

## **Techno-economic and environmental evaluation of producing chemicals and drop-in aviation biofuels via aqueous phase processing**

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### **Supplementary Information\***

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\* Refer to the manuscript for details and references.

**Table S1.** Net aggregated resource requirements to produce 1 MJ of hydrogen in the 12 hydrogen pathways described in the text, and the lifecycle emissions from its production. Negative values are due to co-product displacement. Simulation year: 2015.

Resources		Hydrogen pathways											
		1	2	3	4	5	6	7	8	9	10	11	12
Crude oil	J	4.66E+03	1.57E+04	6.53E+04	2.11E+04	UOP LLC Confidential	2.02E+04	1.21E+06	4.13E+04	7.26E+03	9.00E+02	2.16E+02	4.41E+04
Natural gas		1.49E+06	7.20E+04	6.59E+05	2.02E+06		1.03E+04	1.52E+05	1.48E+05	1.40E+05	1.78E+04	4.57E+03	9.32E+05
Coal		3.13E+04	1.35E+06	1.51E+05	1.33E+05		1.97E+06	3.72E+04	5.04E+04	2.23E+05	2.96E+04	8.82E+03	1.80E+06
Pet coke		8.11E+00	2.73E+01	1.14E+02	3.67E+01		3.51E+01	2.11E+03	7.19E+01	1.26E+01	1.57E+00	3.77E-01	7.68E+01
Bitumen		7.03E+02	2.37E+03	9.85E+03	3.19E+03		3.04E+03	1.83E+05	6.23E+03	1.10E+03	1.36E+02	3.26E+01	6.66E+03
Shale oil		1.07E+03	3.60E+03	1.50E+04	4.84E+03		4.62E+03	2.78E+05	9.46E+03	1.66E+03	2.06E+02	4.96E+01	1.01E+04
Nuclear energy		5.53E+03	2.38E+04	1.67E+04	2.35E+04		2.42E+03	6.68E+03	8.90E+03	1.04E+06	1.20E+06	1.56E+03	3.17E+05
<i>Renewable energy</i>													
Hydroelectric	J	1.93E+03	8.31E+03	5.82E+03	8.18E+03		8.44E+02	2.28E+03	3.10E+03	1.37E+04	1.82E+03	5.42E+02	1.11E+05
Geothermal		1.21E+02	5.20E+02	3.64E+02	5.12E+02		5.28E+01	1.46E+02	1.94E+02	8.58E+02	1.14E+02	3.39E+01	6.92E+03
Solar		1.61E+02	6.94E+02	4.87E+02	6.84E+02		7.06E+01	1.95E+02	2.59E+02	1.15E+03	1.52E+02	1.39E+06	9.25E+03
Wind		1.37E+03	5.92E+03	4.15E+03	5.83E+03		6.02E+02	1.66E+03	2.21E+03	9.77E+03	1.30E+03	3.86E+02	7.88E+04
Unspecified		1.41E+02	6.09E+02	4.27E+02	6.00E+02		6.19E+01	1.71E+02	2.27E+02	1.01E+03	1.33E+02	3.98E+01	8.11E+03
<i>Biomass</i>													
Forest residues	J	3.75E+02	1.62E+03	9.24E+02	1.59E+03		1.64E+02	4.53E+02	6.04E+02	2.67E+03	3.54E+02	1.06E+02	2.15E+04
	g	1.87E-02	8.04E-02	4.59E-02	7.92E-02		8.17E-03	2.25E-02	3.00E-02	1.33E-01	1.76E-02	5.25E-03	1.07E+00
Switchgrass	J	-	-	-	-	-	-	2.38E+06	-	-	-	-	
	g	-	-	-	-	-	-	1.42E+02	-	-	-	-	
Corn	J	-	-	1.99E+06	-	-	-	-	-	-	-	-	
	g	-	-	1.25E+02	-	-	-	-	-	-	-	-	
Soybean	J	-	-	-2.44E+05	-	-	-	-	-	-	-	-	
	g	-	-	-1.32E+01	-	-	-	-	-	-	-	-	
Sugarcane	J	-	-	4.01E+01	-	-	-	-	-	-	-	-	
	g	-	-	1.10E-02	-	-	-	-	-	-	-	-	
Water	cm <sup>3</sup>	1.50E+02	1.42E+02	2.44E+03	1.66E+02	2.55E+02	4.21E+02	2.10E+02	3.46E+02	3.53E+02	9.18E+00	2.09E+03	
Lifecycle emissions	gCO <sub>2</sub> e	92.4	41.7	18.2	135.2	0.11	178.0	182.5	29.8	31.4	4.1	1.2	239.0

