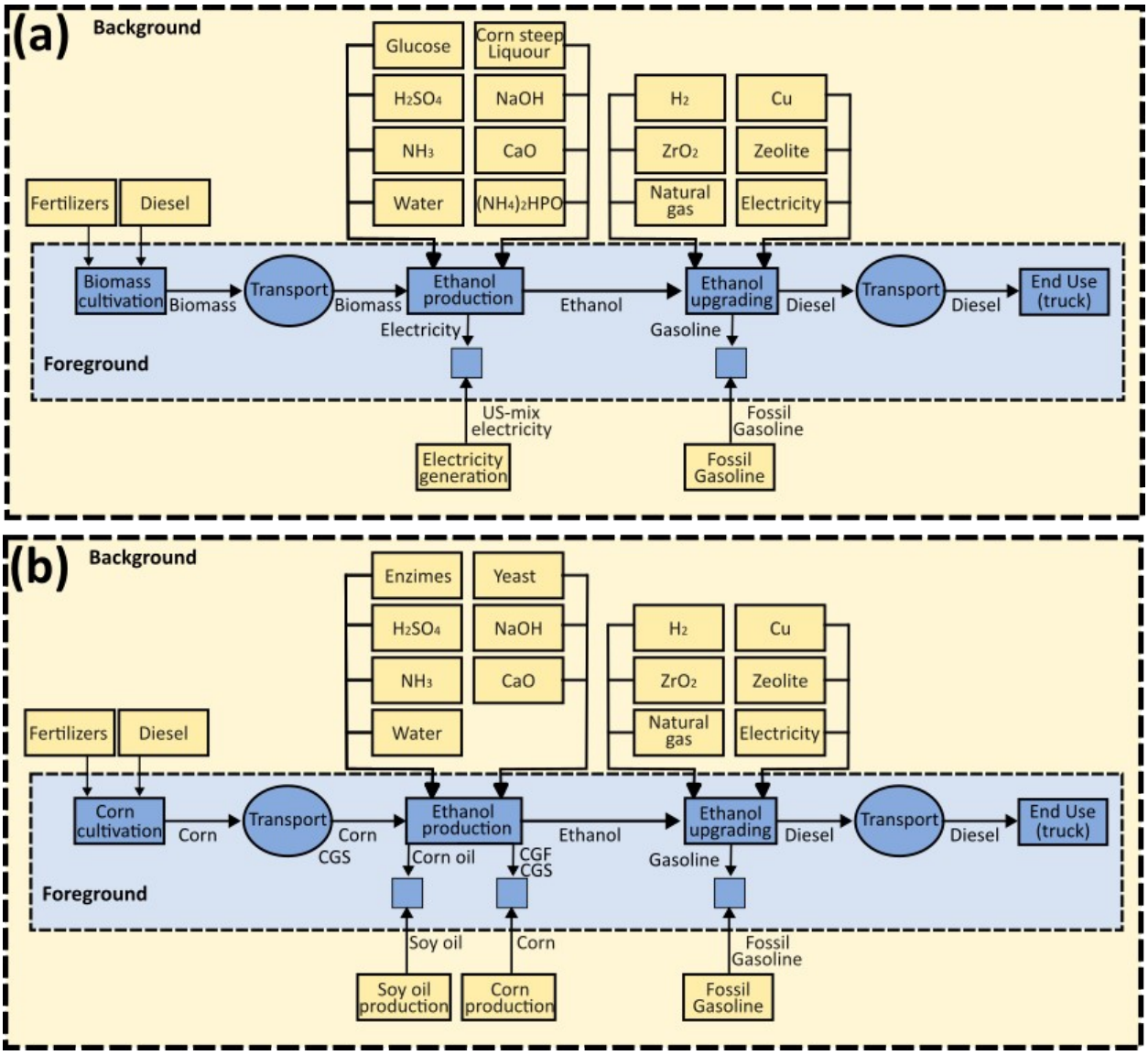

Figure S6. System boundaries (a) systems that use ethanol produced from lignocellulosic biomass (b) systems that use ethanol produced from corn as feedstock.

While the process that we have developed has been optimized to reduce cost and environmental impacts, there are still possible technological developments. Future improvements may lead to even lower environmental impacts. To explore the impact of these potential improvements on GHG emissions, we perform a parametric analysis in Figure S7. In this figure, we focus on two feedstocks, corn ethanol (coupled with carbon capture) and corn stover. We select these feedstocks considering their abundance in the U.S.[8]. In the parametric analysis, we systematically vary the biorefinery energy needs (which can be reduced for example by operating at higher conversions), and the hydrogen consumption in the system (which can be reduced for example by improving the gas separation operations). Two limiting cases are explored, a pessimistic case in which all settings correspond to scenario 1 on Figure 11, and an optimistic case in which settings correspond to scenario 8. In the figure the relative energy and hydrogen consumption with respect to the base case design are systematically

changed in the x-axis and y-axis respectively. Interestingly, in the optimistic case, the carbon footprint is reduced with increased energy consumption. This is explained by considering that the natural gas used in this case has negative emissions.

