Electronic Supplementary Material (ESI) for Green Chemistry

ELECTRONIC SUPPLEMENTARY INFORMATION

A strategy for the simultaneous catalytic conversion of hemicellulose and cellulose from lignocellulosic biomass to liquid transportation fuels

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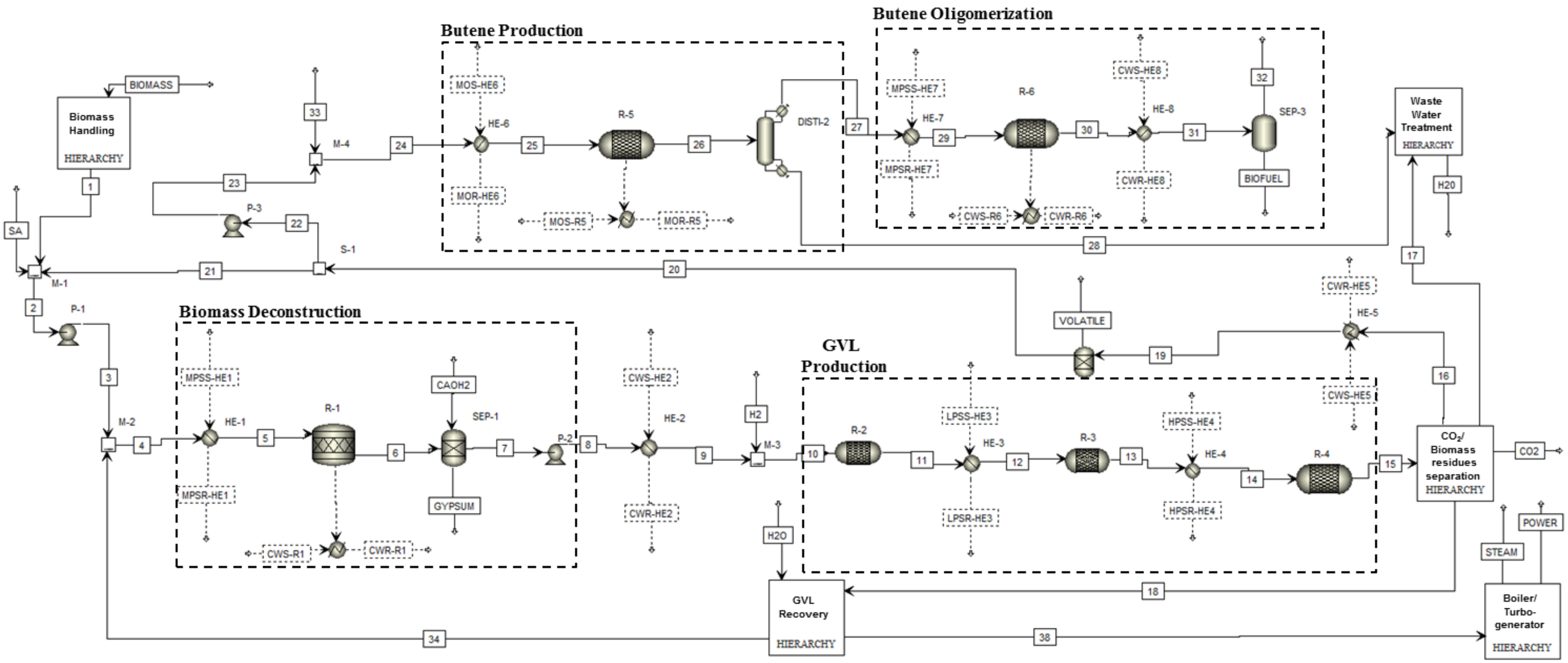
1. Process flow diagram (Basic design)



