Supplementary Information

Superstructure for Thermochemical Process Synthesis with Simultaneous Heat, Power, and Water Integration

The following eleven figures represent the superstructure for thermochemical production of liquid fuels.

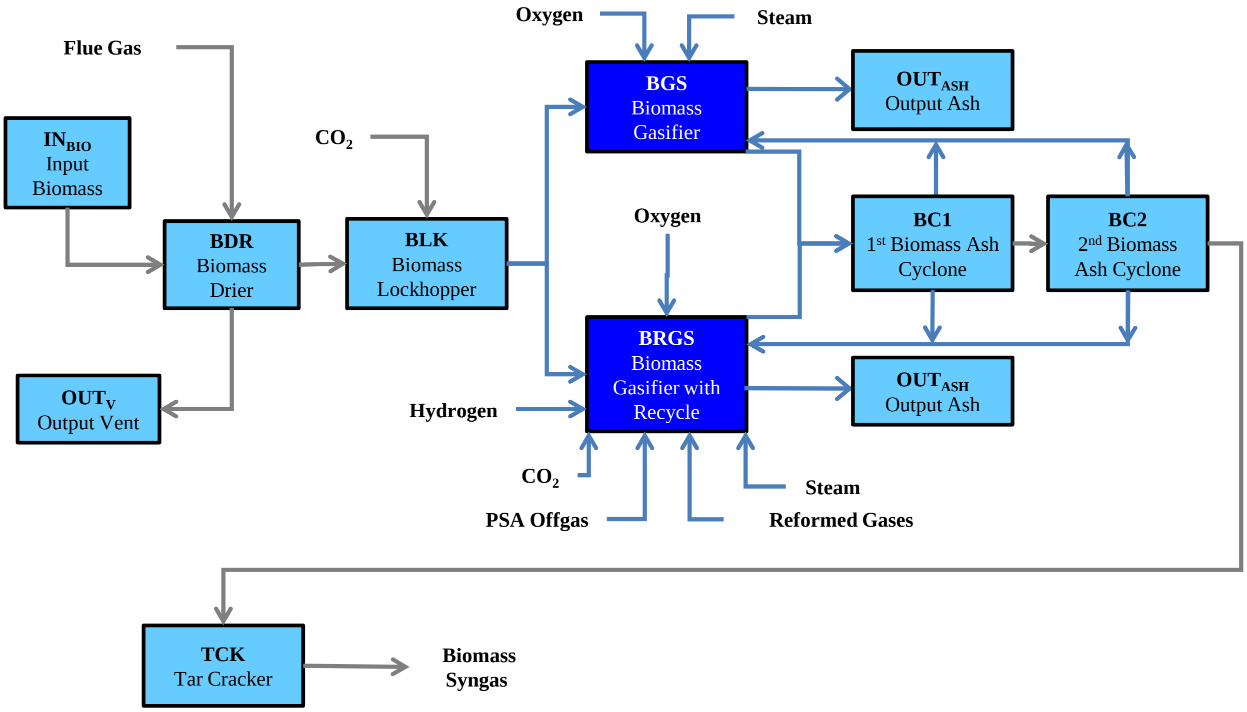

Figure S1: Biomass conversion process flowsheet.

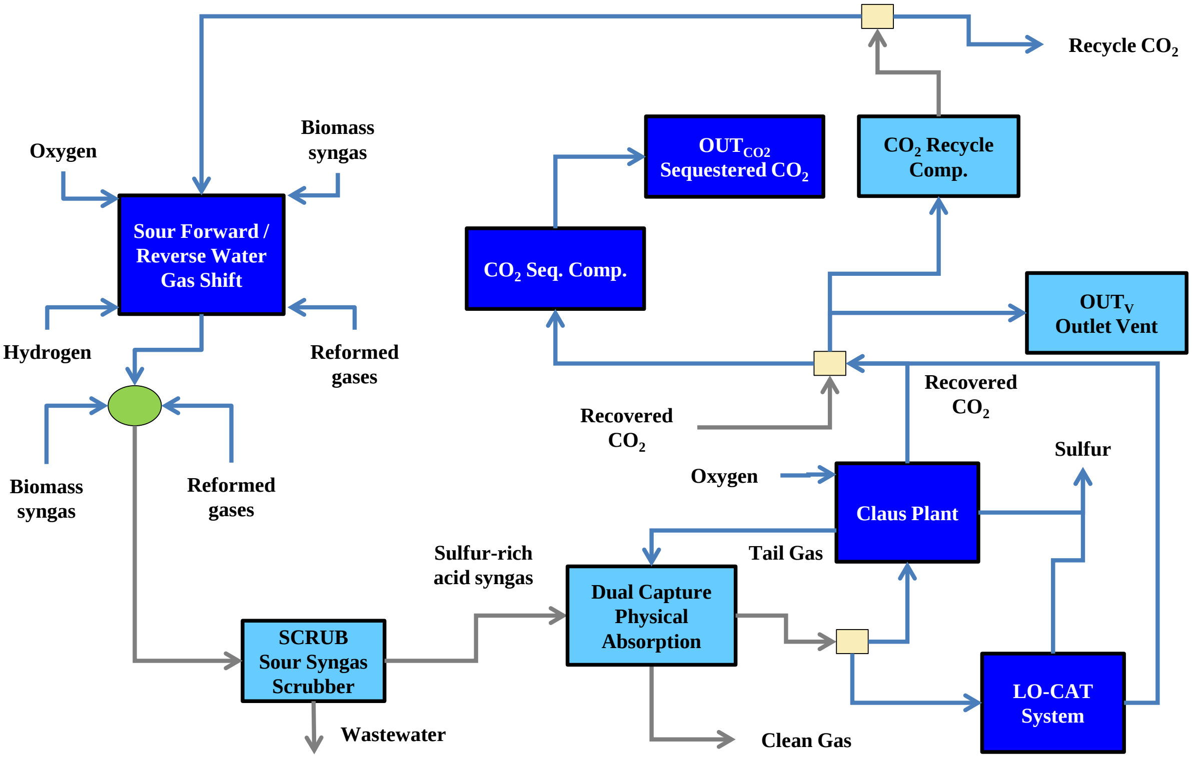

Figure S2: Synthesis gas handling process flowsheet.

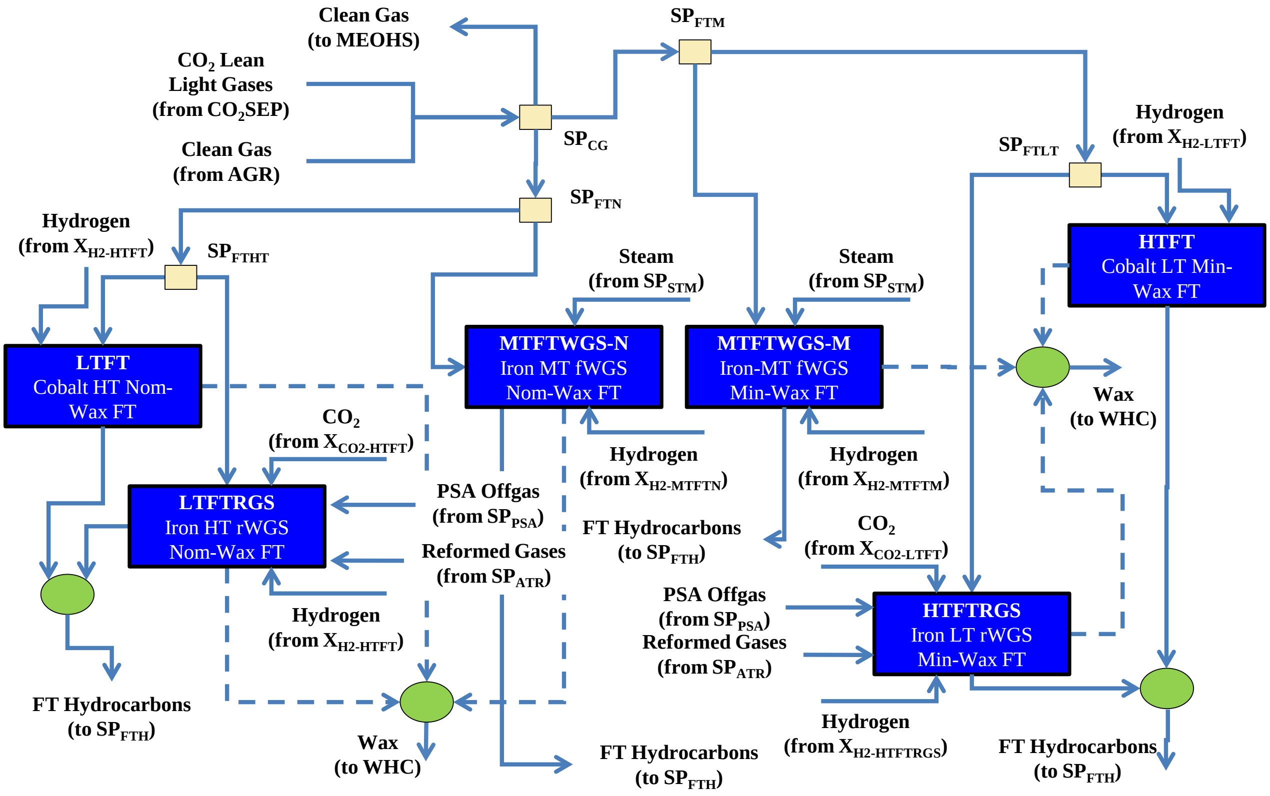

Figure S3: Fischer-Tropsch hydrocarbon production process flowsheet.

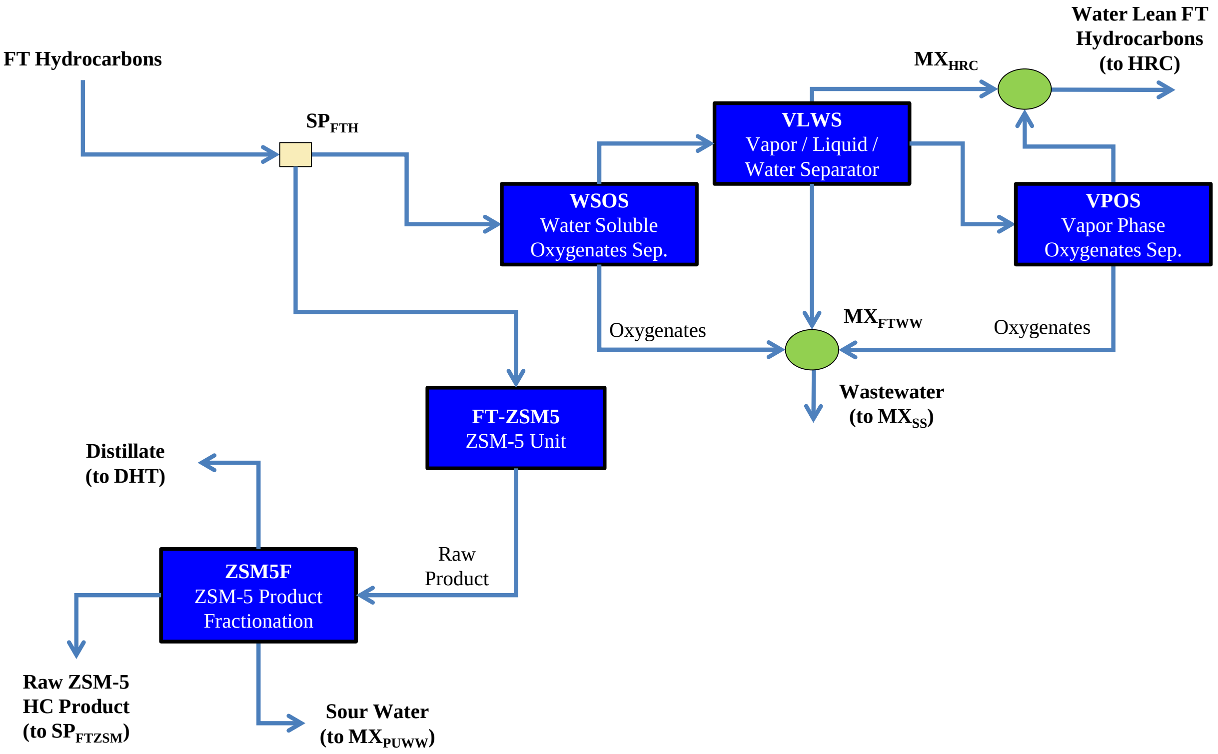

Figure S4: First Fischer-Tropsch hydrocarbon upgrading process flowsheet.

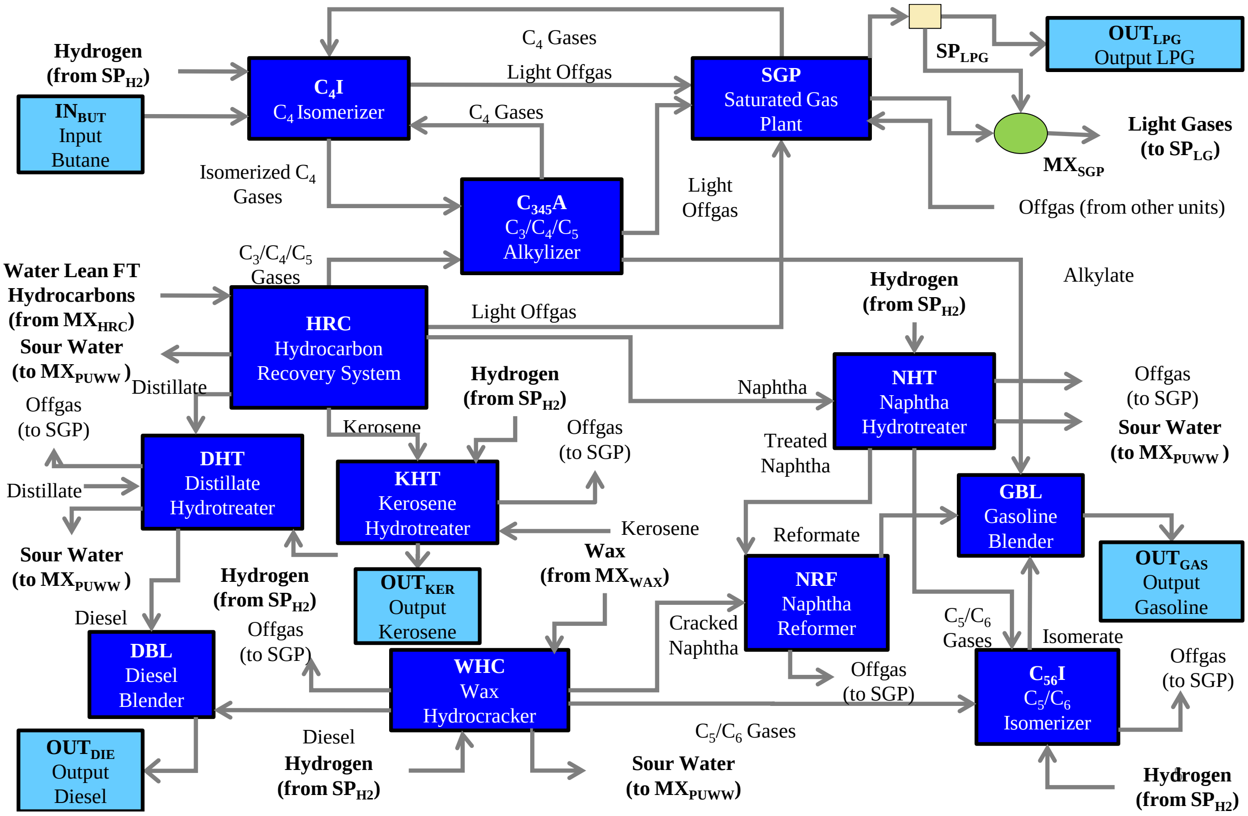

Figure S5: Second Fischer-Tropsch hydrocarbon upgrading process flowsheet.