**Table S2.** Chemical Engineering Plant Cost Index (CEPCI)

	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>
<b>Jan</b>	532.9	564.8	593.6	571.2	572.8	573.1
<b>Feb</b>	539.1	574.6	596.3	569.9	574.9	570.5
<b>Mar</b>	541.8	575.9	596.1	568.3	571.5	568.6
<b>Apr</b>	555.3	582.3	595.9	569.4	573.6	562.9
<b>May</b>	558.2	581.9	593.8	566.5	574.3	560.5
<b>Jun</b>	556.4	588.9	585.6	564.8	576.2	558.3
<b>Jul</b>	550.7	593.2	582.2	564	576.9	556.3
<b>Aug</b>	549.5	596.1	576.6	564.8	578.7	553.9
<b>Sep</b>	552.5	596	577.4	567.3	580.1	550.3
<b>Oct</b>	556.3	594	575.4	567.5	579.7	547.2
<b>Nov</b>	556.7	590.8	570.6	566.6	578.4	542.8
<b>Dec</b>	560.3	590.1	571.9	567.5	575.7	537.1
<b>Ave</b>	550.8	585.7	584.6	567.3	576.1	556.8

**Table S3.** Acetone prices that this study relies on, \$/t.

	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>
<b>Jan</b>	1257	1411	1780	1618	1786	1389
<b>Feb</b>	1301	1543	1548	1755	1830	1213
<b>Mar</b>	1301	1587	1748	1667	1720	1146
<b>Apr</b>	1345	1830	1691	1459	1676	1036
<b>May</b>	1213	1764	1519	1457	1609	970
<b>Jun</b>	1146	1609	1433	1565	1504	970
<b>Jul</b>	1124	1499	1204	1565	1552	992
<b>Aug</b>	1014	1477	1232	1653	1609	926
<b>Sep</b>	1014	1411	1261	1653	1609	794
<b>Oct</b>	1080	1279	1290	1587	1786	750
<b>Nov</b>	1036	1124	1407	1521	1653	794
<b>Dec</b>	1080	1124	1506	1631	1587	794
<b>Ave</b>	1159	1472	1468	1594	1660	981

**Table S4.** Electricity prices that this study relies on, ¢/kWh.

	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>
<b>Jan</b>	6.5	6.53	6.44	6.5	6.98	6.63
<b>Feb</b>	6.55	6.63	6.45	6.66	7.12	6.9
<b>Mar</b>	6.53	6.53	6.46	6.64	6.99	6.81
<b>Apr</b>	6.55	6.53	6.38	6.58	6.77	6.6
<b>May</b>	6.64	6.68	6.53	6.75	6.83	6.71
<b>Jun</b>	6.96	7.14	6.89	7.25	7.39	7.1
<b>Jul</b>	7.23	7.31	7.13	7.45	7.62	7.44
<b>Aug</b>	7.22	7.4	7.08	7.37	7.51	7.32
<b>Sep</b>	7	7.15	6.97	7.22	7.37	7.18
<b>Oct</b>	6.8	6.77	6.62	6.87	7.07	6.88
<b>Nov</b>	6.56	6.53	6.5	6.65	6.75	6.62
<b>Dec</b>	6.6	6.51	6.52	6.66	6.7	6.42
<b>Ave</b>	6.76	6.81	6.66	6.88	7.09	6.88