STREAMS:	1	5	6	7	10	12	14	15	18	20	25	26	29	31	34	36	BIOFUEL
Mass Flow [ton/hr]																	
C6SUGARS	34.2	34.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5SUGARS	20.0	20.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LIGNIN	15.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0	15.0	0.0	0.0	0.0	0.0	0.0	0.0	15.0	0.0
GVL	0.0	343.2	343.2	343.2	343.2	343.2	343.2	359.3	5.5	352.3	15.6	0.2	0.0	0.0	5.3	0.2	0.0
SA	0.0	0.8	0.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER	0.0	86.3	92.5	92.5	92.5	92.5	91.6	94.6	0.1	87.8	10.3	10.3	0.0	0.0	1.3	32.6	0.0
LA	0.0	0.0	13.4	13.4	13.4	13.4	19.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURFURAL	0.0	0.0	7.2	7.2	7.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FA	0.0	0.0	5.3	5.3	5.3	5.3	5.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURFURYL-ALCOHOL	0.0	0.0	0.0	0.0	0.0	6.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MTHF	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	8.7	8.6	0.1	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.1	0.0	0.0	0.0	6.8	6.8	6.8	0.0	0.0	0.4
C8H16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	0.0	0.0	2.5
C12H2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.2	0.0	0.0	2.2
C16H3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.1	0.0	0.0	2.1
C20H4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.6	0.0	0.0	1.6
HUMINS	0.0	0.0	22.1	22.1	22.1	22.8	24.8	24.8	24.7	0.0	0.0	0.0	0.0	0.0	0.0	24.7	0.0
Total Flow [ton/hr]	69.2	499.5	499.5	498.7	498.9	498.9	498.9	498.9	45.3	440.1	25.9	25.9	15.4	15.4	6.6	72.5	8.8
Temperature [C]	25	170	170	170	100	125	220	220	261	122	375	375	170	100	202	183	100
Pressure [bar]	1	16	16	16	35	35	34	34	2	1	37	36	36	36	16	10	35
Enthalpy [MW]	-87	-864	-888	-885	-912	-903	-867	-870	-42	-825	-51	-51	-15	-21	-12	-177	-3

Fig. S.1. Detailed process flow diagram of the basic design with associated streams.

2. Alternative configurations

In addition to the basic design, we generated two alternative configurations, as shown in Figs. S.2 and S.3. In the first alternative configuration, the solid residues are burned in a boiler to satisfy the heating requirement of the process, and the remaining biomass residues are then disposed as waste (Fig. S.4). In the second alternative configuration, the vapor stream containing GVL and H_2O from the evaporator is used for power generation (Fig. S.5).