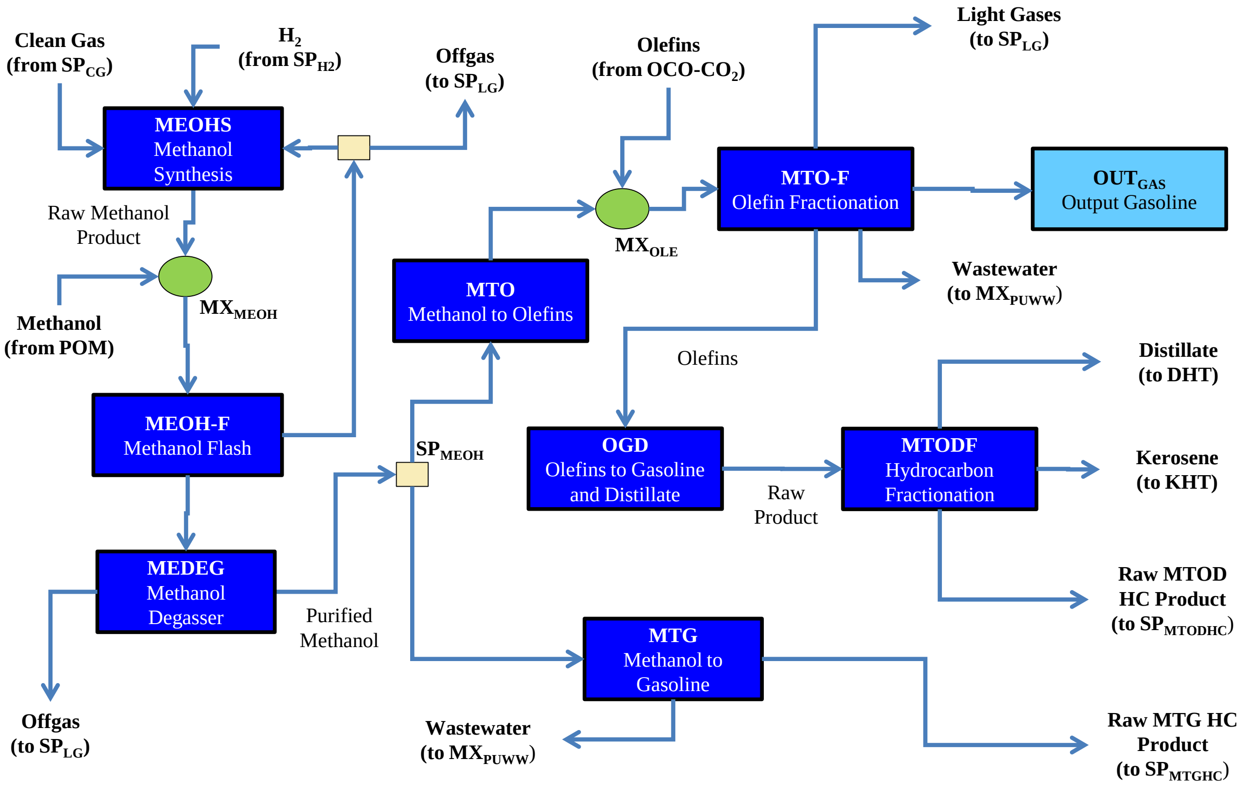

Figure S6: Methanol synthesis and conversion process flowsheet.

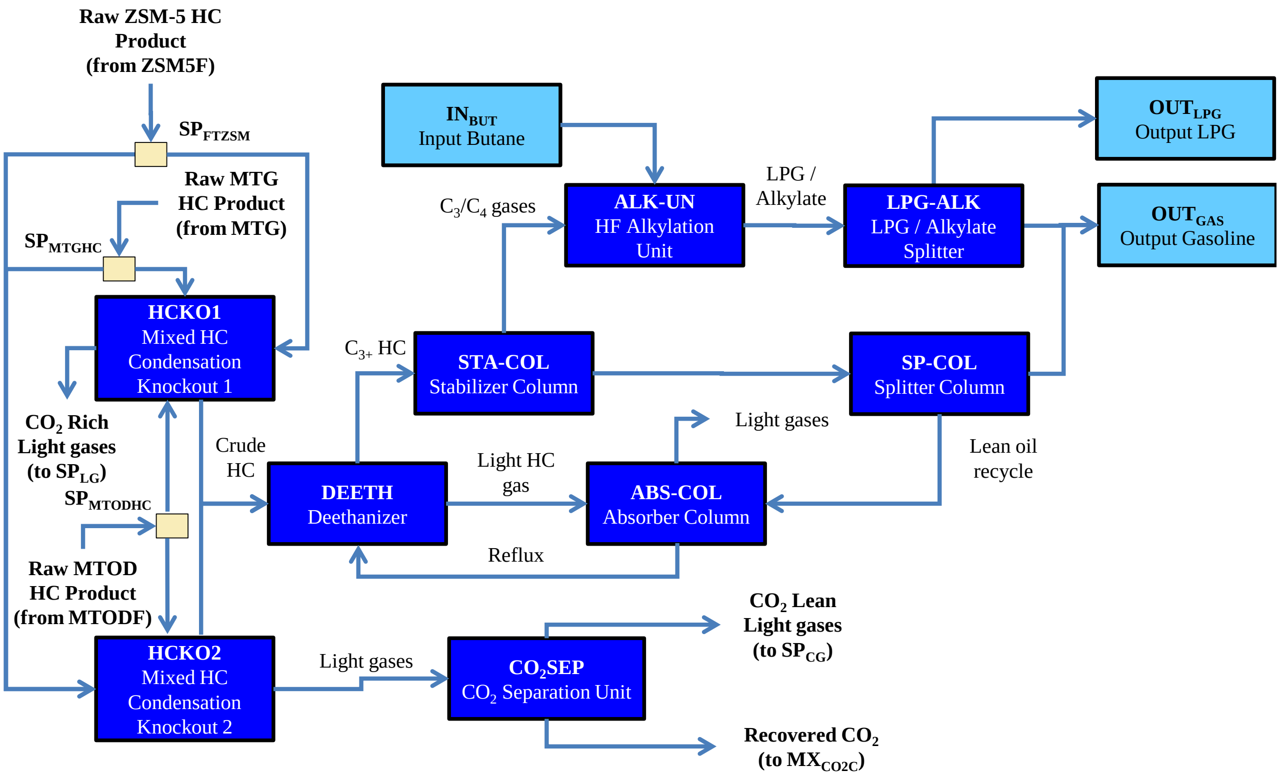

Figure S7: LPG-gasoline separation process flowsheet.

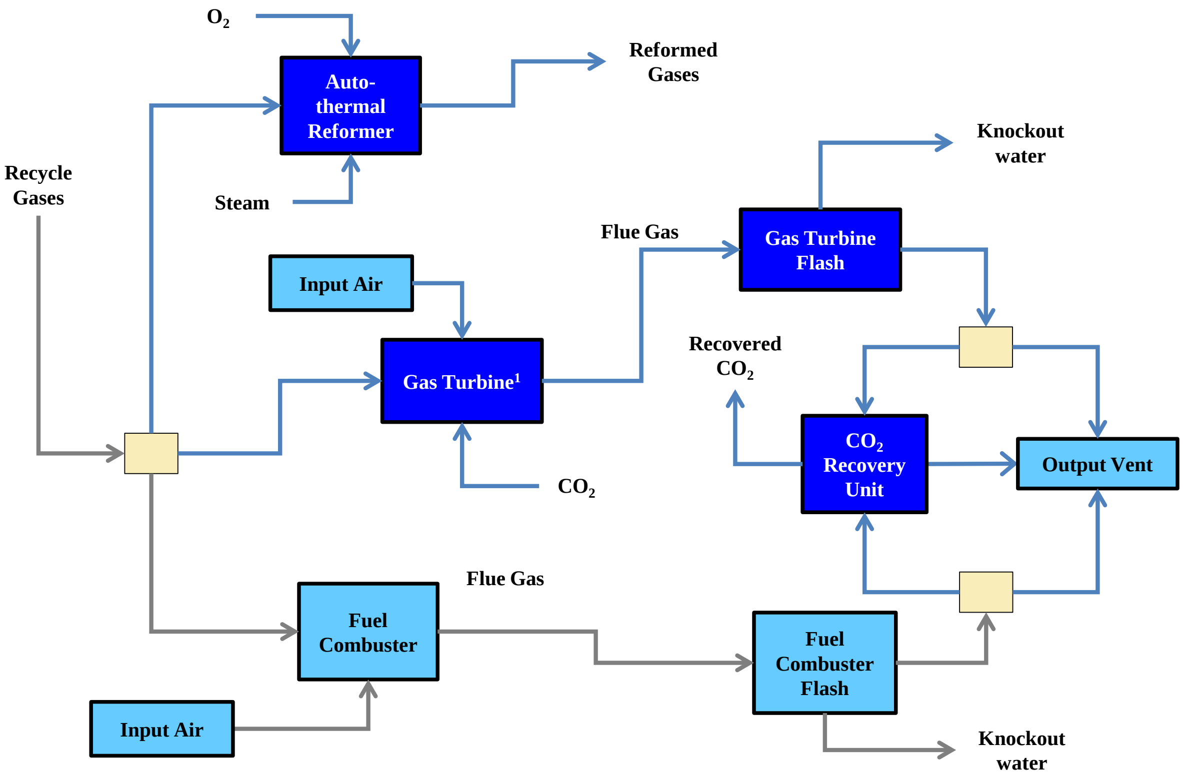

Figure S8: Light gas handling process flowsheet.

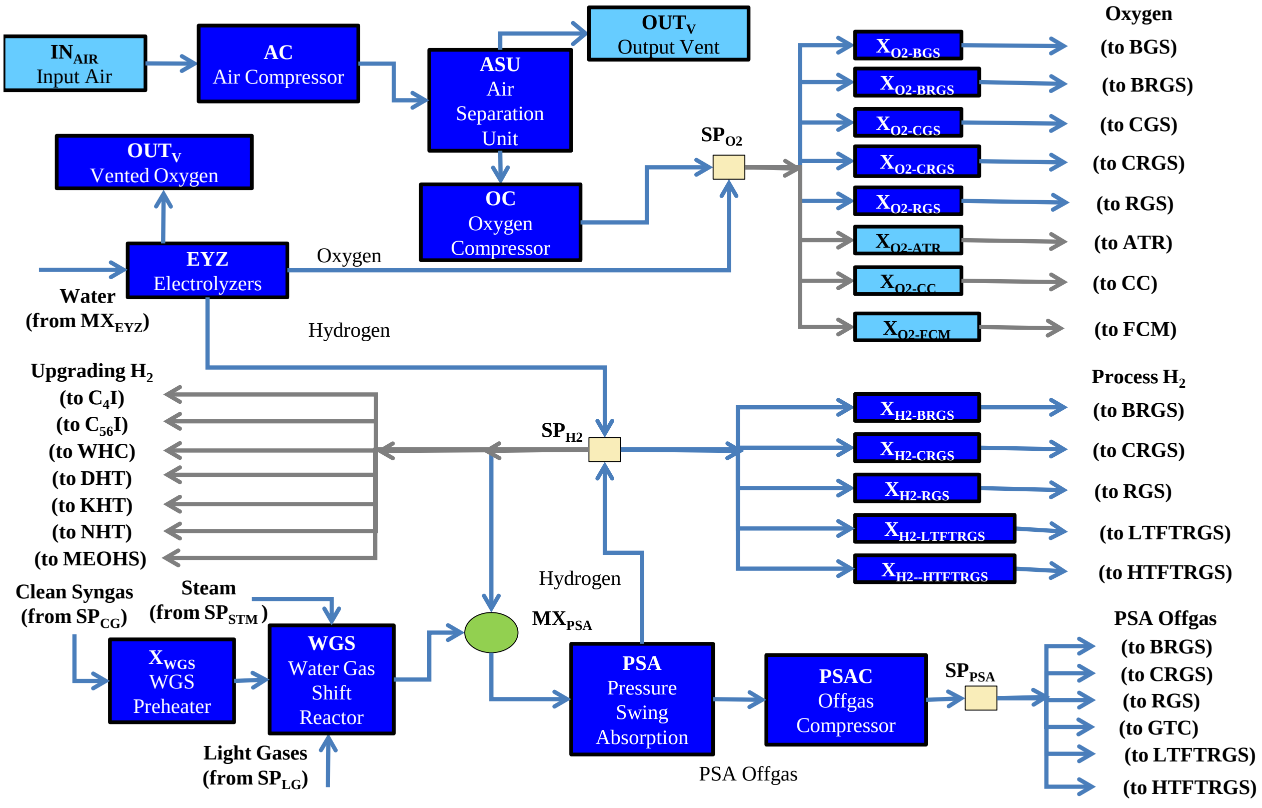

Figure S9: Hydrogen/oxygen production process flowsheet.

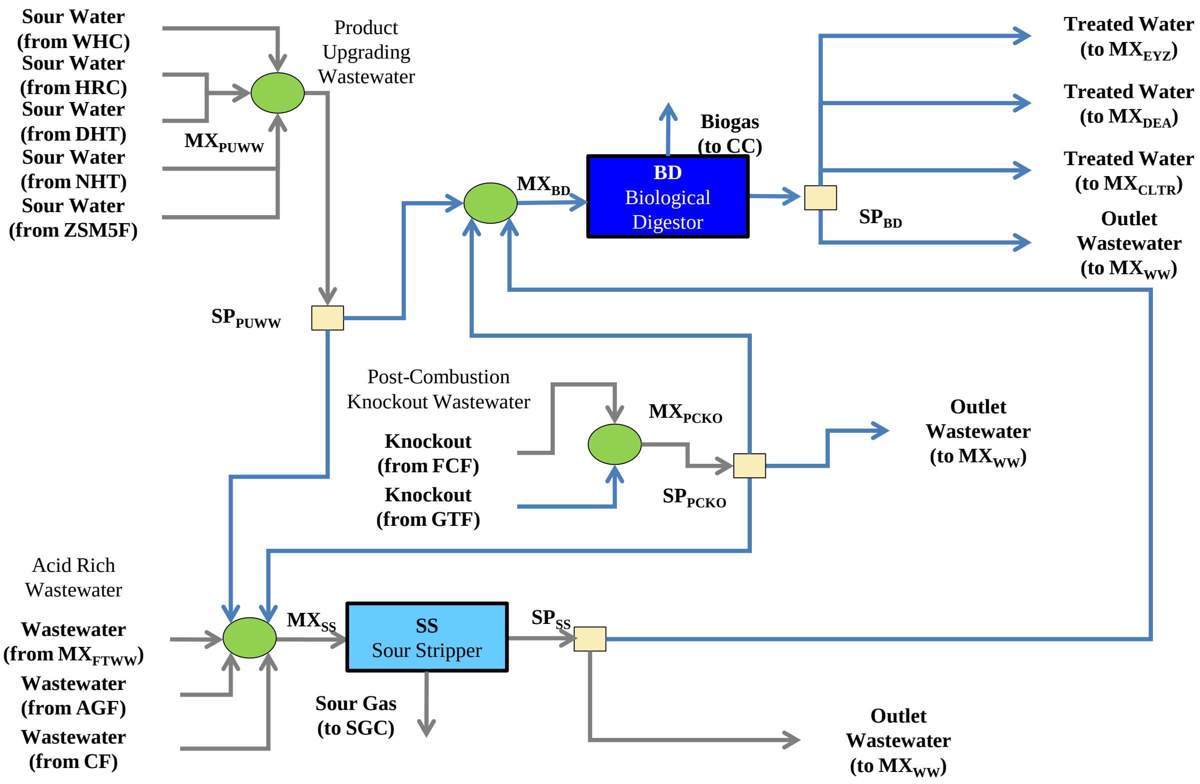

Figure S10: Process wastewater treatment process flowsheet.