**Table S5.** Hydrochloric acid prices that this study relies on, \$/t.

	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>
<b>Jan</b>	151	130	265	232	215	224
<b>Feb</b>	142	130	265	212	207	214
<b>Mar</b>	140	127	265	211	171	153
<b>Apr</b>	140	113	265	208	160	107
<b>May</b>	140	113	264	208	135	98
<b>Jun</b>	140	113	264	208	150	94
<b>Jul</b>	140	113	263	206	176	91
<b>Aug</b>	140	143	254	226	187	80
<b>Sep</b>	137	153	255	226	220	80
<b>Oct</b>	136	170	264	226	242	77
<b>Nov</b>	131	265	264	226	251	61
<b>Dec</b>	130	265	256	215	245	61
<b>Ave</b>	139	153	262	217	197	112

**Table S6.** Ruthenium prices, \$/kg

	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>
<b>Jan</b>	5433	5787	3567	2755	1866	1810
<b>Feb</b>	5892	5787	4088	2733	2045	1800
<b>Mar</b>	6109	5787	4070	2733	2185	1774
<b>Apr</b>	6720	5787	3714	2733	2315	1608
<b>May</b>	7831	5787	3697	2733	2315	1608
<b>Jun</b>	7745	5787	3697	2733	2254	1571
<b>Jul</b>	6766	5787	3697	2699	2189	1426
<b>Aug</b>	6350	5647	3613	2479	2180	1350
<b>Sep</b>	6079	5393	3537	2013	2046	1350
<b>Oct</b>	5718	4731	3537	1833	1894	1350
<b>Nov</b>	5626	4114	3171	1833	1865	1350
<b>Dec</b>	5773	3601	2894	1833	1865	1350
<b>Ave</b>	6337	5333	3607	2426	2085	1529

**Table S7.** Platinum prices, \$/kg

	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>
<b>Jan</b>	50467	57521	48529	52944	45900	40201
<b>Feb</b>	49041	58903	53398	53983	45448	38811
<b>Mar</b>	51498	56912	53518	51023	46870	36893
<b>Apr</b>	55315	57827	51197	47980	46241	37305
<b>May</b>	52606	57610	47438	47727	46988	36965
<b>Jun</b>	50148	57124	46603	46154	46908	35234
<b>Jul</b>	49113	56644	45961	45169	48125	32833
<b>Aug</b>	49639	58201	46857	48191	46786	31882
<b>Sep</b>	51263	56458	52116	47131	44036	31385
<b>Oct</b>	54460	49474	52737	45580	40740	31559
<b>Nov</b>	54587	51428	50759	45821	39127	28815
<b>Dec</b>	55247	47210	51192	43727	39391	27824
<b>Ave</b>	51949	55443	50026	47952	44713	34142

**Table S8.** Acetic acid prices that this study relies on, \$/t.

	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>
<b>Jan</b>	513	650	562	607	725	713
<b>Feb</b>	513	650	590	627	726	700
<b>Mar</b>	537	650	597	682	726	700
<b>Apr</b>	537	651	572	695	739	700
<b>May</b>	537	676	572	659	723	700
<b>Jun</b>	537	625	572	685	733	700
<b>Jul</b>	537	635	572	648	733	700
<b>Aug</b>	537	650	645	667	722	700
<b>Sep</b>	537	650	665	667	703	687
<b>Oct</b>	537	630	608	667	713	687
<b>Nov</b>	537	625	607	708	713	687
<b>Dec</b>	563	625	607	725	713	687
<b>Ave</b>	535	643	597	670	722	697