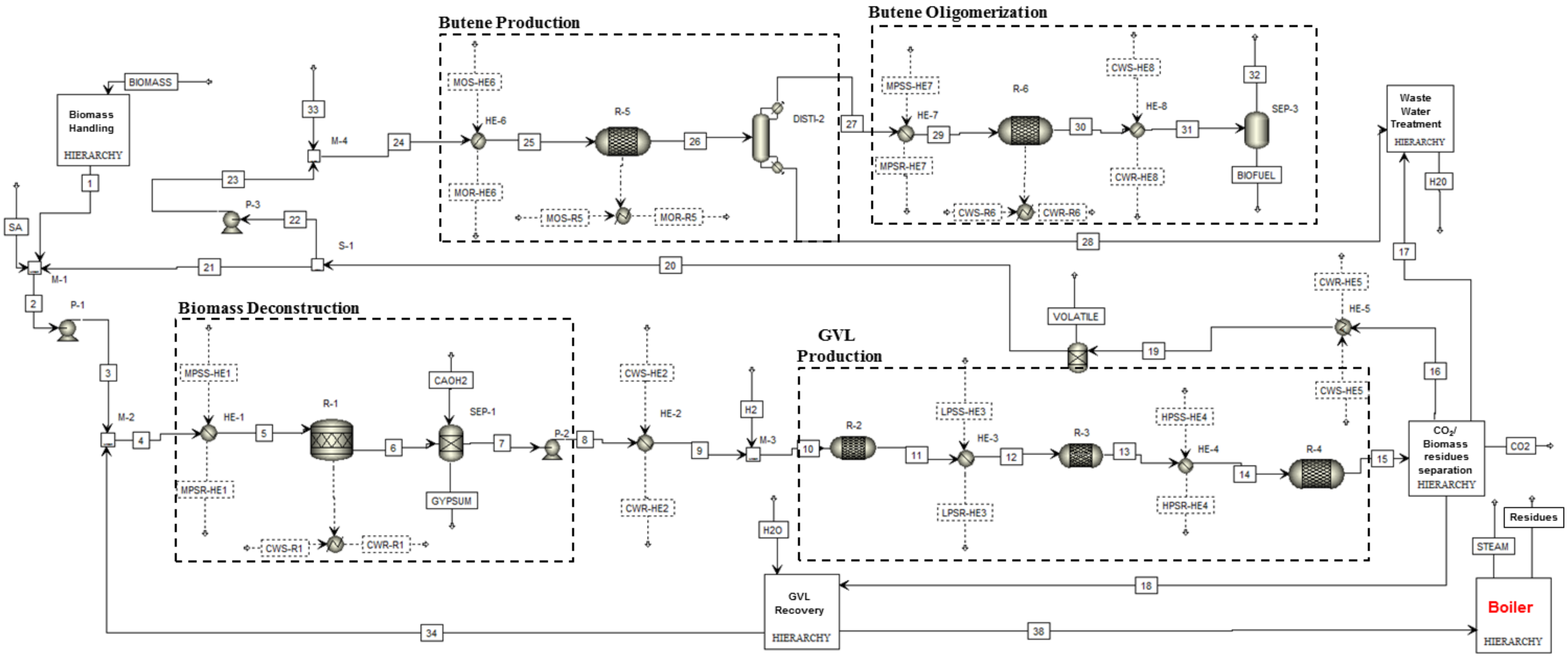


Fig. S.2. Alternative configuration #1- No electricity generation in the plant.

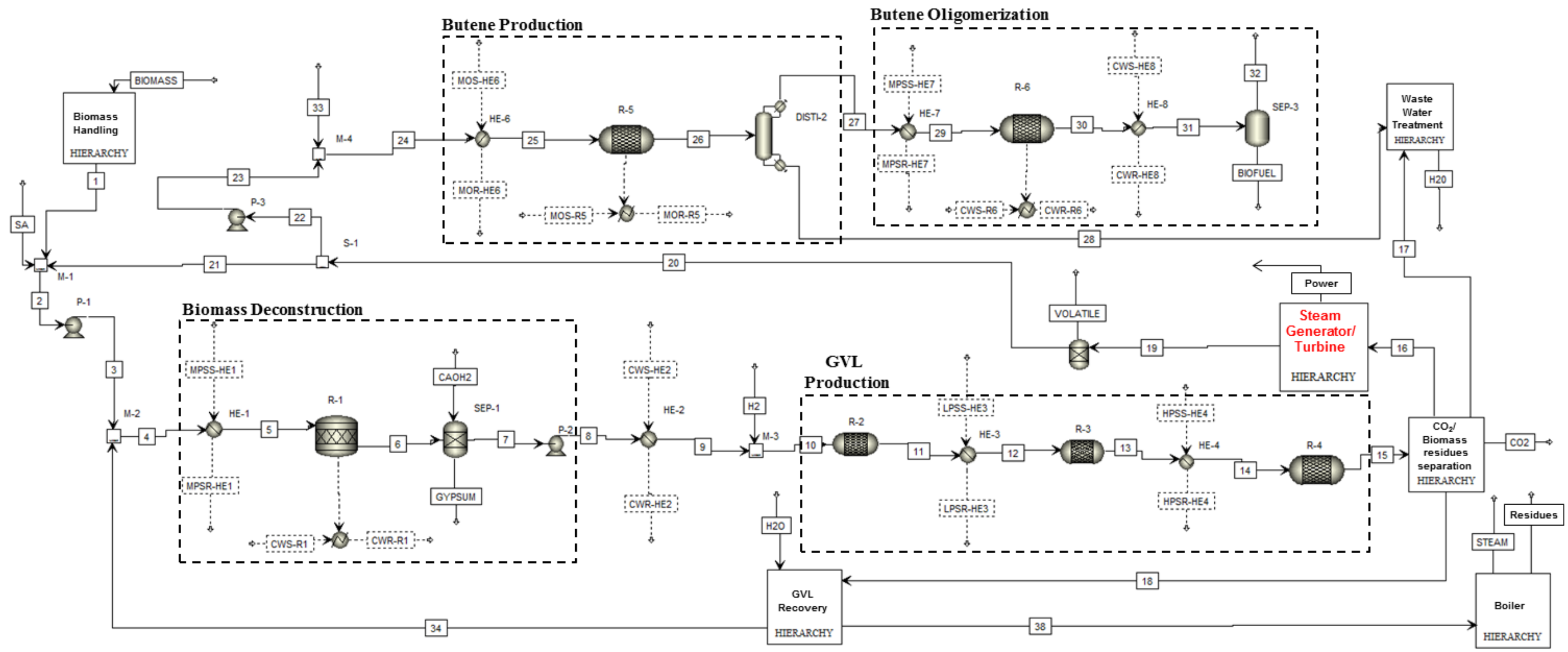
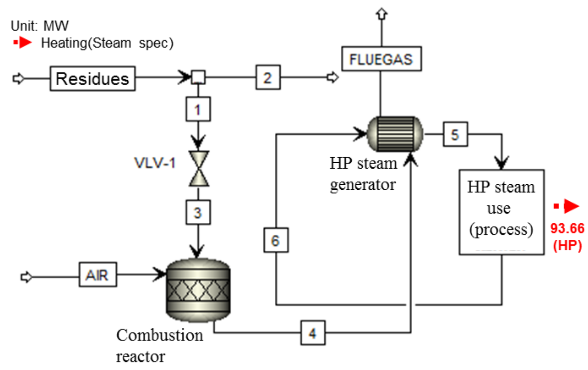