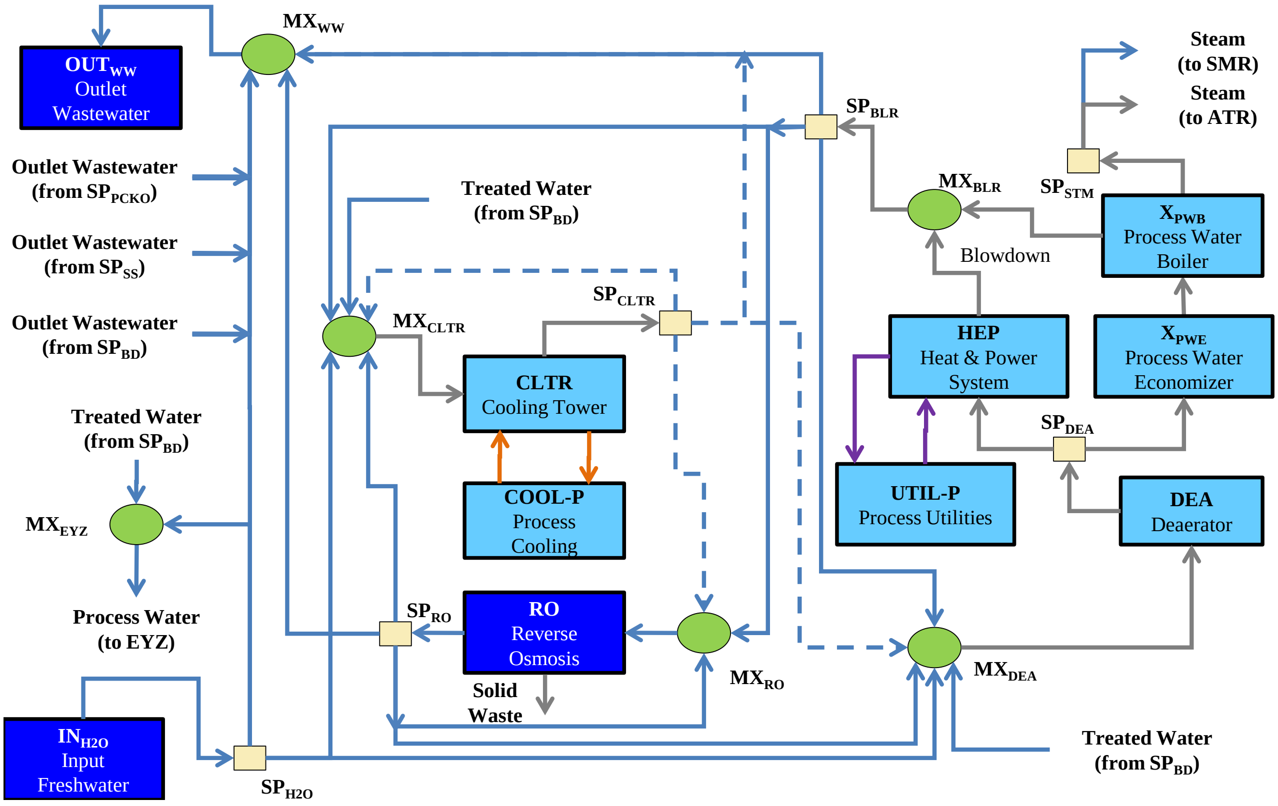

Figure S11: Utility cycle wastewater treatment process flowsheet.

Computational Results for Forty-Eight Case Studies

Forty-eight case studies were performed to demonstrate the capability of the process synthesis model using an average representation of either agricultural residues, forest residues, or perennial crops. The effect of scale on the BTL refinery was examined through four representative capcities of 1 thousand barrels per day (kBD), 5 kBD, 10 kBD, and 50 kBD. The gasoline, diesel, and kerosene compositions output from the refinery were selected to either (a) represent the 2010 United States demand (i.e., 67 vol% gasoline, 22 vol% diesel, 11 vol% kerosene) [1], (b) freely output any unrestricted composition of the products, (c) maximize the diesel production ($\geq 75\%$), or (d) maximize the kerosene production ($\geq 75\%$). The case studies are labeled as $N-C$, where N represents the type of product composition (i.e., R: 2010 U.S. ratios, U: unrestricted composition, D: maximum diesel, K: maximum kerosene) and C represents the capacity in kBD. For example, the U-1 label represents the 1 kBD capacity refinery with an unrestricted product composition.

Tables S1 - S7 detail the results of all forty-eight case studies. The topological results are displayed in Table S1; the overall costs are displayed in Table S2; the investment costs are displayed in Table S3; the material and energy balances are in Tables S4 and S5, respectively; the carbon and GHG balances are in Tables S6 and S7, respectively. Detailed descriptions on the results for the case studies using an unrestricted product composition and the United Stated demand ratios are provided in the main text of the manuscript.

Table S1: Topological information for the optimal solutions for the forty-eight case studies. Biomass conversion (Biomass Conv.) is gasification with a solid (S) or solid/vapor (S/V) fueled system. The temperature (Temp.; °C) of the biomass gasification is selected along with the operating temperature of the water-gas-shift unit (WGS), if utilized. The presence of a CO_2 sequestration system (CO2SEQ) or a gas turbine (GT) is noted using yes (Y) or no (N). The Fischer-Tropsch units will operate at low-temperature (LT) or high-temperature (HT) with a cobalt (Co) or iron (Ir) catalyst. The FT vapor effluent will be upgraded using fractionation into distillate and naphtha (Fract.) or ZSM-5 catalytic conversion. The use of methanol-to-gasoline (MTG) and methanol-to-olefins/olefins-to-gasoline-and-diesel (MTO/MOGD) is noted using yes (Y) or no (N).

Perennial Crops

Case Study	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass Conv.	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S
Biomass Temp.	1100	1100	1000	1000	1100	1100	1000	1000	1100	1100	1000	1000	1100	1100	1000	1000
WGS/RGS Temp.	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Min Wax FT	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Nom. Wax FT	-	-	-	-	-	-	-	-	Co-LTFT	Co-LTFT	Co-LTFT	Co-LTFT	-	Co-LTFT	Co-LTFT	Co-LTFT
FT Upgrading	-	-	-	-	-	-	-	-	Fract.	Fract.	Fract.	Fract.	-	ZSM-5	ZSM-5	ZSM-5
MTG Usage	Y	Y	Y	Y	-	-	-	-	-	-	-	-	Y	Y	Y	Y
MTOD Usage	-	-	-	-	Y	Y	Y	Y	-	-	-	-	Y	-	-	-
CO2SEQ Usage	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
GT Usage	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Forest Residues

Case Study	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass Conv.	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S
Biomass Temp.	900	900	900	900	900	900	900	900	900	900	900	900	900	900	900	900
WGS/RGS Temp.	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Min Wax FT	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Nom. Wax FT	-	-	-	-	-	-	-	-	Co-LTFT	Co-LTFT	Co-LTFT	Co-LTFT	-	Co-LTFT	Co-LTFT	Co-LTFT
FT Upgrading	-	-	-	-	-	-	-	-	Fract.	Fract.	Fract.	Fract.	-	ZSM-5	ZSM-5	ZSM-5
MTG Usage	Y	Y	Y	Y	-	-	-	-	-	-	-	-	Y	Y	Y	Y
MTOD Usage	-	-	-	-	Y	Y	Y	Y	-	-	-	-	Y	-	-	-
CO2SEQ Usage	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
GT Usage	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Agricultural Residues

Case Study	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass Conv.	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S
Biomass Temp.	1100	1100	1000	1000	1100	1100	1000	1000	1100	1100	1000	1000	1100	1100	1000	1000
WGS/RGS Temp.	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Min Wax FT	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Nom. Wax FT	-	-	-	-	-	-	-	-	Co-LTFT	Co-LTFT	Co-LTFT	Co-LTFT	-	Co-LTFT	Co-LTFT	Co-LTFT
FT Upgrading	-	-	-	-	-	-	-	-	Fract.	Fract.	Fract.	Fract.	-	ZSM-5	ZSM-5	ZSM-5
MTG Usage	Y	Y	Y	Y	-	-	-	-	-	-	-	-	Y	Y	Y	Y
MTOD Usage	-	-	-	-	Y	Y	Y	Y	-	-	-	-	Y	-	-	-
CO2SEQ Usage	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y
GT Usage	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Table S2: Overall cost results for the forty-eight case studies. The contribution to the total costs (in \$/GJ) come from biomass, natural gas, butanes, water, CO_2 transportation/storage/monitoring (CO_2 TS&M), investment, and operations/maintenance (O&M). LPG and electricity are sold as byproducts (negative value). The overall costs are reported in (\$/GJ) and (\$/bbl) basis, along with the lower bound values in (\$/GJ) and the optimality gap between the reported solution and the lower bound.

Contribution to Cost	Case Study - Forest Residues															
($/GJ of products)	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass	8.32	8.43	8.44	8.19	8.73	8.71	8.53	8.79	8.46	8.31	8.27	8.40	8.09	8.12	8.23	8.18
Butane	0.61	0.61	0.61	0.61	-0.15	-0.15	-0.15	-0.15	0.00	0.00	0.00	0.00	0.41	0.41	0.41	0.41
Water	0.02	0.02	0.03	0.02	0.02	0.02	0.03	0.02	0.03	0.03	0.02	0.02	0.02	0.03	0.03	0.03
CO_2 TS&M	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Investment	12.00	7.54	6.99	5.90	12.06	7.31	6.72	5.96	13.35	8.23	6.93	5.75	13.08	8.32	6.66	5.74
O&M	3.17	1.99	1.85	1.56	3.19	1.93	1.78	1.58	3.53	2.17	1.83	1.52	3.45	2.20	1.76	1.52
Electricity	-0.61	-0.74	-0.57	-0.57	-0.71	-0.87	-0.59	-0.82	-0.88	-0.60	-0.77	-0.66	-0.91	-0.60	-0.71	-0.83
LPG	-2.25	-1.57	-1.57	-1.12	-0.03	-0.02	-0.02	-0.02	0.00	0.00	0.00	0.00	-0.34	-0.24	-0.24	-0.17
Total ($/GJ)	21.27	16.28	15.77	14.58	23.09	16.93	16.29	15.37	24.49	18.13	16.28	15.03	23.81	18.24	16.15	14.87
Total ($/bbl)	108.43	79.98	77.11	70.30	118.82	83.69	80.05	74.80	126.77	90.56	79.99	72.86	122.89	91.15	79.25	71.96
Lower Bound ($/GJ)	19.92	15.46	14.74	13.86	21.49	15.79	15.37	14.60	23.28	17.18	15.19	14.22	22.50	17.25	15.33	14.12
Gap	6.35%	4.99%	6.57%	4.95%	6.93%	6.74%	5.62%	5.00%	4.92%	5.28%	6.67%	5.41%	5.48%	5.44%	5.07%	5.08%

Contribution to Cost	Case Study - Perennial Crops															
($/GJ of products)	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass	5.81	5.71	5.76	5.78	5.90	6.02	6.12	5.99	5.92	5.81	5.74	5.86	5.80	5.59	5.56	5.75
Butane	0.61	0.61	0.61	0.61	-0.15	-0.15	-0.15	-0.15	0.00	0.00	0.00	0.00	0.41	0.41	0.41	0.41
Water	0.02	0.02	0.02	0.02	0.02	0.02	0.03	0.02	0.02	0.02	0.02	0.02	0.02	0.03	0.02	0.02
CO_2 TS&M	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Investment	12.01	7.50	6.91	5.95	12.11	7.47	6.86	5.84	13.51	8.33	6.77	5.76	13.29	8.20	6.68	5.69
O&M	3.17	1.98	1.83	1.57	3.20	1.97	1.81	1.54	3.57	2.20	1.79	1.52	3.51	2.17	1.77	1.50
Electricity	0.28	0.39	0.29	0.40	0.32	0.42	0.35	0.41	0.42	0.32	0.34	0.41	0.35	0.28	0.28	0.41
LPG	-2.25	-1.57	-1.57	-1.12	-0.03	-0.02	-0.02	-0.02	0.00	0.00	0.00	0.00	-0.34	-0.24	-0.24	-0.17
Total ($/GJ)	19.66	14.64	13.85	13.20	21.36	15.73	14.99	13.64	23.44	16.70	14.67	13.58	23.04	16.44	14.48	13.61
Total ($/bbl)	99.26	70.66	66.15	62.44	108.98	76.84	72.67	64.93	120.80	82.39	70.81	64.60	118.51	80.90	69.73	64.78
Lower Bound ($/GJ)	18.56	13.82	12.89	12.59	20.38	14.83	14.18	12.91	21.99	15.75	13.83	12.74	21.85	15.39	13.73	12.84
Gap	5.60%	5.58%	6.93%	4.63%	4.63%	5.69%	5.44%	5.31%	6.17%	5.68%	5.69%	6.15%	5.14%	6.39%	5.18%	5.63%

Contribution to Cost	Case Study - Agricultural Residues															
($/GJ of products)	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass	10.06	10.13	9.98	10.05	10.27	10.46	10.58	10.29	10.28	10.03	10.01	10.04	9.66	9.97	9.74	9.70
Butane	0.61	0.61	0.61	0.61	-0.15	-0.15	-0.15	-0.15	0.00	0.00	0.00	0.00	0.41	0.41	0.41	0.41
Water	0.02	0.02	0.02	0.02	0.02	0.03	0.02	0.03	0.02	0.02	0.02	0.03	0.03	0.02	0.02	0.02
CO_2 TS&M	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Investment	11.87	7.52	6.91	5.89	12.51	7.45	6.79	5.87	13.46	8.49	6.68	5.82	13.30	8.18	6.76	5.75
O&M	3.14	1.99	1.83	1.56	3.30	1.97	1.79	1.55	3.55	2.24	1.77	1.54	3.51	2.16	1.79	1.52
Electricity	-0.91	-0.88	-0.79	-0.71	-0.91	-0.83	-0.86	-0.62	-0.88	-0.77	-0.75	-0.87	-0.75	-0.59	-0.77	-0.69
LPG	-2.25	-1.57	-1.57	-1.12	-0.03	-0.02	-0.02	-0.02	0.00	0.00	0.00	0.00	-0.34	-0.24	-0.24	-0.17
Total ($/GJ)	22.54	17.81	17.00	16.29	25.01	18.90	18.16	16.96	26.44	20.02	17.73	16.56	25.82	19.92	17.72	16.54
Total ($/bbl)	115.68	88.72	84.08	80.05	129.75	94.95	90.69	83.87	137.91	101.31	88.25	81.58	134.39	100.75	88.22	81.46
Lower Bound ($/GJ)	21.39	16.73	16.05	15.51	23.61	17.96	17.01	16.08	24.76	18.92	16.74	15.74	24.52	18.76	16.77	15.71
Gap	5.08%	6.09%	5.58%	4.79%	5.59%	5.00%	6.32%	5.20%	6.34%	5.48%	5.57%	4.92%	5.03%	5.83%	5.36%	4.99%

Table S3: Breakdown of the investment costs for the forty-eight case studies. The major sections of the plant include the syngas generation section, syngas cleaning, hydrocarbon production, hydrocarbon upgrading, hydrogen/oxygen production, heat and power integration, and wastewater treatment blocks. The values are reported in MM$ and normalized with the amount of fuels produced ($/bpd).