**Table S9.** Furfural and hydroxymethylfurfural prices that this study relies on, \$/t.

	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>
<b>Jan</b>	1237	2655	1982	1380	1627	1639
<b>Feb</b>	1377	2778	1737	1314	1774	1550
<b>Mar</b>	1411	2610	1783	1354	1634	1571
<b>Apr</b>	1432	2698	1869	1564	1583	1637
<b>May</b>	1739	2558	1793	1404	1481	1488
<b>Jun</b>	1446	2539	1587	1484	1399	1485
<b>Jul</b>	1791	2817	1494	1402	1438	1538
<b>Aug</b>	1551	2366	1462	1300	1568	1734
<b>Sep</b>	1615	2188	1398	1466	1343	1487
<b>Oct</b>	1633	2151	1657	1492	1269	1528
<b>Nov</b>	2195	2006	1874	1600	1621	1404
<b>Dec</b>	2532	1975	2101	1572	1670	1828
<b>Ave</b>	1663	2445	1728	1444	1534	1574

**Table S10.** Natural gas prices that this study relies on, \$/mmBtu.

	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>
<b>Jan</b>	5.84	4.49	2.67	3.33	4.7	2.97
<b>Feb</b>	5.32	4.09	2.53	3.33	5.98	2.85
<b>Mar</b>	4.29	3.97	2.16	3.8	4.88	2.80
<b>Apr</b>	4.04	4.24	1.95	4.17	4.63	2.58
<b>May</b>	4.15	4.31	2.43	4.04	4.56	2.84
<b>Jun</b>	4.8	4.54	2.45	3.83	4.57	2.77
<b>Jul</b>	4.63	4.42	2.96	3.62	4.01	2.83
<b>Aug</b>	4.31	4.05	2.84	3.43	3.89	2.76
<b>Sep</b>	3.89	3.89	2.85	3.62	3.92	2.65
<b>Oct</b>	3.43	3.56	3.32	3.67	3.77	2.32
<b>Nov</b>	3.71	3.26	3.54	3.62	4.1	2.08
<b>Dec</b>	4.25	3.16	3.34	4.24	3.43	1.92
<b>Ave</b>	4.39	4	2.75	3.73	4.37	2.61

**Table S11.** Propane prices that this study relies on, \$/gal.

	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>
<b>Jan</b>	1.31	1.35	1.29	0.84	1.4	0.48
<b>Feb</b>	1.28	1.38	1.22	0.86	1.44	0.57
<b>Mar</b>	1.14	1.4	1.26	0.89	1.06	0.54
<b>Apr</b>	1.14	1.45	1.2	0.94	1.1	0.55
<b>May</b>	1.08	1.52	0.95	0.93	1.04	0.47
<b>Jun</b>	1.04	1.52	0.79	0.86	1.05	0.39
<b>Jul</b>	1.01	1.53	0.88	0.92	1.04	0.41
<b>Aug</b>	1.07	1.53	0.9	1.06	1.02	0.37
<b>Sep</b>	1.13	1.56	0.91	1.11	1.06	0.45
<b>Oct</b>	1.23	1.47	0.96	1.14	0.94	0.45
<b>Nov</b>	1.25	1.46	0.89	1.18	0.8	0.43
<b>Dec</b>	1.3	1.4	0.8	1.28	0.56	0.39
<b>Ave</b>	1.17	1.46	1	1	1.04	0.46

**Table S12.** Naphtha prices that this study relies on, \$/gal.

	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>
<b>Jan</b>	1.88	2.36	2.75	2.86	2.68	1.32
<b>Feb</b>	1.93	2.52	2.93	3.16	2.61	1.58
<b>Mar</b>	2.05	2.83	3.01	2.97	2.63	1.56
<b>Apr</b>	2.13	3.03	2.88	2.43	2.66	1.59
<b>May</b>	1.95	2.88	2.66	2.35	2.68	1.74
<b>Jun</b>	1.96	2.69	2.38	2.24	2.76	1.73
<b>Jul</b>	1.91	2.83	2.45	2.61	2.64	1.37
<b>Aug</b>	1.86	2.7	2.86	2.6	2.5	1.2
<b>Sep</b>	1.93	2.61	2.97	2.57	2.41	1.24
<b>Oct</b>	2.06	2.62	2.78	2.54	2.02	1.25
<b>Nov</b>	2.12	2.5	2.78	2.51	1.83	1.26
<b>Dec</b>	2.29	2.56	2.83	2.74	1.32	1.12
<b>Ave</b>	2.01	2.68	2.77	2.63	2.4	1.41