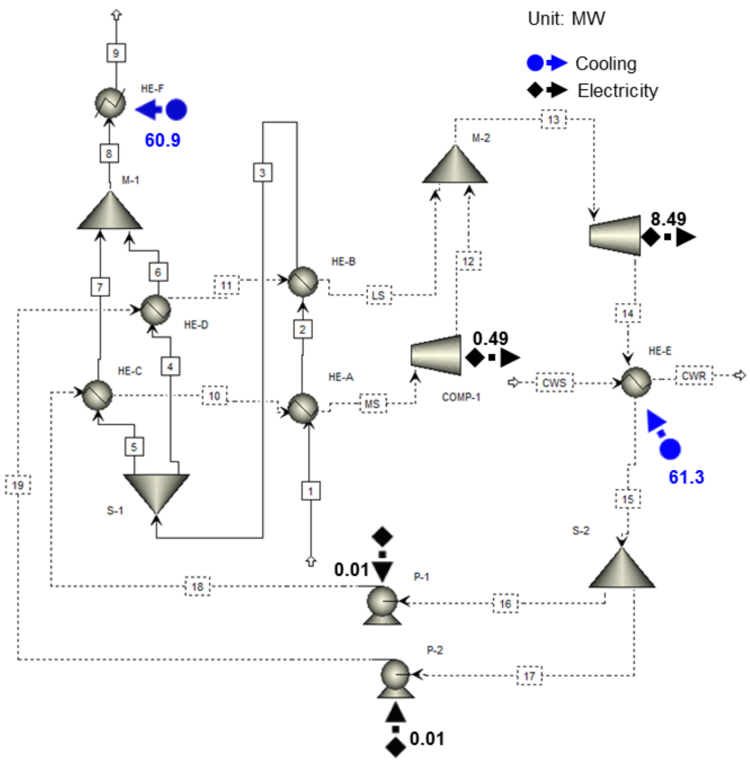
Fig. S.3. Alternative configuration #2- Electricity generation using the heat from the vapor stream of GVL/H_2O.



STREAMS:	Residues	1	3	4	5	6
Mass Flow [ton/hr]						
CO2	0.0	0.0	0.0	47.1	0.0	0.0
H2O	32.6	21.5	21.5	36.1	168.6	168.6
N2	0.0	0.0	0.0	183.9	0.0	0.0
O2	0.0	0.0	0.0	20.5	0.0	0.0
GVL	0.2	0.1	0.1	0.0	0.0	0.0
Lignin	15.0	9.9	9.9	0.0	0.0	0.0
HUMINS	24.7	16.3	16.3	0.0	0.0	0.0
Total Flow [ton/hr]	72.5	47.8	47.8	287.5	168.6	168.6
Temperature [C]	183	183	105	932	399	267
Pressure [bar]	10	10	1	1	53	53
Enthalpy [MW]	-200	-132	-132	-132	-599	-693

Fig. S.4. Detailed process flow diagram of the boiler subsystem in the alternative configuration #1.

This design of steam generator/turbine comprises two steam generators, two preheaters, two coolers, two pumps, and a combination of back-pressure (non-condensing) and condensing turbines connected in series. The hot water is vaporized in the medium-pressure steam generator, and then expanded through a back-pressure turbine to generate power. The outlet of the turbine is mixed with a low-pressure steam, and the mixture is expanded through a condensing turbine to obtain the maximum power output. Later, it is condensed to a saturated liquid, and pumped back to each steam generator to start the cycle again.