Contribution to Cost (MM $)	Case Study - Forest Residues															
	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Syngas Generation	41	124	275	1173	40	121	342	1531	43	134	228	974	42	138	214	945
Syngas Cleaning	31	99	178	748	33	97	142	650	33	102	165	667	31	94	152	644
Hydrocarbon Production	22	67	143	570	20	66	117	478	23	72	122	511	25	79	122	498
Hydrocarbon Upgrading	6	20	18	79	7	20	16	66	11	36	62	253	11	36	64	262
Hydrogen/Oxygen Production	16	56	94	391	18	52	73	333	19	59	103	418	19	60	98	446
Heat and Power Integration	16	51	96	423	16	48	84	375	17	50	87	344	17	50	82	358
Wastewater Treatment	7	22	10	45	7	22	9	36	8	25	39	178	8	25	43	184
Total (MM $)	140	438	813	3430	140	425	781	3468	155	478	806	3344	152	484	775	3336
Total ($/bpd)	139562	87659	81333	68591	140223	84958	78149	69352	155269	95698	80568	66881	152060	96761	77501	66717

Contribution to Cost (MM $)	Case Study - Perennial Crops															
	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Syngas Generation	41	127	263	1153	40	124	354	1506	44	134	218	928	44	135	216	921
Syngas Cleaning	31	96	181	767	33	101	147	624	33	101	164	696	31	96	156	663
Hydrocarbon Production	21	67	139	593	21	65	111	474	24	75	122	520	25	77	119	506
Hydrocarbon Upgrading	6	20	18	82	6	20	16	67	12	37	59	253	11	35	61	260
Hydrogen/Oxygen Production	17	54	95	406	18	54	77	328	20	61	98	419	19	58	101	429
Heat and Power Integration	16	50	98	412	16	49	84	359	17	52	85	360	16	51	83	352
Wastewater Treatment	7	21	10	43	7	21	8	35	8	25	41	174	8	24	42	177
Total (MM $)	140	436	804	3457	141	434	797	3395	157	485	787	3351	155	477	777	3307
Total ($/bpd)	139652	87270	80399	69149	140791	86873	79745	67890	157080	96924	78727	67023	154558	95367	77696	66146

Contribution to Cost (MM $)	Case Study - Agricultural Residues															
	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Syngas Generation	41	125	251	1133	42	119	337	1482	44	136	217	946	44	129	222	920
Syngas Cleaning	31	100	189	754	34	103	151	650	33	102	161	704	31	97	162	659
Hydrocarbon Production	21	69	142	578	21	68	116	471	24	76	119	531	25	80	118	504
Hydrocarbon Upgrading	6	20	18	79	7	20	16	69	12	38	60	241	12	36	58	272
Hydrogen/Oxygen Production	17	52	96	413	18	53	79	338	20	62	94	419	19	60	100	448
Heat and Power Integration	15	50	99	425	16	48	82	369	16	54	84	370	16	49	86	360
Wastewater Treatment	7	21	10	45	7	22	8	36	8	25	43	176	8	25	40	178
Total (MM $)	138	437	804	3426	145	433	790	3415	156	494	777	3387	155	476	787	3342
Total ($/bpd)	138048	87465	80410	68519	145427	86635	78951	68292	156463	98776	77721	67734	154706	95178	78654	66834

Table S4: Overall material balance for the forty-eight case studies. The inputs to the BTL refinery are biomass, butane, and water, while the outputs include gasoline, diesel, kerosene, LPG, sequestered CO_2, and vented CO_2.

Material Balances								Case Study - Forest Residues								
	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass (dt/hr)	21.74	110.10	220.38	1069.56	22.79	113.76	222.73	1148.00	22.10	108.47	215.86	1097.13	21.14	106.05	214.91	1068.16
Butane (kBD)	0.05	0.23	0.45	2.26	0.01	0.06	0.11	0.57	0.00	0.00	0.00	0.00	0.03	0.15	0.30	1.52
Water (kBD)	1.63	6.34	18.18	75.05	1.37	8.67	20.51	81.72	2.05	9.92	14.68	69.21	1.43	9.42	19.51	102.57
Gasoline (kBD)	1.00	5.00	10.00	50.00	0.25	1.25	2.50	12.50	0.25	1.25	2.50	12.50	0.67	3.36	6.72	33.60
Diesel (kBD)	0.00	0.00	0.00	0.00	0.75	3.75	7.50	37.50	0.00	0.00	0.00	0.00	0.22	1.08	2.15	10.77
Kerosene (kBD)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.75	3.75	7.50	37.50	0.11	0.56	1.13	5.63
LPG (kBD)	0.10	0.49	0.99	4.95	0.00	0.01	0.01	0.07	0.00	0.00	0.00	0.00	0.01	0.07	0.15	0.74
Seq. CO_2 (tonne/hr)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Vented CO_2 (tonne/hr)	14.72	75.55	151.35	711.48	15.11	75.31	143.91	767.65	14.82	71.30	141.08	730.38	13.94	70.16	144.27	712.37

Material Balances								Case Study - Perennial Crops								
	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass (dt/hr)	21.69	106.44	215.05	1077.31	22.00	112.26	228.24	1117.80	22.09	108.47	214.32	1093.17	21.62	104.25	207.29	1073.12
Butane (kBD)	0.05	0.23	0.45	2.26	0.01	0.06	0.11	0.57	0.00	0.00	0.00	0.00	0.03	0.15	0.30	1.52
Water (kBD)	1.70	7.84	14.51	74.21	1.57	7.67	20.01	70.88	1.77	8.67	16.51	80.88	1.30	9.67	15.18	72.55
Gasoline (kBD)	1.00	5.00	10.00	50.00	0.25	1.25	2.50	12.50	0.25	1.25	2.50	12.50	0.67	3.36	6.72	33.60
Diesel (kBD)	0.00	0.00	0.00	0.00	0.75	3.75	7.50	37.50	0.00	0.00	0.00	0.00	0.22	1.08	2.15	10.77
Kerosene (kBD)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.75	3.75	7.50	37.50	0.11	0.56	1.13	5.63
LPG (kBD)	0.10	0.49	0.99	4.95	0.00	0.01	0.01	0.07	0.00	0.00	0.00	0.00	0.01	0.07	0.15	0.74
Seq. CO_2 (tonne/hr)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Vented CO_2 (tonne/hr)	14.64	70.43	143.89	722.32	14.01	73.21	151.63	725.39	14.81	71.30	138.92	724.83	14.61	67.64	133.60	719.31

Material Balances								Case Study - Agricultural Residues								
	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass (dt/hr)	21.89	110.23	217.27	1093.34	22.35	113.78	230.22	1120.10	22.38	109.19	217.77	1092.19	21.02	108.44	212.06	1055.47
Butane (kBD)	0.05	0.23	0.45	2.26	0.01	0.06	0.11	0.57	0.00	0.00	0.00	0.00	0.03	0.15	0.30	1.52
Water (kBD)	1.50	8.01	17.84	80.05	1.43	10.42	17.01	102.57	1.78	7.42	17.51	94.23	1.82	8.26	14.18	83.39
Gasoline (kBD)	1.00	5.00	10.00	50.00	0.25	1.25	2.50	12.50	0.25	1.25	2.50	12.50	0.67	3.36	6.72	33.60
Diesel (kBD)	0.00	0.00	0.00	0.00	0.75	3.75	7.50	37.50	0.00	0.00	0.00	0.00	0.22	1.08	2.15	10.77
Kerosene (kBD)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.75	3.75	7.50	37.50	0.11	0.56	1.13	5.63
LPG (kBD)	0.10	0.49	0.99	4.95	0.00	0.01	0.01	0.07	0.00	0.00	0.00	0.00	0.01	0.07	0.15	0.74
Seq. CO_2 (tonne/hr)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Vented CO_2 (tonne/hr)	14.93	75.72	147.00	744.76	14.50	75.33	154.39	728.60	15.22	72.31	143.76	723.47	13.76	73.51	140.28	694.61

Table S5: Overall energy balance for the forty-eight studies (MW). The energy inputs to the BTL refinery come from biomass, butane or electricity. The energy outputs are gasoline, diesel, kerosene, LPG, or electricity. Input energy for electricity is denoted as a positive value while output electricity is denoted as a negative value. The energy efficiency of the process is calculated by dividing the total energy output with the total energy inputs to the process.

Energy Balances	Case Study - Forest Residues															
	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass	122	620	1242	6027	128	641	1255	6469	125	611	1216	6182	119	598	1211	6019
Butane	3	14	27	137	1	3	7	34	0	0	0	0	2	9	18	92
Gasoline	64	319	637	3186	16	80	159	796	16	80	159	796	43	214	428	2141
Diesel	0	0	0	0	53	267	533	2667	0	0	0	0	15	77	153	766
Kerosene	0	0	0	0	0	0	0	0	52	260	519	2596	8	39	78	390
LPG	6	30	60	300	0	0	1	4	0	0	0	0	1	4	9	45
Electricity	-2	-13	-19	-98	-2	-15	-20	-139	-3	-10	-26	-113	-3	-10	-24	-141
Efficiency (%)	57.33%	56.95%	56.45%	58.14%	55.60%	56.10%	56.55%	55.46%	56.90%	57.18%	57.92%	56.69%	57.81%	56.76%	56.31%	56.99%

Energy Balances	Case Study - Perennial Crops															
	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass	127	622	1256	6293	128	656	1333	6529	129	634	1252	6385	126	609	1211	6268
Butane	3	14	27	137	1	3	7	34	0	0	0	0	2	9	18	92
Gasoline	64	319	637	3186	16	80	159	796	16	80	159	796	43	214	428	2141
Diesel	0	0	0	0	53	267	533	2667	0	0	0	0	15	77	153	766
Kerosene	0	0	0	0	0	0	0	0	52	260	519	2596	8	39	78	390
LPG	6	30	60	300	0	0	1	4	0	0	0	0	1	4	9	45
Electricity	1	7	10	68	1	7	12	70	1	6	12	69	1	5	10	69
Efficiency (%)	53.14%	53.82%	53.55%	53.16%	52.84%	51.54%	50.86%	51.77%	51.49%	52.67%	53.27%	52.04%	51.23%	53.29%	53.59%	51.45%

Energy Balances	Case Study - Agricultural Residues															
	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass	123	621	1224	6161	126	641	1297	6311	126	615	1227	6154	118	611	1195	5947
Butane	3	14	27	137	1	3	7	34	0	0	0	0	2	9	18	92
Gasoline	64	319	637	3186	16	80	159	796	16	80	159	796	43	214	428	2141
Diesel	0	0	0	0	53	267	533	2667	0	0	0	0	15	77	153	766
Kerosene	0	0	0	0	0	0	0	0	52	260	519	2596	8	39	78	390
LPG	6	30	60	300	0	0	1	4	0	0	0	0	1	4	9	45
Electricity	-3	-15	-27	-121	-3	-14	-29	-105	-3	-13	-26	-148	-3	-10	-26	-118
Efficiency (%)	57.74%	57.28%	57.84%	57.28%	57.20%	55.97%	55.41%	56.30%	56.16%	57.27%	57.37%	57.52%	57.69%	55.49%	57.22%	57.27%

Table S6: Carbon balances (in kg/s) for the optimal solutions for the forty-eight case studies. Carbon is input to the process via biomass or butanes and exits the process as liquid product, LPG byproduct, vented CO_2, or sequestered (Seq.) CO_2. The small amount of CO_2 input to the system in the purified oxygen stream ($< 0.01\%$) is neglected.

Carbon Balances	Case Study - Forest Residues															
	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass	2.31	11.68	23.37	113.44	2.42	12.07	23.62	121.76	2.34	11.50	22.89	116.36	2.24	11.25	22.79	113.29
Butane	0.04	0.21	0.41	2.07	0.01	0.05	0.10	0.52	0.00	0.00	0.00	0.00	0.03	0.14	0.28	1.39
Gasoline	1.16	5.79	11.58	57.91	0.29	1.45	2.90	14.48	0.29	1.45	2.90	14.48	0.78	3.89	7.78	38.91
Diesel	0.00	0.00	0.00	0.00	0.99	4.96	9.91	49.56	0.00	0.00	0.00	0.00	0.28	1.42	2.85	14.24
Kerosene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.93	4.65	9.30	46.52	0.14	0.70	1.40	6.98
LPG	0.07	0.37	0.73	3.66	0.00	0.01	0.01	0.05	0.00	0.00	0.00	0.00	0.01	0.05	0.11	0.55
Vented CO_2	1.12	5.73	11.47	53.93	1.15	5.71	10.91	58.19	1.12	5.40	10.69	55.37	1.06	5.32	10.94	54.00
Seq. CO_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
% Conversion	52.47%	51.81%	51.77%	53.31%	52.80%	52.89%	54.02%	52.41%	52.05%	53.02%	53.29%	52.42%	53.46%	53.29%	52.60%	52.91%

Carbon Balances	Case Study - Perennial Crops															
	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass	2.30	11.29	22.81	114.26	2.33	11.91	24.21	118.55	2.34	11.50	22.73	115.94	2.29	11.06	21.99	113.82
Butane	0.04	0.21	0.41	2.07	0.01	0.05	0.10	0.52	0.00	0.00	0.00	0.00	0.03	0.14	0.28	1.39
Gasoline	1.16	5.79	11.58	57.91	0.29	1.45	2.90	14.48	0.29	1.45	2.90	14.48	0.78	3.89	7.78	38.91
Diesel	0.00	0.00	0.00	0.00	0.99	4.96	9.91	49.56	0.00	0.00	0.00	0.00	0.28	1.42	2.85	14.24
Kerosene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.93	4.65	9.30	46.52	0.14	0.70	1.40	6.98
LPG	0.07	0.37	0.73	3.66	0.00	0.01	0.01	0.05	0.00	0.00	0.00	0.00	0.01	0.05	0.11	0.55
Vented CO_2	1.11	5.34	10.91	54.75	1.06	5.55	11.49	54.99	1.12	5.40	10.53	54.94	1.11	5.13	10.13	54.53
Seq. CO_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
% Conversion	52.59%	53.56%	53.03%	52.93%	54.69%	53.59%	52.72%	53.82%	52.07%	53.02%	53.67%	52.61%	52.28%	54.20%	54.51%	52.67%

Carbon Balances	Case Study - Agricultural Residues															
	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass	2.32	11.69	23.04	115.96	2.37	12.07	24.42	118.80	2.37	11.58	23.10	115.84	2.23	11.50	22.49	111.94
Butane	0.04	0.21	0.41	2.07	0.01	0.05	0.10	0.52	0.00	0.00	0.00	0.00	0.03	0.14	0.28	1.39
Gasoline	1.16	5.79	11.58	57.91	0.29	1.45	2.90	14.48	0.29	1.45	2.90	14.48	0.78	3.89	7.78	38.91
Diesel	0.00	0.00	0.00	0.00	0.99	4.96	9.91	49.56	0.00	0.00	0.00	0.00	0.28	1.42	2.85	14.24
Kerosene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.93	4.65	9.30	46.52	0.14	0.70	1.40	6.98
LPG	0.07	0.37	0.73	3.66	0.00	0.01	0.01	0.05	0.00	0.00	0.00	0.00	0.01	0.05	0.11	0.55
Vented CO_2	1.13	5.74	11.14	56.46	1.10	5.71	11.70	55.23	1.15	5.48	10.90	54.84	1.04	5.57	10.63	52.65
Seq. CO_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
% Conversion	52.12%	51.75%	52.50%	52.17%	53.83%	52.88%	52.27%	53.71%	51.39%	52.67%	52.82%	52.66%	53.78%	52.13%	53.30%	53.54%

Table S7: Greenhouse gas (GHG) balances for the optimal solutions for the forty-eight case studies. The total GHG emissions (in CO_2 equivalents - kg CO_2eq/s) for feedstock acquisition and transportation, biomass carbon storage, product transportation and use, CO_2 sequestration, and process venting are shown for each study. Process feedstocks include biomass and butane while products include gasoline, diesel, kerosene, and LPG.