**Table S13.** Jet fuel prices that this study relies on, \$/gal.

	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>
<b>Jan</b>	2.05	2.62	3.09	3.09	2.92	1.5
<b>Feb</b>	1.99	2.84	3.21	3.22	2.97	1.76
<b>Mar</b>	2.11	3.13	3.26	2.97	2.89	1.63
<b>Apr</b>	2.24	3.27	3.23	2.81	2.89	1.7
<b>May</b>	2.06	3.09	2.97	2.73	2.87	1.85
<b>Jun</b>	2.06	3.05	2.68	2.77	2.88	1.73
<b>Jul</b>	2.02	3.13	2.89	2.89	2.82	1.54
<b>Aug</b>	2.08	3.01	3.16	3	2.84	1.39
<b>Sep</b>	2.11	2.95	3.19	2.93	2.73	1.39
<b>Oct</b>	2.25	2.97	3.11	2.89	2.46	1.39
<b>Nov</b>	2.32	3.05	2.96	2.83	2.3	1.33
<b>Dec</b>	2.45	2.87	2.94	2.96	1.8	1.08
<b>Ave</b>	2.15	3	3.06	2.92	2.7	1.52



**Table S14.** Diesel fuel prices that this study relies on, \$/gal.

	<b>2010</b>	<b>2011</b>	<b>2012</b>	<b>2013</b>	<b>2014</b>	<b>2015</b>
<b>Jan</b>	2.07	2.64	3.08	3.1	3.12	1.68
<b>Feb</b>	2.04	2.84	3.22	3.24	3.23	1.99
<b>Mar</b>	2.16	3.13	3.3	3.04	2.99	1.86
<b>Apr</b>	2.28	3.27	3.24	2.9	2.96	1.84
<b>May</b>	2.14	3.04	2.99	2.89	2.94	1.97
<b>Jun</b>	2.11	3.05	2.71	2.89	2.96	1.89
<b>Jul</b>	2.07	3.17	2.92	3.02	2.88	1.68
<b>Aug</b>	2.12	3.01	3.18	3.07	2.85	1.52
<b>Sep</b>	2.18	2.98	3.23	3.05	2.74	1.51
<b>Oct</b>	2.3	3.01	3.24	3	2.53	1.47
<b>Nov</b>	2.38	3.1	3.18	2.94	2.43	1.41
<b>Dec</b>	2.5	2.94	3.07	3.05	2.03	1.14
<b>Ave</b>	2.2	3.02	3.11	3.02	2.81	1.66

















**Table S22.** Representative red maple wood composition adjusted based on Zhang et al. 2013. Uronic acids are assumed to be the only extractives (Jara 2010). Moisture content is assumed to be 7.3%.

<b>Dry composition</b>	<b>%</b>
Cellulose (glucan)	44.1
Hemicellulose (xylan)	18.7
Lignin	24.8
Soluble lignin	2.1
Acetate	5.2
Uronic acids	2.8
Ash	2.3
Total	100.0

**Table S23.** Pretreatment reactor material inputs based on 100 a.u. of dry red maple wood, reactions, reactor conditions and yields for different pretreatment techniques.