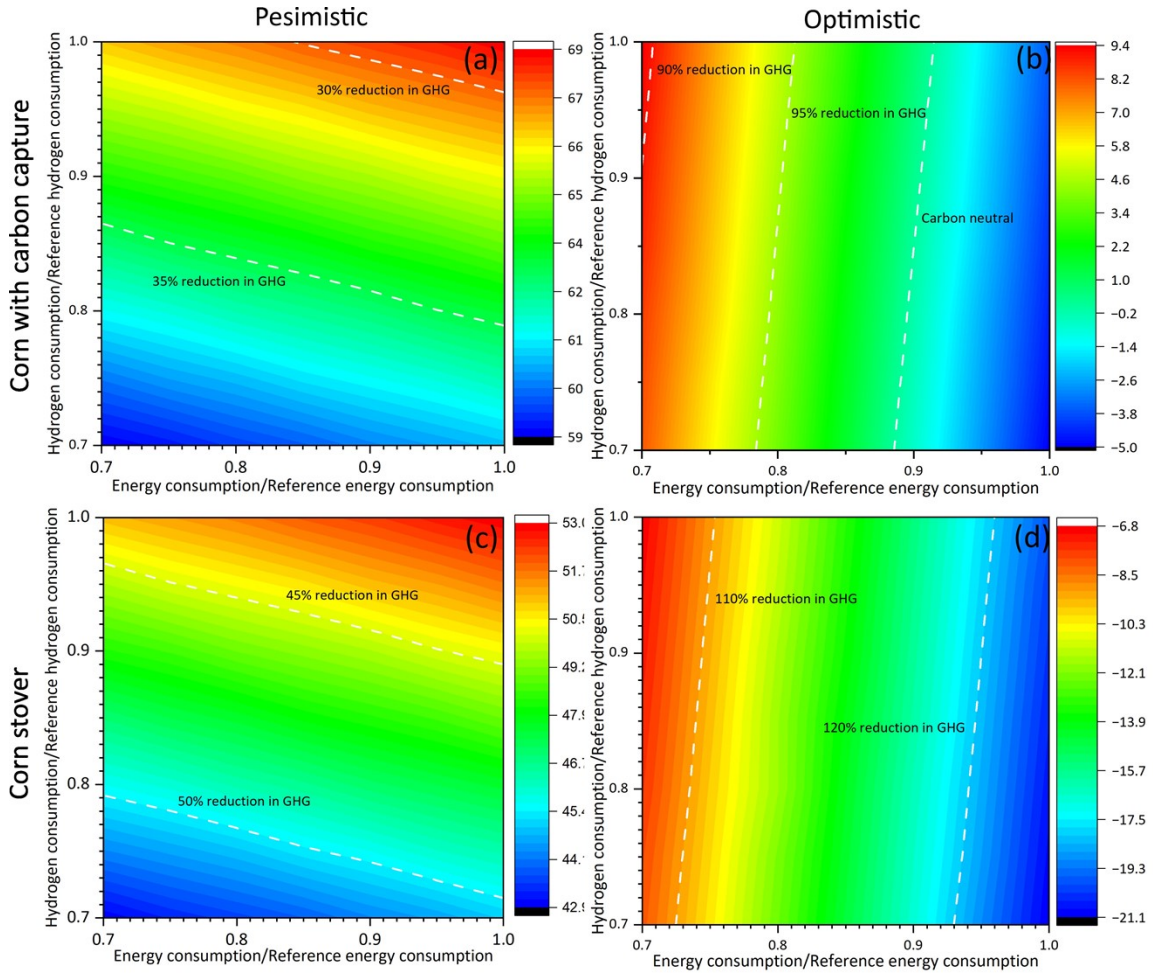

Figure S7. Sensitivity analysis showing the GHG emissions as a function of energy (x-axis) and hydrogen consumed (y-axis). Both axes are normalized with respect to the reference design. (a) Corn with carbon capture pessimistic scenario (b) Corn with carbon capture optimistic scenario (c) Corn stover pessimistic scenario (d) Corn stover optimistic scenario.

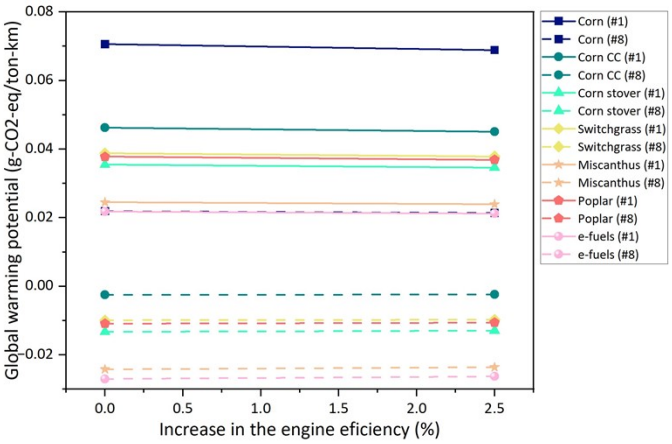

Figure S8. GHG emissions throughout the life cycle as a function of engine energy efficiency.

S6. Engine performance

Table S13. Engine geometry

Parameter	**Units**	**Value**
Bore	mm	82
Stroke	mm	90.4
Displacement	cm^3	475
Compression Ratio	-	17:1
Swirl Ratio	-	Variable 2.3-5.6
IVC/IVO	CAD	-132˚/ 350
EVO/EVC	CAD	112˚/ -332

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