STREAMS:	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	LS	MS
Mass Flow [ton/hr]																					
C6SUGARS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5SUGARS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LIGNIN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GVL	352.3	352.3	352.3	244.8	107.5	244.8	107.5	352.3	352.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER	87.8	87.8	87.8	61.0	26.8	61.0	26.8	87.8	87.8	29.5	67.0	29.5	96.4	96.4	96.4	34.3	62.2	34.3	62.2	67.0	29.5
LA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURFURAL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURFURYL-ALCOHOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MTHF	0.1	0.1	0.1	0.1	0.0	0.1	0.0	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	0.6	0.6	0.6	0.4	0.2	0.4	0.2	0.6	0.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C8H16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C12H2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C16H3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C20H4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HUMINS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow [ton/hr]	440.8	440.8	440.8	306.3	134.5	306.3	134.5	440.8	440.8	29.5	67.0	29.5	96.4	96.4	96.4	34.3	62.2	34.3	62.2	67.0	29.5
Temperature [C]	261	187	166	166	166	155	155	155	122	156	156	159	159	46	46	46	46	46	46	159	184
Pressure [bar]	2	1	1	1	1	1	1	1	1	11	6	6	6	0	0	0	0	11	6	6	11
Enthalpy [MW]	-687	-705	-744	-516	-228	-525	-231	-756	-819	-126	-285	-108	-354	-360	-423	-150	-273	-150	-273	-246	-108

Fig. S.5. Detailed process flow diagram of the steam generator/turbine subsystem in the alternative configuration #2.

3. Heat exchanger network design

The aim of heat exchanger network design is to minimize external utility requirements by maximizing heat recovery between process streams (i.e. hot steams and cold streams) through heat integration. Hot steams (e.g. overhead vapor in distillation column) need to be cooled, while cold streams (e.g. bottom liquid in distillation column) need to be heated. Utility streams (e.g. steam, cooling water) are used to heat the cold streams or cool the hot streams. For heat transfer between process streams, the temperature of hot stream must be higher than that of cold stream. Thus, a feasible heat exchanger design has a minimum temperature difference (ΔT_{min}), which represents the bottleneck in the heat recovery. With a given value of ΔT_{min}, the minimum energy requirement or maximum energy recovery can be evaluated from a composite curve, which consists of temperature and enthalpy profiles of hot streams and cold streams in the process. The composite curve for basic design is obtained by using ASPEN Energy Analyzer[1], assuming that the ΔT_{min} is 10 K for the process (Fig. S.6). The total minimum hot utility requirement (QHmin) is 93.7 MW and total minimum cold utility requirement (QCmin) is 139.5 MW. We can also verify a feasible heat exchanger network design through a grid diagram, which represents which hot streams can be matched to cold steams *via* heat recovery (Fig. S.7). Once the unit price of each utility is given, the total utility cost can be estimated using the following equation.

$$\text{Total Utility Cost} = \sum_{m} UP_m \times QHmin_m + \sum_{n} UP_n \times QCmin_n$$

where UP_m = Unit price of hot utility *m*, (in \$/MW)

UP_n = Unit price of cold utility *n*, (in \$/MW)

$QHmin_m$ = Total minimum requirement of hot utility *m*, (in MW)

$QCmin_n$ = Total minimum requirement of cold utility *n*, (in MW)

As shown in Fig. S.6, the hot and cold composite curves have enthalpy intervals, in which each composite curve does not change slope. Total minimum area requirement (A_{min}) of the heat exchanger network can be calculated using the following equation.[2]