GHG Balances	Case Study - Forest Residues															
	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass	-11.23	-56.88	-113.85	-552.53	-11.77	-58.77	-115.06	-593.05	-11.42	-56.04	-111.51	-566.77	-10.92	-54.78	-111.02	-551.81
Butane	0.01	0.03	0.05	0.25	0.00	0.01	0.01	0.06	0.00	0.00	0.00	0.00	0.00	0.02	0.03	0.17
Gasoline	4.24	21.22	42.44	212.20	1.06	5.30	10.61	53.05	1.06	5.30	10.61	53.05	2.85	14.26	28.52	142.59
Diesel	0.00	0.00	0.00	0.00	3.63	18.16	36.32	181.60	0.00	0.00	0.00	0.00	1.04	5.22	10.43	52.17
Kerosene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.41	17.05	34.09	170.47	0.51	2.56	5.12	25.58
LPG	0.27	1.34	2.69	13.43	0.00	0.02	0.04	0.19	0.00	0.00	0.00	0.00	0.04	0.20	0.40	2.01
Vented CO_2	4.09	20.98	42.04	197.63	4.20	20.92	39.98	213.24	4.12	19.81	39.19	202.88	3.87	19.49	40.07	197.88
Seq. CO_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LGHG	-2.62	-13.30	-26.63	-129.02	-2.88	-14.36	-28.11	-144.92	-2.83	-13.88	-27.62	-140.37	-2.60	-13.04	-26.45	-131.41
GHGAF	6.39	31.93	63.87	319.34	6.35	31.76	63.53	317.64	6.21	31.07	62.15	310.74	6.12	30.61	61.22	306.08
GHGAE	0.21	1.27	1.95	9.88	0.25	1.49	2.03	14.06	0.30	1.04	2.63	11.40	0.31	1.04	2.43	14.31
GHGI	-0.40	-0.40	-0.40	-0.39	-0.44	-0.43	-0.43	-0.44	-0.43	-0.43	-0.43	-0.44	-0.40	-0.41	-0.42	-0.41

GHG Balances	Case Study - Perennial Crops															
	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass	-7.13	-35.00	-70.72	-354.28	-7.23	-36.92	-75.06	-367.60	-7.26	-35.67	-70.48	-359.50	-7.11	-34.28	-68.17	-352.90
Butane	0.01	0.03	0.05	0.25	0.00	0.01	0.01	0.06	0.00	0.00	0.00	0.00	0.00	0.02	0.03	0.17
Gasoline	4.24	21.22	42.44	212.20	1.06	5.30	10.61	53.05	1.06	5.30	10.61	53.05	2.85	14.26	28.52	142.59
Diesel	0.00	0.00	0.00	0.00	3.63	18.16	36.32	181.60	0.00	0.00	0.00	0.00	1.04	5.22	10.43	52.17
Kerosene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.41	17.05	34.09	170.47	0.51	2.56	5.12	25.58
LPG	0.27	1.34	2.69	13.43	0.00	0.02	0.04	0.19	0.00	0.00	0.00	0.00	0.04	0.20	0.40	2.01
Vented CO_2	4.07	19.56	39.97	200.65	3.89	20.34	42.12	201.50	4.11	19.81	38.59	201.34	4.06	18.79	37.11	199.81
Seq. CO_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LGHG	1.45	7.15	14.42	72.24	1.35	6.91	14.04	68.79	1.32	6.49	12.82	65.37	1.40	6.76	13.45	69.42
GHGAF	6.39	31.93	63.87	319.34	6.35	31.76	63.53	317.64	6.21	31.07	62.15	310.74	6.12	30.61	61.22	306.08
GHGAE	-0.10	-0.67	-1.00	-6.90	-0.11	-0.72	-1.22	-7.09	-0.14	-0.56	-1.18	-7.03	-0.12	-0.48	-0.96	-6.96
GHGI	0.23	0.23	0.23	0.23	0.22	0.22	0.23	0.22	0.22	0.21	0.21	0.22	0.23	0.22	0.22	0.23

GHG Balances	Case Study - Agricultural Residues															
	U-1	U-5	U-10	U-50	D-1	D-5	D-10	D-50	K-1	K-5	K-10	K-50	R-1	R-5	R-10	R-50
Biomass	-6.78	-34.17	-67.34	-338.89	-6.93	-35.27	-71.36	-347.18	-6.94	-33.84	-67.50	-338.53	-6.51	-33.61	-65.73	-327.15
Butane	0.01	0.03	0.05	0.25	0.00	0.01	0.01	0.06	0.00	0.00	0.00	0.00	0.00	0.02	0.03	0.17
Gasoline	4.24	21.22	42.44	212.20	1.06	5.30	10.61	53.05	1.06	5.30	10.61	53.05	2.85	14.26	28.52	142.59
Diesel	0.00	0.00	0.00	0.00	3.63	18.16	36.32	181.60	0.00	0.00	0.00	0.00	1.04	5.22	10.43	52.17
Kerosene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	3.41	17.05	34.09	170.47	0.51	2.56	5.12	25.58
LPG	0.27	1.34	2.69	13.43	0.00	0.02	0.04	0.19	0.00	0.00	0.00	0.00	0.04	0.20	0.40	2.01
Vented CO_2	4.15	21.03	40.83	206.88	4.03	20.93	42.89	202.39	4.23	20.09	39.93	200.96	3.82	20.42	38.97	192.95
Seq. CO_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LGHG	1.88	9.46	18.66	93.86	1.80	9.15	18.51	90.10	1.76	8.59	17.14	85.95	1.76	9.06	17.74	88.32
GHGAF	6.39	31.93	63.87	319.34	6.35	31.76	63.53	317.64	6.21	31.07	62.15	310.74	6.12	30.61	61.22	306.08
GHGAE	0.31	1.52	2.71	12.28	0.31	1.42	2.94	10.64	0.30	1.33	2.58	14.94	0.26	1.01	2.63	11.90
GHGI	0.28	0.28	0.28	0.28	0.27	0.28	0.28	0.27	0.27	0.27	0.26	0.26	0.28	0.29	0.28	0.28

Process Units

The nomenclature for all terms in the mathematical model for process synthesis with simultaneous heat, power, and water integration is shown below. All constraints included in the model are listed subsequently with a corresponding description of how that particular equation governs proper operation of the process design. For a more extensive discussion of the mathematical model, the reader is directed to previously published works [2, 3, 4, 5, 6, 7].

The set of units, U, is presented in full detail in Table S8 and defined formally in Equation S1. Note that several units in Table S8 are listed as u_n. The n subscript represents the consideration of multiple forms of the same process unit, each with a distinct set of operating conditions (e.g., temperature and pressure). Though these unit properties are generally given as continuous variables in a process synthesis problem, they have been assumed to take discrete choices and will be modeled using binary variables.

$$u \in U = \{\text{Complete set of process units listed in Table S8}\} \tag{S1}$$

Table S8: Process units present in the BTL synthesis problem. The subscript n corresponds to multiple forms of the same process unit, each with a distinct set of operating conditions or ratios of feedstock. Distinct process units are used in lieu of continuous variables representing the process operating conditions. This will prevent the use of bilinear terms when specifying feedstock ratios or highly non-linear equations when specifying equilibrium constants or species enthalpies.

Unit Name	Unit Index	Unit Name	Unit Index
	Process Inlets		
Inlet Air	IN_{AIR}	Inlet Natural Gas	IN_{NG}
Inlet Water	IN_{H2O}	Inlet Butane	IN_{BUT}
	Process Outlets		
Outlet Gasoline	OUT_{GAS}	Outlet Diesel	OUT_{DIE}
Outlet Kerosene	OUT_{KER}	Outlet Ash	OUT_{ASH}
Outlet Sulfur	OUT_{S}	Outlet Scrubbed HCl	OUT_{SCR}
Outlet Vent	OUT_{V}	Outlet Propane	OUT_{PRO}
Outlet Sequestered CO_2	OUT_{CO_2}	Outlet Wastewater	OUT_{WW}

Table S8: (continued)

Unit Name	Unit Index	Unit Name	Unit Index
		Biomass conversion	
Biomass Dryer	BDR	Biomass Dryer Air Heater	X_{BDR}
Biomass Lockhopper	BLK	Biomass Gasifier	BGS_n
First Biomass Vapor Cyclone	BC_1	Second Biomass Vapor Cyclone	BC_2
Tar Cracker	TCK	Tar Cracker Splitter	SP_{TCK}
Tar Cracker Cooler	X_{TCK}		
		Syngas Cleaning	
Reverse Water Gas Shift Unit	RGS_n	RGS Effluent Cooler	X_{RGS}
COS-HCN Hydrolyzer	CHH	HCl Scrubber	HSC
Acid Gas Flash Vapor Cooler	X_{AGF}	Acid Gas Flash 2-Phase Cooler	X_{AGF_n}
Acid Gas Flash Unit	AGF	Acid Gas Thermal Analyzer	X_{AGR}
Acid Gas Removal Unit	AGR	First CO_2 Compressor	CO_2C
CO_2 Recycle Compressor	CO_2RC	CO_2 Sequestration Compressor	CO_2SC
Acid Gas Compressor	AGC		
		Sulfur Recovery	
Acid Gas Splitter	SP_{AG}	Acid Gas Preheater	X_{AG}
Claus Combustor	CC	First Sulfur Convertor	SC_1
First Sulfur Separator	SS_1	Second Sulfur Convertor Heater	X_{SC_2}
Second Sulfur Convertor	SC_2	Second Sulfur Separator	SS_2
Third Sulfur Convertor Heater	X_{SC_3}	Third Sulfur Convertor	SC_3
Third Sulfur Separator	SS_3	Sulfur Pit	SPT
Tail Gas Hydrolyzer	TGH	Tail Gas Flash Vapor Cooler	X_{TGF}
Tail Gas Flash 2-Phase Cooler	X_{TGF_n}	Tail Gas Flash Unit	TGF
Tail Gas Compressor	TGC		
		Hydrocarbon Production	
Iron MT fWGS nominal wax FT	MTFTWGS-N	Iron MT fWGS minimal was FT	MTFTWGS-M
Fischer-Tropsch Compressor	FTC	Fischer-Tropsch Splitter	SP_{FT}
Low-Temperature Preheater	X_{LTFT}	Low-Temperature Splitter	SP_{LTFT}
Low-Temperature Iron-Based FT	LTFT	Low-Temperature Cobalt-Based FT	LTFTRGS
High-Temperature Preheater	X_{HTFT}	High-Temperature Splitter	SP_{HTFT}

Table S8: (continued)

Unit Name	Unit Index		Unit Name	Unit Index
High-Temperature Iron-Based FT	HTFT		High-Temperature Cobalt-Based FT	HTFTRGS
ZSM-5 hydrocarbon conversion unit	FT-ZSM5		ZSM-5 product fractionation	ZSM5F
Methanol synthesis unit	MEOHS		Methanol flash unit	MEOH-F
Methanol degasser	MEDEG		Methanol to gasoline ZSM-5 reactor	MTG
Methanol to olefins ZSM-5 reactor	MTO		MTO fractionation	MTO-F
Low-Temperature Effluent Cooler	X_{LTFTC}		High-Temperature Effluent Cooler	X_{HTFTC}
Water-Soluble Oxygenates Separator	WSOS		Vapor-Phase Oxygenates Separator	VPOS
Primary Vapor-Liquid-Water Separator	VLWS			
		Hydrocarbon Recovery		
Hydrocarbon Recovery Column	HRC		Wax Hydrocracker	WHC
Distillate Hydrotreater	DHT		Kerosene Hydrotreater	KHT
Naphtha Hydrotreater	NHT		Naphtha Reformer	NRF
C_4 Isomerizer	C_4I		C_5-C_6 Isomerizer	$C_{56}I$
C_3-C_4-C_5 Alkylation Unit	$C_{345}A$		Saturated Gas Plant	SGP
Diesel Blender	DBL		Gasoline Blender	GBL
Olefins to gasoline/distillate	OGD		OGD fractionation	OGD-F
Mixed hydrocarbon knockout 1	HCKO1		Mixed hydrocarbon knockout 2	
De-ethanizer	DEETH		Absorber column	ABS-COL
1-stage Rectisol CO_2 separation	CO_2SEP		Stabilizer column	
HF alkylation unit	ALK-UN		LPG/Alkylate splitter	LPG-ALK
Splitter column	SP-COL			
		Recycle Gas Treatment		
Light Gas Compressor	LGC		Light Gas Splitter	SP_{LG}
Fuel Combustor	FCM		Fuel Combuster Effluent Cooler	X_{FCM}
Fuel Combustor Flash Unit	FCF		First Gas Turbine Air Compressor	$GTAC_1$
Second Gas Turbine Air Compressor	$GTAC_2$		Gas Turbine Combustor	GTC
First Gas Turbine	GT_1		Second Gas Turbine	GT_2
Gas Turbine Effluent Cooler	X_{GT}		Gas Turbine Flash Unit	GTF
Gas Turbine Effluent Compressor	GTEC		CO_2 Recovery Unit	CO_2R
Water Gas Shift Unit	WGS	Auto-thermal Reactor	ATR	
		Water Treatment		
Biological Digestor	BD		Reverse Osmosis	RO
Cooling Tower	CLTR		Process Cooling	COOL-P
Heat & Power System	HEP		Heat & Power Utilities	HEAT-P
Deaerator	DEA		Process Water Economizer	X_{WPR}
Process Water Boiler	X_{WBL}			

Table S8: (continued)

Unit Name	Unit Index	Unit Name	Unit Index
Hydrogen/Oxygen Production			
PSA Effluent Splitter	SP_{PSA}	Pressure-swing Absorption Unit	PSA
PSA Hydrogen Preheater	X_{H_2P}	PSA Hydrogen Splitter	SP_{H_2P}
Electrolyzer	EYZ	Electrolyzer Oxygen Preheater	X_{O_2E}
Electrolyzer Oxygen Splitter	SP_{O_2E}	Electrolyzer Hydrogen Preheater	X_{H_2E}
Electrolyzer Hydrogen Splitter	SP_{H_2E}	Air Compressor	AC
Air Separation Unit	ASU	Oxygen Compressor	OC
ASU Oxygen Preheater	X_{O_2A}	OC Oxygen Splitter	SP_{O_2C}
OC Oxygen Preheater	X_{O_2C}		

Process Species

The set of all species, S, is listed in Table S9 and defined formally in Equation S2.

$$s \in S = \{\text{Complete set of species listed in Table S9}\} \tag{S2}$$

Table S9: Species present in the BTL synthesis problem. The molecular formula of the pseudocomponent hydrocarbons and oxygenates are given by Bechtel. The formula for the biomass and coal species are derived from the ultimate analysis assuming that the “atomic” weight of ash is 1.0 g/mol.