		Pretreatment techniques			
		Hot water	Oxalic acid	Hydro-chloric acid	Sulfuric acid
		Biorefinery model			
		1-4	5	6	7
Material inputs, a.u.	Dry biomass	100	100	100	100
	Moisture in biomass	7.9	7.9	7.9	7.9
	Additional water	124.6	124.0	124.0	124.0
	Acid	-	0.7	0.7	0.7
Reactor conditions	Temperature, °C	200	160	140	160
	Pressure, psi (kPa)	235 (1620)	235 (1620)	235 (1620)	235 (1620)
	Residence time, min	11.2	27.5	51	27.5
Reactions and % yields	Cellulose → Glucooligomers	6.2	3	15.4	8.9
	Glucooligomers + H <sub>2</sub> O → Glucose	100.0	100.0	100.0	100.0
	Glucose → HMF + 3 H <sub>2</sub> O	41.7	29.6	23.3	30.4
	Xylan → Xylooligomers	87.1	92.5	94.4	91.0
	Xylooligomers + H <sub>2</sub> O → Xylose	21.9	85.5	81.9	93.9
	Xylose → Furfural + 3 H <sub>2</sub> O	30.1	8.0	14.4	9.2
	Acetate → Acetic acid	100.0	100.0	100.0	100.0

**Table S24.** Cellulose deconstruction reactions and percent reaction yields for low and high yield cases. All reactions take place under 200°C and 230 psi (1586 kPa) at a residence time of 1 hour.

	<b>Low yield</b>	<b>High yield</b>
Biorefinery model	3	Others
Cellulose → Glucooligomers	100.0	100.0
Glucooligomers + H <sub>2</sub> O → Glucose	100.0	100.0
Glucose → Levulinic acid + Formic acid + H <sub>2</sub> O	55.0	75.0
Glucose → C <sub>6</sub> Humins	45.0	25.0

**Table S25.** Percent conversion and molar selectivities derived from experimental data (Xing et al. 2010) to be applied in the hydrodeoxygenation reactor for the low and high yield cases.

**% Molar selectivity of alkanes based on carbon number**

C <sub>1</sub>	C <sub>2</sub>	C <sub>3</sub>	C <sub>4</sub>	C <sub>5</sub>	C <sub>6</sub>	C <sub>7</sub>	C <sub>8</sub>	C <sub>9</sub>	C <sub>10</sub>	C <sub>11</sub>	C <sub>12</sub>	C <sub>13</sub>
15.7	0.10	1.90	7.40	0.22	1.58	1.11	0.44	0.85	0.75	1.08	13.0	55.9

**% Conversion**

Low yield	High yield
91	95

**Table S26.** Lifecycle production emissions of biorefinery products in gCO<sub>2e</sub>/kg for chemicals and gCO<sub>2e</sub>/MJ for fuels compared with their conventional counterparts.

Products	Conv.	Biorefineries						
		1	2	3	4	5	6	7
Acetic acid	620 <sup>a,d</sup>	267	272	281	92.4	276	262	267
HMF		416	425	439	144	430	410	416
Furfural		N/A	N/A	N/A	160	N/A	N/A	N/A
Natural gas	17.5 <sup>b,d</sup>	49.3	48.4	53.5	N/A	51.4	47.9	47.1
Propane		49.2	48.3	53.5	N/A	51.4	47.8	47.1
Naphtha	16.9 <sup>c,d</sup>	50.3	49.4	54.4	37.2	52.5	48.8	48.1
Jet fuel	13.5 <sup>c,e</sup>	53.6	52.8	58.0	38.2	55.9	52.1	51.5
Diesel	18.0 <sup>c,d</sup>	49.8	48.9	54.0	36.7	52.0	48.3	47.7

<sup>a</sup>Acetic acid production from methanol carboxylation.

<sup>b</sup>Natural gas from shale and crude oil.

<sup>c</sup>Product from crude oil refining.

<sup>d</sup>Data from GREET.net.

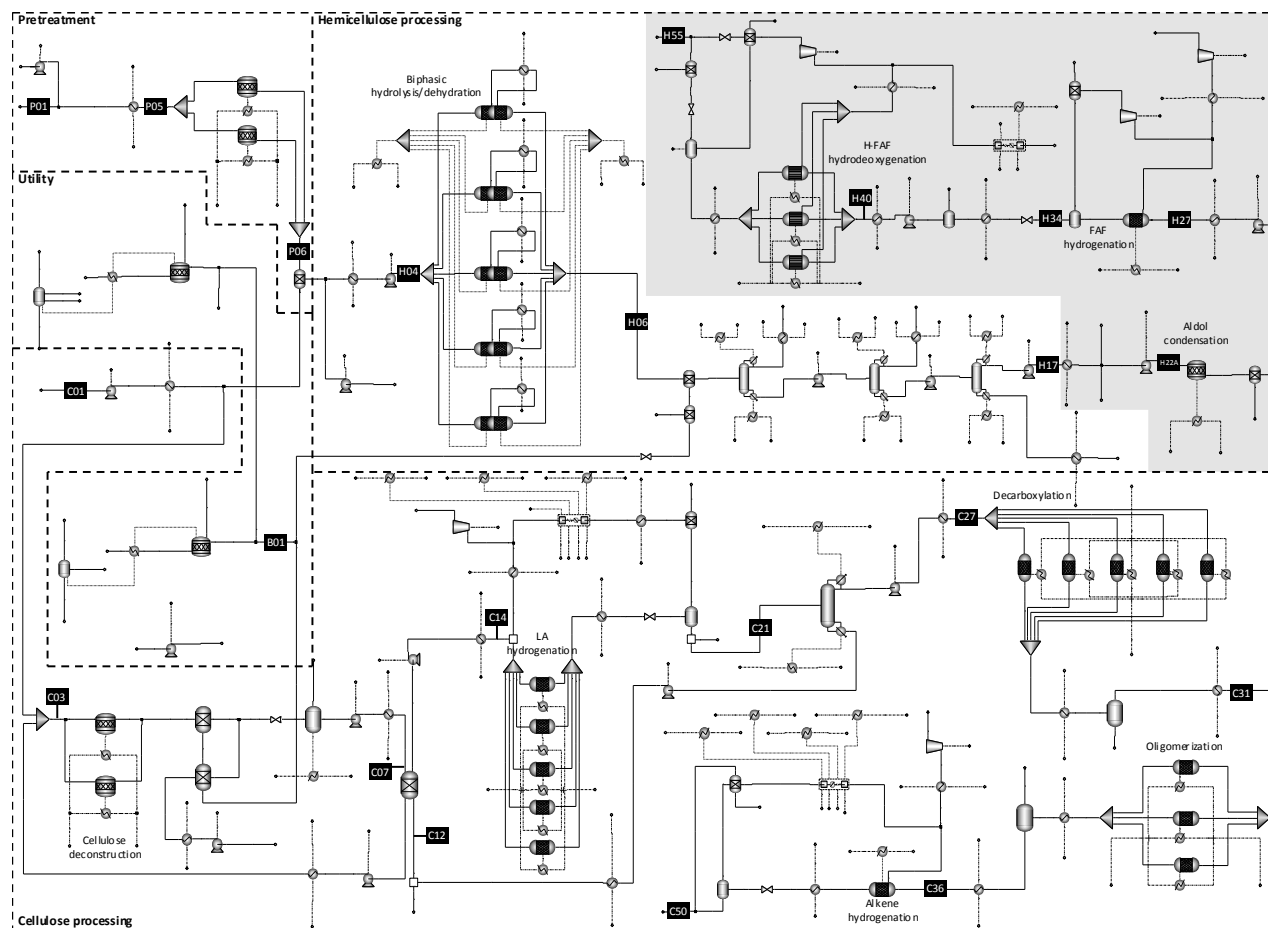
<sup>e</sup>Data from Stratton et al. 2010.

**Table S27.** Cost of hydrogen in 2010 USD/kg based on the Hydrogen Analysis (H2A) carried out by the U.S. Department of Energy. A large-scale central plant is assumed unless noted otherwise. Start of production is assumed to take place in 2010. Plant sizes (kg/day) have been rounded. CCS: Carbon capture and storage.