Species Name	Species Index	Species Name	Species Index	Species Name	Species Index
Light Non-Hydrocarbon Gases					
Oxygen	O_2	Nitrogen	N_2	Argon	Ar
Nitric Oxide	NO	Nitrous Oxide	N_2O	Water	H_2O
Carbon Monoxide	CO	Hydrogen	H_2	Carbon Dioxide	CO_2

Table S9: (continued)

Species Name	Species Index	Species Name	Species Index	Species Name	Species Index
		Hydrocarbons			
Methane	CH_4	Acetylene	C_2H_2	Ethylene	C_2H_4
Ethane	C_2H_6	Propylene	C_3H_6	Propane	C_3H_8
Isobutylene	iC_4H_8	1-Butene	nC_4H_8	Isobutane	iC_4H_{10}
n-Butane	nC_4H_{10}	1-Pentene	C_5H_{10}	2-Methylbutane	iC_5H_{12}
n-Pentane	nC_5H_{12}	1-Hexene	C_6H_{12}	2-Methylpentane	iC_6H_{14}
n-Hexane	nC_6H_{14}	1-Heptene	C_7H_{14}	n-Heptane	C_7H_{16}
1-Octene	C_8H_{16}	n-Octane	C_8H_{18}	1-Nonene	C_9H_{18}
n-Nonane	C_9H_{20}	1-Decene	$C_{10}H_{20}$	n-Decane	$C_{10}H_{22}$
1-Undecene	$C_{11}H_{22}$	n-Undecane	$C_{11}H_{24}$	1-Dodecene	$C_{12}H_{24}$
n-Dodecane	$C_{12}H_{26}$	1-Tridecene	$C_{13}H_{26}$	n-Tridecane	$C_{13}H_{28}$
1-Tetradecene	$C_{14}H_{28}$	n-Tetradecane	$C_{14}H_{30}$	1-Pentadecene	$C_{15}H_{30}$
n-Pentadecane	$C_{15}H_{32}$	1-Hexadecene	$C_{16}H_{32}$	n-Hexadecane	$C_{16}H_{34}$
1-Heptadecene	$C_{17}H_{34}$	n-Heptadecane	$C_{17}H_{36}$	1-Octadecene	$C_{18}H_{36}$
n-Octadecane	$C_{18}H_{38}$	1-Nonadecene	$C_{19}H_{38}$	n-Nonadecane	$C_{19}H_{40}$
1-Eicosene	$C_{20}H_{40}$	n-Eicosane	$C_{20}H_{42}$	C_{21} Pseudocomponent	$C_{21}OP$
C_{22} Pseudocomponent	$C_{22}OP$	C_{23} Pseudocomponent	$C_{23}OP$	C_{24} Pseudocomponent	$C_{24}OP$
C_{25} Pseudocomponent	$C_{25}OP$	C_{26} Pseudocomponent	$C_{26}OP$	C_{27} Pseudocomponent	$C_{27}OP$
C_{28} Pseudocomponent	$C_{28}OP$	C_{29} Pseudocomponent	$C_{29}OP$	C_{30+} Pseudocomponent	$C_{30}Wax$
VP Oxygenate	OXVAP	HP Oxygenate	OXHC	AP Oxygenate	OXH2O
Methanol	CH_3OH				
		Products			
Gasoline	GAS	Diesel	DIE	Kerosene	KER
LPG	LPG				

Indices/Sets

The indices are used throughout the mathematical model are listed below.

u : Process unit index

s : Species index

a : Atom index

p : Proximate analysis index

r : Reaction index

i : General counting index

The set, U, is defined as the complete set of process units. Several subsets of units are then defined for specific areas of the BTL process as presented below.

$$
\begin{aligned}
u_{RGS} &= \{u : u = \mathrm{RGS}_n\} \\
u_{ATR} &= \{u : u = \mathrm{ATR}_n\}
\end{aligned}
$$

The set of all atoms, A, includes C, H, O, N, S, Cl, and Ar.

$$a \in A = \{\mathrm{C, H, O, N, S, Cl, Ar}\}$$

The list of all unit connections, UC, is derived below.

$$UC = \{(u,u') : \exists \text{ a connection between unit } u \text{ and unit } u' \text{ in the superstructure}\}$$

Using *a priori* knowledge about the operations of each unit in the BTL process, the complete set of species that can possibly exist in a stream from unit u to unit u' is defined as $S^{UC}_{u,u'}$. The set $(u,u',s) \in S^{UF}$ is then constructed from all streams in UC along with the set of all species s that exist within a given unit u (S^U).

$$
\begin{aligned}
S^{UF} &= \{(u,u',s) : \exists s \in S^{UC}_{u,u'}\} \\
S^{U} &= \{(s,u) : \exists (u,u',s) \in S^{UF} \text{ or } \exists (u',u,s) \in S^{UF}\}
\end{aligned}
$$

Parameters

With the exception of all the pseudocomponents, the molecular formula is equal to the species index defined in Table S9. The pseudocomponent hydrocarbons and oxygenate formulas are given by Bechtel while the formulas for biomass and coal compounds are derived from the ultimate analysis and normalized to one mole of carbon. Char has been assumed to consist completely of carbon and ash has been assigned a generic molecular weight of 1.0 g/mol. The atomic ratio ($AR_{s,a}$) of atom a in species s is derived from the molecular formulas in Table S9.

$AR_{s,a}$: Atomic ratio of atom a in species s

Using the appropriate atomic weight of atom a (AW_a), the molecular weight of all species s (MW_s) is defined using Equation S3.

AW_a : Atomic weight of atom a

$$MW_s = \sum_a AW_a \cdot AR_{s,a} \tag{S3}$$

Variables

Continuous variables are used in the mathematical model to describe the species molar flow rates ($N^S_{u,u',s}$), the total molar flow rates ($N^T_{u,u'}$), the extent of reaction in a process unit (ξ^u_r), the molar composition of a stream ($x^S_{u,u',s}$), the split fraction of a stream between two units ($sp_{u,u'}$), the total stream enthalpy flow rate ($H^T_{u,u'}$), the heat lost from a unit (Q^L_u), the heat transferred to or absorbed from a unit (Q_u), the delivered cost of feedstock ($Cost^F_s$), the cost of CO_2 sequestration ($Cost^{Seq}$), the cost of electricity ($Cost^{El}$), and the levelized unit investment cost ($Cost^U_u$). Note that the subscripts u and u' are both used to denote an element of the set U and can be used interchangeably in the stream flow indices.

$N^S_{u,u',s}$: Molar flow of species s from unit u to unit u'
$N^T_{u,u'}$: Total molar flow from unit u to unit u'
ξ^u_r : Extent of reaction r in unit u
$x^S_{u,u',s}$: Molar composition of species s from unit u to unit u'
$sp_{u,u'}$: Split fraction of stream going from unit u to unit u'
$H^T_{u,u'}$: Total enthalpy flow from unit u to unit u'
Q^L_u : Heat lost from unit u

Q_u : Heat transferred to or absorbed from from unit u

$Cost^F_s$: Total delivered cost of feedstock s

$Cost^{Seq}$: Total sequestration cost of CO_2

$Cost^{El}$: Total cost of electricity

$Cost^U_u$: Total levelized cost of unit u

Binary variables (y_u) are introduced to represent the logical use of a process unit u. These binary variables are only needed for specific process units since many of the units in the BTL process will always be required. The units that require binary variables include the reverse water gas shift unit, the Fischer-Tropsch units, the autothermal reformer, the steam reformer, the gas turbine, the methanol synthesis unit, the methanol conversion units, and each of the hydrocarbon upgrading units.

y_u : Logical existence of process unit u (i.e., it takes the value of one if unit u is selected and zero otherwise)

General Constraints

Material Balances

Species Balances

$$\sum_{(u',u)\in UC} N^S_{u',u,s} - \sum_{(u,r,s')\in R^U} \frac{\nu_{r,s}}{\nu_{r,s'}} \cdot \xi^u_r - \sum_{(u,u')\in UC} N^S_{u,u',s} = 0 \quad \forall s \in S^U_u, u \in U^{Bal}_{Sp} \tag{S4}$$

Extent of Reaction

$$\xi^u_r - fc^u_r \cdot \sum_{(u',u,s)\in S^{UF}} N^S_{u',u,s} = 0 \quad \forall (u,r,s) \in R^U \tag{S5}$$

Atom Balances

$$\sum_{(u',u,s)\in S^{UF}} AR_{s,a} \cdot N^S_{u',u,s} - \sum_{(u,u',s)\in S^{UF}} AR_{s,a} \cdot N^S_{u,u',s} = 0 \quad \forall a \in A^U_u, u \in U^{Bal}_{At} \tag{S6}$$

Total Mole Balance

$$N^{T}_{u',u} - \sum_{(u,u',s)\in S^{UF}} N^{S}_{u',u,s} \quad = 0 \quad \forall (u,u') \in UC \tag{S7}$$

Process Splitters

Set Unit Split Fractions

$$N^{S}_{u,u',s} - x^{S}_{u_I,u,s} \cdot N^{T}_{u,u'} \quad = 0 \quad \forall (u,u',s) \in S^{UF}, u \in U_{Sp} \tag{S8}$$

Split Fractions Sum to 1

$$\sum_{(u,u',s)\in S^{UF}} x^{S}_{u,u',s} - 1 \quad = 0 \quad \forall (u,u') \in UC_{Comp} \tag{S9}$$

Flash Units

Upper Bound of Liquid Phase Split Fraction

$$x^{S}_{u,u_L,s} - min\{1, \frac{1}{K^{VLE}_{u,s}}\} \quad \leq 0 \quad \forall (u,u_L,s) \in S^{UF}, u \in U_{Fl} \tag{S10}$$

Upper Bound of Vapor Phase Split Fraction

$$x^{S}_{u,u_V,s} - min\{1, K^{VLE}_{u,s}\} \quad \leq 0 \quad \forall (u,u_V,s) \in S^{UF}, u \in U_{Fl} \tag{S11}$$

Set Liquid Phase Split Fraction

$$x^{S}_{u,u_L,s} \cdot N^{T}_{u,u_L} - N^{S}_{u,u_L,s} \quad = 0 \quad \forall u \in U_{Fl} \tag{S12}$$

Set Vapor Phase Split Fraction

$$x^{S}_{u,u_V,s} \cdot N^{T}_{u,u_V} - N^{S}_{u,u_V,s} \quad = 0 \quad \forall u \in U_{Fl} \tag{S13}$$

Set Phase Equilibrium

$$x^S_{u,u_V,s} - K^{VLE}_{u,s} \cdot x^S_{u,u_L,s} \quad = 0 \quad \forall u \in U_{Fl} \tag{S14}$$

Heat Balances

Conservation of Energy

$$\sum_{(u,u') \in UC} H^T_{u,u'} - \sum_{(u',u) \in UC} H^T_{u',u} - Q_u - Q^L_u - Wu \quad = 0 \quad \forall u \in U/U_{Agg} \tag{S15}$$

Total Heat Balance

$$H^T_{u,u'} - \sum_{(u,u',s) \in S^{UF}} H^S_{u,u',s} \quad = 0 \quad \forall (u,u') \in UC \tag{S16}$$

Logical Unit Existence

Bound on Molar Flows

$$\sum_{(u',u) \in UC} N^T_{u',u} - UB^N_u \cdot y_u \quad \leq 0 \quad \forall u \in U^{Ex} \tag{S17}$$

Upper Bound on Inlet Enthalpy Flow

$$H^T_{u',u} - UB^H_{u',u} \cdot y_u \quad \leq 0 \quad \forall (u',u) \in UC, u \in U^{Ex} \tag{S18}$$

Lower Bound on Inlet Enthalpy Flow

$$LB^H_{u',u} \cdot y_u - H^T_{u',u} \quad \leq 0 \quad \forall (u',u) \in UC, u \in U^{Ex} \tag{S19}$$

Upper Bound on Outlet Enthalpy Flow

$$H^T_{u,u'} - UB^H_{u',u} \cdot y_u \quad \leq 0 \quad \forall (u,u') \in UC, u \in U^{Ex} \tag{S20}$$

Lower Bound on Outlet Enthalpy Flow

$$LB^{H}_{u,u'} \cdot y_u - H^{T}_{u,u'} \quad \leq 0 \quad \forall (u,u') \in UC, u \in U^{Ex} \tag{S21}$$

Process Inlets

Biomass Moisture Content

$$MW_{\mathrm{H_2O}} \cdot N^{S}_{u,u',\mathrm{H_2O}} - \sum_{s \in S_{Bio}} PA^{M}_{s} \cdot MW_s \cdot N^{S}_{u,u',s} \quad = 0 \quad (u,u') = (\mathrm{IN_{BIO}},\mathrm{BDR}) \tag{S22}$$

Known Stream Compositions

Set Stream Compositions for Inlet Streams

$$N^{S}_{u,u',s} - x^{K}_{u,s} \cdot N^{T}_{u,u'} \quad = 0 \quad \forall (u,u',s) \in S^{UF}, u = \{\mathrm{IN_{AIR}},\mathrm{IN_{NG}},\mathrm{IN_{BUT}}\} \tag{S23}$$

Greenhouse Gas Emissions Reduction

Set Reduction from Petroleum Based Processes

$$GHG_{BTL} - GHG_{Red} \cdot (GHG_{Pet} + GHG_{Elec}) \quad = 0 \tag{S24}$$

Sum Emissions from GTL Components

$$GHG_{BTL} - GHG^{Seq} - GHG^{Proc} - GHG^{Feed} \quad = 0 \tag{S25}$$

Set Emissions from Feedstock Acquisition

$$GHG^{Feed} - \sum_{u \in U_{In}} \sum_{(u,u',s) \in S^{UF}} GHG^{T}_{s} \cdot MW_s * N^{S}_{u,u',s} \quad = 0 \tag{S26}$$

Set Emissions from CO_2 Sequestration

$$GHG^{Seq} - GHG^{T}_{\mathrm{CO_2}} \cdot MW_{\mathrm{CO_2}} \cdot N^{S}_{\mathrm{CO_2SC},\mathrm{OUT_{CO_2}},\mathrm{CO_2}} \quad = 0 \tag{S27}$$

Set Emissions from CO_2 Venting

$$GHG^{Proc} - MW_{\mathrm{CO_2}} \cdot N^S_{\mathrm{CO_2R,OUT_V,CO_2}} \quad = 0 \tag{S28}$$

Process Outlet Fuel Ratios

Set Gasoline to Diesel Output Ratio

$$MW_{\mathrm{GAS}} \cdot N^S_{\mathrm{GBL,OUT_{GAS},GAS}} - Rat_{G-D} \cdot MW_{\mathrm{DIE}} \cdot N^S_{\mathrm{DBL,OUT_{DIE},DIE}} \quad = 0 \tag{S29}$$

Set Diesel to Kerosene Output Ratio

$$MW_{\mathrm{DIE}} \cdot N^S_{\mathrm{DBL,OUT_{DIE},DIE}} - Rat_{D-K} \cdot MW_{\mathrm{KER}} \cdot N^S_{\mathrm{KHT,OUT_{KER},KER}} \quad = 0 \tag{S30}$$

Biomass Conversion

Biomass Drier

Upper Bound for Biomass Drier Activation

$$\begin{aligned} & MW_{\mathrm{H_2O}} \cdot N^S_{u,u',\mathrm{H_2O}} - \\ & MT_{\mathrm{Bio}} \cdot \sum_{(u,u',s) \in S^{UF}} MW_s \cdot N^S_{u,u',s} - UB \cdot y_u \end{aligned} \quad \leq 0 \quad (u,u') = (\mathrm{IN_{BIO}},\mathrm{BDR}) \tag{S31}$$

Lower Bound for Biomass Drier Activation

$$\begin{aligned} & MT_{\mathrm{Bio}} \cdot \sum_{(u,u',s) \in S^{UF}} MW_s \cdot N^S_{u,u',s} - \\ & MW_{\mathrm{H_2O}} \cdot N^S_{u,u',\mathrm{H_2O}} - UB \cdot (1 - y_u) \end{aligned} \quad \leq 0 \quad (u,u') = (\mathrm{IN_{BIO}},\mathrm{BDR}) \tag{S32}$$

Upper Bound for Biomass Drier Moisture Evaporation

$$\begin{aligned} & MT_{\mathrm{Bio}} \cdot \sum_{(u,u',s) \in S^{UF}} MW_s \cdot N^S_{u,u',s} - \\ & MW_{\mathrm{H_2O}} \cdot N^S_{u,u',\mathrm{H_2O}} - UB \cdot (1 - y_u) \end{aligned} \quad \leq 0 \quad (u,u') = (\mathrm{BDR},\mathrm{BLK}) \tag{S33}$$

Lower Bound for Biomass Drier Moisture Evaporation

$$\begin{aligned} & MW_{\mathrm{H_2O}} \cdot N^S_{u,u',\mathrm{H_2O}} - \\ & MT_{\mathrm{Bio}} \cdot \sum_{(u,u',s)\in S^{UF}} MW_s \cdot N^S_{u,u',s} - UB \cdot (1-y_u) \end{aligned} \quad \leq 0 \quad (u,u') = (\mathrm{BDR,BLK}) \tag{S34}$$

Gasifier Lockhopper

Set CO_2 Lockhopper Flow Rate

$$MW_{\mathrm{CO_2}} \cdot N^S_{\mathrm{CO_2C_2,BLK,CO_2}} - mf_u \cdot \sum_{s\in S_{Bio}} MW_s \cdot N^S_{\mathrm{BDR,BLK},s} \quad = 0 \tag{S35}$$

Biomass Gasifier

Water-Gas-Shift Equilibrium

$$N_{u,\mathrm{BC1,CO}} \cdot N_{u,\mathrm{BC1,H_2O}} - K^{RGS}_u \cdot N_{u,\mathrm{BC1,CO_2}} \cdot N_{u,\mathrm{BC1,H_2}} \quad = 0 \quad \forall u \in U_{BGS} \tag{S36}$$

Hydrocarbon Conversion Fraction

$$MW_s \cdot N_{u,\mathrm{BC1},s} - \sum_{(u',u,s)\in S^{UF}} cf^{HC}_{u,s} \cdot M^{S,Calc}_s \quad = 0 \quad \forall s \in S_{HC}, u \in U_{BGS} \tag{S37}$$

Hydrocarbon Generation from Pyrolysis

$$M^{S,Calc}_s - \sum_{s'\in S_{Bio}} \sum_{(u',u,s')\in S^{UF}} Pyr^{HC}_{s,s'} \cdot MW_s \cdot N^S_{u',u,s'} - \sum_{(u',u)\in UC} MW_s \cdot N^S_{u',u,s} \quad = 0 \quad u \in U_{BGS} \tag{S38}$$

Set Ratio of NO to N_2O

$$N_{u,\mathrm{BC1,NO}} - sr_{u,\frac{\mathrm{NO}}{\mathrm{N_2O}}} \cdot N_{u,\mathrm{BC1,N_2O}} \quad = 0 \quad \forall u \in U_{BGS} \tag{S39}$$

Set Ratio of HCN to NH_3

$$N_{u,\mathrm{BC1,HCN}} - sr_{u,\frac{\mathrm{HCN}}{\mathrm{NH_3}}} \cdot N_{u,\mathrm{BC1,NH_3}} \quad = 0 \quad \forall u \in U_{BGS} \tag{S40}$$

Set Amount Input Nitrogen to NH_3 and N_2

$$N_{u,\mathrm{BC1,NH_3}} + 2 \cdot N_{u,\mathrm{BC1,N_2}} - nf_u \cdot \sum_{(u,\mathrm{BC1},s) \in S^{UF}} N^S_{u,\mathrm{BC1},s} \cdot AR_{s,\mathrm{N}} \quad = 0 \quad \forall u \in U_{BGS} \tag{S41}$$

Set Ratio of NH_3 to N_2

$$N_{u,\mathrm{BC1,NH_3}} - (a^1_{u,\mathrm{N_2}} + a^2_{u,\mathrm{N_2}} \cdot T_u) \cdot (N_{u,\mathrm{BC1,NH_3}} + 2 \cdot N_{u,\mathrm{BC1,N_2}}) \quad = 0 \quad \forall u \in U_{BGS} \tag{S42}$$

Set Ratio of COS to H_2S

$$N_{u,\mathrm{BC1,COS}} - sr_{u,\frac{\mathrm{COS}}{\mathrm{H_2S}}} \cdot N_{u,\mathrm{BC1,H_2S}} \quad = 0 \quad \forall u \in U_{BGS} \tag{S43}$$

Amount of Char Production

$$MW_{\mathrm{Char}} \cdot N^S_{u,\mathrm{BC1,Char}} - (a^1_{u,\mathrm{Char}} + a^2_{u,\mathrm{Char}} \cdot T_u) \cdot \sum_{s \in S_{Bio}} MW_s \cdot N^S_{\mathrm{BLK},u,s} \quad = 0 \quad \forall u \in U_{BGS} \tag{S44}$$

Rate of Ash Removal

$$N^S_{u,\mathrm{OUT_{ASH},Ash}} - sf_{u,\mathrm{Ash}} \cdot \sum_{(u',u) \in UC} N^S_{u',u,\mathrm{Ash}} \quad = 0 \quad \forall u \in U_{BGS} \tag{S45}$$

Gasifier Heat Loss

$$Q^L_u + hl_u \cdot \sum_{s \in S_{Bio}} MW_s \cdot N^S_{\mathrm{BLK},u,s} \cdot LHV_s \quad = 0 \quad \forall u \in U_{BGS} \tag{S46}$$

Logical Use of One Gasifier Temperature

$$\sum_{u \in U_{BGS}} y_u - 1 \quad = 0 \tag{S47}$$

Biomass Gasifier Solids

Removal of Solids from First Cyclone

$$rf_{BC1}\cdot N^T_{\mathrm{BGS,BC1}} - N^T_{\mathrm{BC1,BGS}} \quad = 0 \tag{S48}$$

Removal of Solids from Second Cyclone

$$rf_{BC2}\cdot N^T_{\mathrm{BC1,BC2}} - N^T_{\mathrm{BC2,BGS}} \quad = 0 \tag{S49}$$

Natural gas conversion

Auto-Thermal Reactor

Logical Use of One Temperature

$$\sum_{u\in U_{\mathrm{ATR}}} y_u - 1 \quad = 0 \tag{S50}$$

Water-Gas-Shift Equilibrium

$$N^S_{u,u',\mathrm{CO_2}}\cdot N^S_{u,u',\mathrm{H_2}} - K^{RGS}_u\cdot N^S_{u,u',\mathrm{CO}}\cdot N^S_{u,u',\mathrm{H_2O}} \quad = 0 \quad \forall (u,u')\in UC, u\in U_{ATR} \tag{S51}$$

CH_4 Steam Reforming Equilibrium

$$x^S_{u,u',\mathrm{CO}}\cdot {x^S_{u,u',\mathrm{H_2}}}^3 - K^{SR}_{u,\mathrm{CH_4}}\cdot x^S_{u,u',\mathrm{CH_4}}\cdot x^S_{u,u',\mathrm{H_2O}} \quad = 0 \quad \forall (u,u')\in UC, u\in U_{ATR} \tag{S52}$$

Bypass of Inert Species

$$\sum_{(u',u,s)\in S^{UF}} N^S_{u',u,s} - \sum_{(u,u',s)\in S^{UF}} N^S_{u,u',s} \quad = 0 \quad \forall u\in U_{\mathrm{ATR}}, s\in S^{In}_{ATR} \tag{S53}$$

Steam Reformer

Logical Use of One Temperature

$$\sum_{u \in U_{\mathrm{SMR}}} y_u - 1 \quad = 0 \tag{S54}$$

Water-Gas-Shift Equilibrium

$$N^S_{u,u',\mathrm{CO_2}} \cdot N^S_{u,u',\mathrm{H_2}} - K^{RGS}_u \cdot N^S_{u,u',\mathrm{CO}} \cdot N^S_{u,u',\mathrm{H_2O}} \quad = 0 \quad \forall (u,u') \in UC, u \in U_{SMR} \tag{S55}$$

CH_4 Steam Reforming Equilibrium

$$x^S_{u,u',\mathrm{CO}} \cdot {x^S_{u,u',\mathrm{H_2}}}^3 - K^{SR}_{u,\mathrm{CH_4}} \cdot x^S_{u,u',\mathrm{CH_4}} \cdot x^S_{u,u',\mathrm{H_2O}} \quad = 0 \quad \forall (u,u') \in UC, u \in U_{SMR} \tag{S56}$$

Bypass of Inert Species

$$\sum_{(u',u,s) \in S^{UF}} N^S_{u',u,s} - \sum_{(u,u',s) \in S^{UF}} N^S_{u,u',s} \quad = 0 \quad \forall u \in U_{\mathrm{SMR}}, s \in S^{In}_{SMR} \tag{S57}$$

Partial oxidation to methanol

Conversion of methane

$$N^S_{\mathrm{POM},u,\mathrm{CH_4}} \quad = fc_{\mathrm{POM,CH_4}} \cdot \sum_{(u',\mathrm{POM,CH_4}) \in S^{UF}} N^S_{u',\mathrm{POM,CH_4}} \tag{S58}$$

Selectivity to products

$$N^S_{\mathrm{POM},u,s} \cdot AR_{s,\mathrm{C}} \quad = cd_{\mathrm{POM,CH_4}} \cdot \sum_{(u',\mathrm{POM,CH_4}) \in S^{UF}} N^S_{u',\mathrm{POM,CH_4}} \quad \forall s \in S^{Ef}_{\mathrm{POM}} \tag{S59}$$

Oxidative coupling to olefins

Conversion of alkanes

$$N^S_{\mathrm{OCO},u,s} \quad = fc_{\mathrm{OCO},s} \cdot \sum_{(u',\mathrm{OCO},s) \in S^{UF}} N^S_{u',\mathrm{OCO},s} \quad \forall s \in S^{HC}_{\mathrm{OCO}} \tag{S60}$$

Selectivity to products

$$N^S_{\mathrm{OCO},u,s} \cdot AR_{s,\mathrm{C}} \quad = cd_{\mathrm{OCO},s} \cdot \sum_{s \in S^{HC}_{\mathrm{OCO}}} \sum_{(u',\mathrm{OCO},s) \in S^{UF}} N^S_{u',\mathrm{OCO},s} \quad \forall s \in S^{Ef}_{\mathrm{OCO}} \tag{S61}$$

Acid Gas Recovery

Set CO_2 Molar Fraction in Clean Output

$$N^S_{\mathrm{AGR},\mathrm{SP}_{\mathrm{AGR}},\mathrm{CO_2}} - rf_{\mathrm{AGR}} \cdot N^T_{\mathrm{AGR},\mathrm{SP}_{\mathrm{CG}}} \quad = 0 \tag{S62}$$

Set CO_2 Output Flow Rates

$$N^T_{\mathrm{AGR},\mathrm{CO_2C}} - sf_{\mathrm{AGR}} \cdot (N^T_{\mathrm{AGR},\mathrm{CO_2C}} + N^T_{\mathrm{AGR},\mathrm{MX}_{\mathrm{CO2RC}}}) \quad = 0 \tag{S63}$$

Claus Sulfur Recovery

Set Inlet Combustor Oxygen Level

$$\sum_{(u,\mathrm{CC}) \in UC} N^S_{u,\mathrm{CC},\mathrm{O_2}} - er_{\mathrm{CC}} \cdot \sum_{(u,\mathrm{CC},s) \in S^{UF}} N^S_{u,\mathrm{CC},s} \cdot sor_s \quad = 0 \tag{S64}$$

Hydrocarbon Production

Fischer-Tropsch

Set Ratio of H_2 to CO in Cobalt-Based Inlet

$$\sum_{(u',u,\mathrm{H_2}) \in S^{UF}} - FTR_{u,\mathrm{CO}} \cdot \sum_{(u',u,\mathrm{CO}) \in S^{UF}} \quad = 0 \quad \forall u \in U_{CoFT} \tag{S65}$$

Set Ratio of H_2 to CO and CO_2 in Iron-Based Inlet

$$\sum_{(u',u,\mathrm{H_2}) \in S^{UF}} - FTR_{u,\mathrm{CO}} \cdot \sum_{(u',u,\mathrm{CO}) \in S^{UF}} - FTR_{u,\mathrm{CO_2}} \cdot \sum_{(u',u,\mathrm{CO_2}) \in S^{UF}} \quad = 0 \quad \forall u \in U_{IrFT} \tag{S66}$$

Adjust Weight Fraction of C_1 Species

$$W_1 = \frac{1}{2}(1 - \sum_{n=5}^{\infty} W_n) \tag{S67}$$

Adjust Weight Fraction of C_2 Species

$$W_2 = \frac{1}{6}(1 - \sum_{n=5}^{\infty} W_n) \tag{S68}$$

Adjust Weight Fraction of C_3 Species

$$W_3 = \frac{1}{6}(1 - \sum_{n=5}^{\infty} W_n) \tag{S69}$$

Adjust Weight Fraction of C_4 Species

$$W_4 = \frac{1}{6}(1 - \sum_{n=5}^{\infty} W_n) \tag{S70}$$

Set Weight Fraction of C_n Species from Anderson-Schultz-Flory Distribution

$$W_n = n(1-\alpha)^2\alpha^{n-1} \qquad \forall 5 \leq n \leq 29 \tag{S71}$$

Set Weight Fraction of Wax

$$W_{Wax} = \sum_{n=30}^{\infty} n(1-\alpha)^2\alpha^{n-1} \tag{S72}$$

Set Carbon Distribution from Weight Fractions

$$cr_n = \frac{n \cdot W_n}{\sum_{n=1}^{29} n \cdot W_n + n_{Wax} \cdot W_{Wax}} \tag{S73}$$

Set Exactly One Low-Temperature Unit

$$y_{\text{LTFT}} + y_{\text{LTFTRGS}} - 1 \quad = 0 \tag{S74}$$

Set Exactly One High-Temperature Unit

$$y_{\text{HTFT}} + y_{\text{HTFTRGS}} - 1 \quad = 0 \tag{S75}$$

Aqueous Phase Oxygenates Separator

Removal of Aqueous Phase Oxygenates

$$N^{S}_{\text{WSOS},\text{VLWS},s} \quad = 0 \quad \forall s \in S_{APO} \tag{S76}$$

Vapor Phase Oxygenates Separator

Removal of Vapor Phase Oxygenates

$$N^{S}_{\text{VPOS},\text{HRC},s} \quad = 0 \quad \forall s \in S_{VPO} \tag{S77}$$

Hydrocarbon Upgrading

Hydrocarbon Upgrading Units

Set Carbon Distribution Fractions of Total Input

$$N^{S}_{u,u',s} \cdot AR_{s,\text{C}} - cf_{u,u',s} \cdot \sum_{(u'',u,s') \in S^{UF}} N^{S}_{u'',u,s'} \cdot AR_{s',\text{C}} \quad = 0 \quad \forall u \in U_{UG}, (u,u',s) \in s^{UF} \tag{S78}$$

Saturated Gas Plant

Set Fractional Recovery of Light Gases

$$N^{S}_{\text{SGP},\text{C}_4\text{I},s} - rf_s \cdot \sum_{(u,\text{SGP},s) \in S^{UF}} N^{S}_{u,\text{SGP},s} \quad = 0 \quad \forall s \in S_{C_4} \tag{S79}$$

Recycle Gas Treatment

Fuel Combustor

Set Inlet Combustor Oxygen Level

$$\sum_{(u,\mathrm{FCM})\in UC} N^S_{u,\mathrm{FCM},\mathrm{O_2}} - er_{\mathrm{FCM}} \cdot \sum_{(\mathrm{SP_{LG}},\mathrm{FCM},s)\in S^{UF}} N^S_{\mathrm{SP_{LG}},\mathrm{FCM},s} \cdot sor_s \quad = 0 \tag{S80}$$

Gas Turbine

Set Air Leakage From First Compressor

$$N^S_{\mathrm{GTAC_1},\mathrm{OUT_V},s} - lk_{\mathrm{GTAC_1}} \cdot N^S_{\mathrm{IN_{AIR}},\mathrm{GTAC_1},s} \quad = 0 \quad \forall(\mathrm{GTAC_1},s) \in S^U \tag{S81}$$

Set Air Bypass From First Compressor

$$N^S_{\mathrm{GTAC_1},\mathrm{GT_2},s} - by_{\mathrm{GTAC_1}} \cdot N^S_{\mathrm{IN_{AIR}},\mathrm{GTAC_1},s} \quad = 0 \quad \forall(\mathrm{GTAC_1},s) \in S^U \tag{S82}$$

Set Inlet Oxygen Flow Rate in Combustor

$$er_{\mathrm{GTC}} \cdot \sum_{(u,\mathrm{GTC},s)\in S^{UF}} sor_s \cdot N^S_{u,\mathrm{GTC},s} - \sum_{(u,\mathrm{GTC},s)\in S^{UF}} N^S_{u,\mathrm{GTC},\mathrm{O_2}} \quad = 0 \tag{S83}$$

Set Heat Loss in Combustor

$$Q^L_{\mathrm{GTC}} - hl_{\mathrm{GTC}} \cdot (H^T_{\mathrm{SP_{LG}},\mathrm{GTC}} - H^T_{\mathrm{X_{GTF}},\mathrm{GTF}}) \quad = 0 \tag{S84}$$