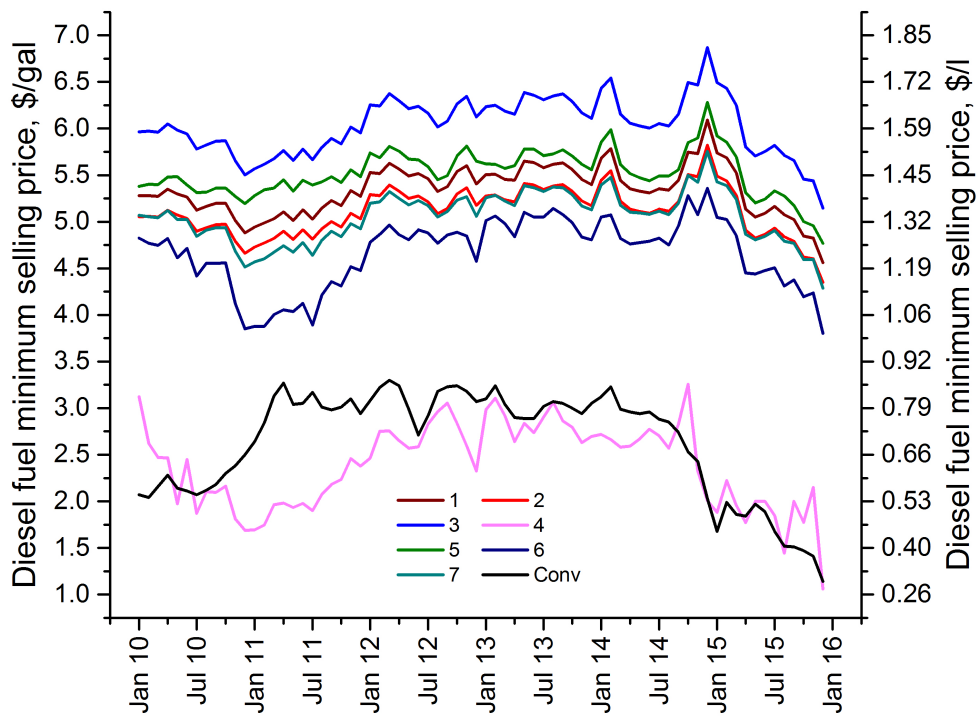
<b>Feedstock/Utility</b>	<b>Technology</b>	<b>Plant size</b>	<b>Notes</b>	<b>H<sub>2</sub> cost</b>
Natural gas	Steam reforming	380,000	-	1.78
		380,000	With CCS	2.19
		380,000	Improved efficiency	1.69
		380,000	With CCS, improved efficiency	2.11
		1,500	Small-scale distributed plant	4.46
Biomass, hybrid poplar	Gasification	150,000	-	2.39
		150,000	Improved efficiency	2.16
Coal	Gasification	300,000	-	1.41
		300,000	With CCS	2.05
		250,000	Improved efficiency	1.43
		250,000	With CCS, improved efficiency	1.97
Water/Grid electricity	PEM electrolysis	50,000	-	5.37
		50,000	With future efficiency	4.04
	Solid oxide electrolysis	50,000	-	5.04
		50,000	With improved efficiency	3.72
	Photoelectrochemical	50,000	Technology option 1	4.82
		50,000	Technology option 2	5.99
Water/Solar energy	Thermolysis	100,000	-	4.03



**Figure S1.** Process overview of the 12 hydrogen pathways employed in the lifecycle analysis calculations. Note that many lifecycle steps have been omitted for simplicity (e.g. transportation steps, water gas shift reaction, etc.).



**Figure S2.** Aspen Plus® process flow diagram (PFD) of a single train outlining the four processing sections (pretreatment, cellulose processing, hemicellulose processing, utility) and the reactors. Unit operations in the shaded area do not exist in Biorefinery 4. Details of the streams shown are given for each Biorefinery model from Table S15 to Table S21. Recycle of streams utilized via calculator blocks are not visible in this PFD.



**Figure S3.** Minimum selling prices (MSP) of diesel fuels from the biorefinery models under consideration for the time period from January 2010-December 2015. Also shown are the conventional diesel fuel prices for comparison purposes.