Wastewater Treatment

Biological Digestor

Set Biogas Ratio of CH_4 to CO_2

$$N^S_{\mathrm{BD},\mathrm{CC},\mathrm{CH_4}} - cr_{\mathrm{BD}} \cdot N^S_{\mathrm{BD},\mathrm{CC},\mathrm{CO_2}} \quad = 0 \tag{S85}$$

Reverse Osmosis

Set Removal Fraction of Solids

$$N^{S}_{\mathrm{RO,SP_{RO}},s} - rf_{\mathrm{RO}} \cdot N^{S}_{\mathrm{MX_{RO},RO},s} \quad = 0 \quad \forall s \in S_{Sol} \tag{S86}$$

Cooling Cycle

Cooling Tower Flow Rate from Energy Requirement

$$Q_C - hr_{\mathrm{COOL\text{-}P}} \cdot N^{S}_{\mathrm{CLTR,COOL\text{-}P,H_2O}} \quad = 0 \tag{S87}$$

Cooling Tower Evaporation Loss

$$N^{Evap}_{\mathrm{CLTR}} - 0.00085 \cdot \Delta T_{\mathrm{CLTR}} \cdot N^{S}_{\mathrm{CLTR,COOL\text{-}P,H_2O}} \quad = 0 \tag{S88}$$

Cooling Tower Drift Loss

$$N^{Drift}_{\mathrm{CLTR}} - 0.001 \cdot N^{S}_{\mathrm{MX_{CLTR},CLTR,H_2O}} \quad = 0 \tag{S89}$$

Sum Total Cooling Tower Losses

$$N^{Evap}_{\mathrm{CLTR}} + N^{Drift}_{\mathrm{CLTR}} - N^{S}_{\mathrm{CLTR,OUT_V,H_2O}} \quad = 0 \tag{S90}$$

Set Known Cooling Tower Output Solid Concentrations

$$x^{Kn}_{\mathrm{CLTR,SP_{CLTR}},s} \cdot N^{T}_{\mathrm{CLTR,SP_{CLTR}}} - N^{S}_{\mathrm{CLTR,SP_{CLTR}},s} \quad = 0 \quad \forall s \in S_{Sol} \tag{S91}$$

Steam Cycle

Set Known Process Steam Boiler Output Solid Concentrations

$$x^{Kn}_{\mathrm{XPWB,MX_{BLR}},s} \cdot N^{T}_{\mathrm{XPWB,MX_{BLR}}} - N^{S}_{\mathrm{XPWB,MX_{BLR}},s} \quad = 0 \quad \forall s \in S_{Sol} \tag{S92}$$

Set Known Heat Engine Boiler Output Solid Concentrations

$$x^{Kn}_{\mathrm{HEP,MX_{BLR}},s} \cdot N^{T}_{\mathrm{HEP,MX_{BLR}}} - N^{S}_{\mathrm{HEP,MX_{BLR}},s} \quad = 0 \quad \forall s \in S_{Sol} \tag{S93}$$

Outlet Wastewater

Upper Bound on Output Wastewater Concentrations

$$N^{S}_{\mathrm{MX_{WW},OUT_V},s} - x^{Max}_{\mathrm{MX_{WW},OUT_V},s} \cdot N^{T}_{\mathrm{MX_{WW},OUT_V}} \quad \leq 0 \quad \forall s \in S_{WW} \tag{S94}$$

Hydrogen/Oxygen Production

Pressure-Swing Absorption

Set Recovery Fraction of H_2 from Inlet

$$N^{S}_{\mathrm{PSA,SP_{H_2P},H_2}} - Rev^{\mathrm{H_2}}_{\mathrm{PSA}} \cdot \sum_{(u,\mathrm{PSA}) \in UC} N^{S}_{u,\mathrm{PSA,H_2}} \quad = 0 \tag{S95}$$

Set Inlet Mole Fraction of H_2

$$\sum_{(u,\mathrm{PSA}) \in UC} N^{S}_{u,\mathrm{PSA,H_2}} - In^{\mathrm{H_2}}_{\mathrm{PSA}} \cdot \sum_{(u,\mathrm{PSA}) \in UC} N^{T}_{u,\mathrm{PSA}} \quad = 0 \tag{S96}$$

Air Separation Unit

Recovery Fraction of O_2

$$N^{S}_{\mathrm{ASU,OUT_V},s} - (1 - sf_{\mathrm{ASU}}) \cdot N^{S}_{\mathrm{AC,ASU},s} \quad = 0 \quad \forall s \in S^{U}_{ASU} \tag{S97}$$

Process Hot/Cold/Power Utility Requirements

Set Electricity Needed for Process Units

$$Q^{El}_{P} - \sum_{u \in U_{Util}} S_u \cdot El^{Base}_{u} \quad = 0 \tag{S98}$$

Set Cooling Water Needed for Process Units

$$Q_P^{CW} - \sum_{u \in U_{Util}} S_u \cdot CW_u^{Base} \quad = 0 \tag{S99}$$

Set Heating Fuel Needed for Process Units

$$Q_{\text{FCM}} - \sum_{u \in U_{Util}} S_u \cdot F_u^{Base} \quad = 0 \tag{S100}$$

Set Utilities Needed for Process Units

$$Q_{u,ut}^{HU} - S_u \cdot U_{u,ut}^{Base} \quad = 0 \quad \forall ut, u \in U_{Util} \tag{S101}$$

Process Costs

Feedstock Costs

Levelized Cost of Biomass Feedstock

$$Cost_s^F = \frac{MW_s \cdot N_{\text{IN}_{\text{BIO}},\text{BDR},s}^S \cdot C_s^F}{Prod \cdot LHV_{Prod}} \quad \forall s \in S_{Bio} \tag{S102}$$

Levelized Cost of Coal Feedstock

$$Cost_s^F = \frac{MW_s \cdot N_{\text{IN}_{\text{COAL}},\text{CDR},s}^S \cdot C_s^F}{Prod \cdot LHV_{Prod}} \quad \forall s \in S_{Coal} \tag{S103}$$

Levelized Cost of Natural Gas Feedstock

$$Cost_s^F = \sum_{(\text{IN}_{\text{NG}},u) \in UC} \frac{MW_s \cdot N_{\text{IN}_{\text{NG}},u,s}^S \cdot C_s^F}{Prod \cdot LHV_{Prod}} \quad \forall s \in S_{NG} \tag{S104}$$

Levelized Cost of Freshwater Feedstock

$$Cost_{\text{H}_2\text{O}}^F = \frac{MW_{\text{H}_2\text{O}} \cdot N_{\text{IN}_{\text{H}_2\text{O}},\text{SP}_{\text{WRI}},\text{H}_2\text{O}}^S \cdot C_{\text{H}_2\text{O}}^F}{Prod \cdot LHV_{Prod}} \tag{S105}$$

Electricity Costs

Levelized Cost of Electricity

$$Cost^{El} = \frac{F_{In}^{El} \cdot C_{In}^{El} - F_{Out}^{El} \cdot C_{Out}^{El}}{Prod \cdot LHV_{Prod}} \tag{S106}$$

CO$_2$ Sequestration Costs

Levelized Cost of CO$_2$ Sequestration

$$Cost^{Seq} = \frac{MW_{\mathrm{CO_2}} \cdot N^{S}_{\mathrm{CO_2SC,OUT_{CO_2},CO_2}} \cdot C^{Seq}}{Prod \cdot LHV_{Prod}} \tag{S107}$$

Levelized Investment Costs

Total Overnight Cost of Process Units

$$TOC_u = (1 + IC_u) \cdot (1 + BOP_u) \cdot C_{o,u} \cdot \frac{S_u}{S_{o,u}}^{sf_u} \tag{S108}$$

Variable Capital Costs of Process Units

$$CC_u = LCCR \cdot IDCF \cdot TOC_u \tag{S109}$$

Levelized Cost of Process Units

$$Cost_u^U = \frac{CC_u \cdot (1 + OM)}{CAP \cdot Prod \cdot LHV_{Prod}} \tag{S110}$$

Objective Function

Levelized Cost of Fuel Production

$$\mathrm{MIN} \sum_{u \in U_{In}} \sum_{(u,s) \in S^U} Cost_s^F + Cost^{El} + Cost^{Seq} + \sum_{u \in U_{Inv}} Cost_u^U \tag{S111}$$

Simultaneous Heat and Power Integration

Pinch Points

Set Pinch Points Based on Inlet Temperatures

$$\left\{\begin{array}{l} T_{pi} = T_{u,u'}^{HP-in} \quad \forall (u,u') \in HP; \quad T_{pi} = T_u \quad \forall u \in HPt^{HB}; \\ T_{pi} = T_{ut} \quad \forall (ut,pi) \in HPt - PI^{Ut}; \quad T_{pi} = T_{b,c,t}^{PC-in} \quad \forall (b,c,t) \in HEP; \quad T_{pi} = T_c \\ T_{pi} = T_{u,u'}^{CP-in} + \Delta T \quad \forall (u,u') \in CP; \quad T_{pi} = T_{b,c}^{EC-in} + \Delta T \quad \forall (b,c) \in CP^{EC}; \\ T_{pi} = T_{b,t}^{SH-in} + \Delta T \quad \forall (b,t) \in CP^{SH}; \quad T_{pi} = T_{ut} + \Delta T \quad \forall (ut,pi) \in CPt - PI^{Ut}; \\ T_{pi} = T_b + \Delta T \end{array}\right\} \tag{S112}$$

Temperature Differences

Process Unit Hot Stream Inlets

$$\Delta T_{u,u',pi}^{HP-in} = \max\{0, T_{u,u'}^{HP-in} - T_{pi}\} \tag{S113}$$

Process Unit Hot Stream Outlets

$$\Delta T_{u,u',pi}^{HP-out} = \max\{0, T_{u,u'}^{HP-out} - T_{pi}\} \tag{S114}$$

Process Unit Cold Stream Inlets

$$\Delta T_{u,u',pi}^{CP-in} = \max\{0, T_{u,u'}^{CP-in} - (T_{pi} - \Delta T)\} \tag{S115}$$

Process Unit Cold Stream Outlets

$$\Delta T_{u,u',pi}^{CP-out} = \max\{0, T_{u,u'}^{CP-out} - (T_{pi} - \Delta T)\} \tag{S116}$$

Heat Engine Precooler Inlets

$$\Delta T_{b,c,t,pi}^{PC-in} = \max\{0, T_{b,c,t}^{PC-in} - T_{pi}\} \tag{S117}$$

Heat Engine Precooler Outlets

$$\Delta T_{b,c,t,pi}^{PC-out} = \max\{0, T_{b,c,t}^{PC-out} - T_{pi}\} \tag{S118}$$

Heat Engine Economizer Inlets

$$\Delta T_{b,c,pi}^{EC-in} = \max\{0, T_{b,c}^{EC-in} - (T_{pi} - \Delta T)\} \tag{S119}$$

Heat Engine Economizer Outlets

$$\Delta T_{b,c,pi}^{EC-out} = \max\{0, T_{b,c}^{EC-out} - (T_{pi} - \Delta T)\} \tag{S120}$$

Heat Engine Superheater Inlets

$$\Delta T_{b,t,pi}^{SH-in} = \max\{0, T_{b,t}^{SH-in} - (T_{pi} - \Delta T)\} \tag{S121}$$

Heat Engine Superheater Outlets

$$\Delta T_{b,t,pi}^{SH-out} = \max\{0, T_{b,t}^{SH-out} - (T_{pi} - \Delta T)\} \tag{S122}$$

Heat Engine Logical Existence

Bound on Heat Engine Flow Rate

$$F_{b,c,t}^{Up} \cdot y_{b,c,t}^{En} \geq F_{b,c,t}^{En} \quad \forall (b,c,t) \in HEP \tag{S123}$$

Bound on Total Amount of Heat Engines

$$\sum_{(b,c,t) \in HEP} y_{b,c,t}^{En} \leq EnMax \tag{S124}$$

Heat Balances

Heat Engine Electricity Balance

$$\sum_{(b,c,t)\in HEP} (w^{Tur}_{b,c,t} - w^{Pum}_{b,c,t}) \cdot F^{En}_{b,c,t} \quad = F_{El} \tag{S125}$$

Upper Heat Balance for Pinch Points

$$\begin{aligned} Q^{H}_{pi} = \quad & \sum_{(u,u')\in HP} \sum_{s} N^{s}_{u,u',s} \cdot Cp^{P}_{u,u',s} \cdot (\Delta T^{HP-in}_{u,u',pi} - \Delta T^{HP-out}_{u,u',pi}) \\ & + \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot Cp^{HE-P} \cdot (\Delta T^{PC-in}_{b,c,t,pi} - \Delta T^{PC-out}_{b,c,t,pi}) \\ & + \sum_{(ut,pi)\in HPt-PI^{Ut}} \sum_{(u,ut)\in HPt} Q^{HU}_{u,ut} + \\ & + \sum_{(u,pi)\in HPt-PI^{HB}} Q_{u} + \sum_{b} \sum_{(c,pi)\in HPt-PI^{C}} \sum_{t} F^{En}_{b,c,t} \cdot dH^{C}_{c} \end{aligned} \tag{S126}$$

Lower Heat Balance for Pinch Points

$$\begin{aligned} Q^{C}_{pi} = \quad & \sum_{(u,u')\in CP} \sum_{s} N^{s}_{u,u',s} \cdot Cp^{P}_{u,u',s} \cdot (\Delta T^{CP-out}_{u,u',pi} - \Delta T^{CP-in}_{u,u',pi}) \\ & + \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot Cp^{HE-E} \cdot (\Delta T^{EC-out}_{b,c,pi} - \Delta T^{EC-in}_{b,c,pi}) \\ & + \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot Cp^{HE-S} \cdot (\Delta T^{SH-out}_{b,t,pi} - \Delta T^{SH-in}_{b,t,pi}) \\ & + \sum_{(ut,pi)\in CPt-PI^{Ut}} \sum_{(u,ut)\in CPt} Q^{HU}_{u,ut} + \sum_{(b,pi)\in CPt-PI^{B}} \sum_{c} \sum_{t} F^{En}_{b,c,t} \cdot dH^{B}_{b} \end{aligned} \tag{S127}$$

Pinch Point Heating Deficit

$$z_{pi} = Q^{C}_{pi} - Q^{H}_{pi} \tag{S128}$$

Negativity of Pinch Deficits

$$z_{pi} \leq 0 \tag{S129}$$

Total Heating Deficit

$$\Omega - Q_c = 0 \tag{S130}$$

Total Heat Balance

$$\begin{aligned}
\Omega = \quad & \sum_{(u,u')\in HP} \sum_{s} N^{s}_{u,u',s} \cdot Cp^{P}_{u,u',s} \cdot (T^{HP-in}_{u,u'} - T^{HP-out}_{u,u'}) \\
& + \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot Cp^{HE-P} \cdot (T^{PC-in}_{b,c,t} - T^{PC-out}_{b,c,t}) \\
& + \sum_{(u,ut)\in HPt} Q^{HU}_{u,ut} + \sum_{u\in HPt^{HB}} Q_u + \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot dH^{C}_{c} \\
& - \sum_{(u,u')\in CP} \sum_{s} N^{s}_{u,u',s} \cdot Cp^{P}_{u,u',s} \cdot (T^{CP-out}_{u,u'} - T^{CP-in}_{u,u'}) \\
& - \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot Cp^{HE-E} \cdot (T^{EC-out}_{b,c} - T^{EC-in}_{b,c}) \\
& - \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot Cp^{HE-S} \cdot (T^{SH-out}_{b,t} - T^{SH-in}_{b,t}) \\
& - \sum_{(u,ut)\in CPt} Q^{HU}_{u,ut} - \sum_{(b,c,t)\in HEP} F^{En}_{b,c,t} \cdot dH^{B}_{b}
\end{aligned} \tag{S131}$$

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