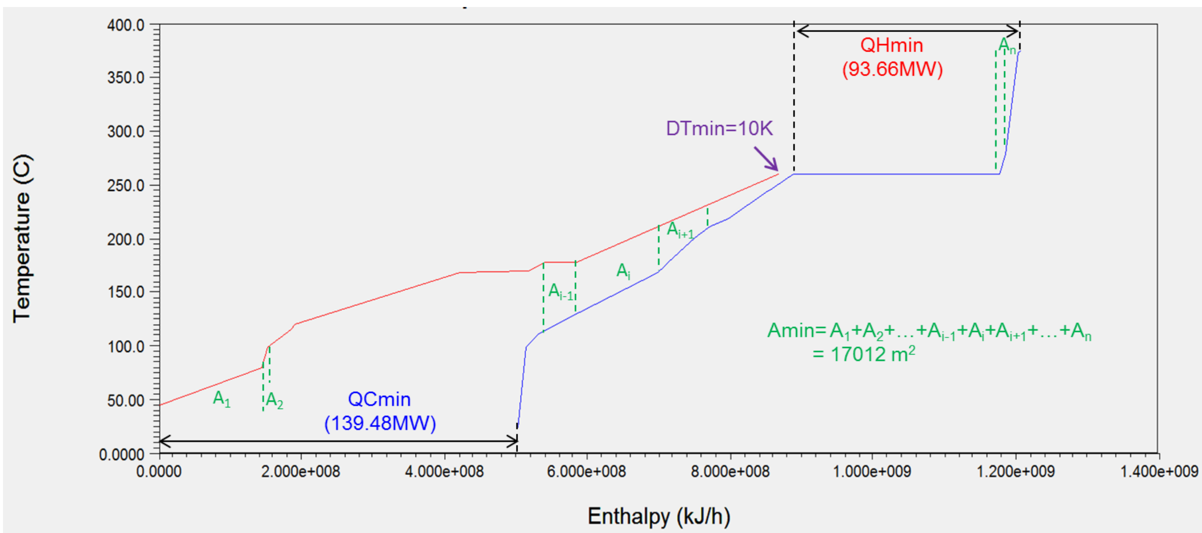
$$A_{min} = \sum_{i} \frac{\nabla Q_i}{U_i \nabla T_{LM\,i}}$$

where U_i, ΔQ_i, $\Delta T_{LM\,i}$ are the overall heat-transfer coefficient, enthalpy change, log-mean temperature difference (LMTD) for enthalpy interval *i*, respectively. The A_{min} for basic design is estimated to be 17012 m^2 using ASPEN Energy Analyzer (Fig. S.6). Once the A_{min} is known, the total capital cost of the heat exchanger network can be estimated using the equation below.[2]

$$\text{Total Capital Cost} = a + b \times (A_{min})^{c}$$

where the cost parameters a, b and c depend on specific materials of construction and types of heat exchanger.

An increase in ΔT_{min} value leads to a higher utility cost and a lower capital cost for the heat exchanger network, while a decrease in ΔT_{min} value leads to a lower utility cost and a higher capital cost. Thus, an optimum ΔT_{min} exists where total cost, which is sum of the utility costs and capital costs, is at its minimum value. The MSP of butene oligomers for the basic design using hybrid poplar feedstock is calculated by varying the ΔT_{min} values (Fig. S.8). The optimum ΔT_{min} value is estimated to be 7.75 K, which leads to a 0.06% reduction in the MSP.



Process Streams		Inlet T[C]	Outlet T[C]	Enthalpy[Kj/h]
4 => 5	↗	112.0	169.9	77231740
R1 5 => 6	↙	170.4	169.9	80893685
8 => 9	↙	170.8	99.9	94137714
11 => 12	↗	99.9	124.9	31479430
13 => 14	↗	124.9	219.9	137159244
SEP2_EV1 12 => 75	↗	260.6	261.1	289466816
SEP2_HE1 13 => 41	↙	213.9	185.5	3481682
SEP2_HE2 9 => 12	↗	212.2	261.1	79944840
16 => 19	↙	261.1	121.6	475560472
24 => 25	↗	174.5	375.0	38651548
R5 25 => 26	↗	374.5	375.0	1395209
27 => 29	↗	116.5	169.9	1254491
R6 29 => 30	↙	170.4	169.9	9464995
30 => 31	↙	169.9	99.9	2136849
DS1 Reboiler	↗	244.5	247.0	5749506
DS1 Condenser	↙	116.5	45.0	33306576
REC_DS2 Reboiler	↗	201.3	279.1	16952404
REC_DS2 Condenser	↙	178.8	178.4	40404459
H2-Makeup	↗	25.0	99.9	256342
H2O-Makeup	↗	25.0	178.4	23713652
Power cycle	↙	80.4	45.8	128817313

Utility Streams		Inlet T[C]	Outlet T[C]	Cp[Kj/kg C]
Cooling water	↗	25.0	35.0	3.86
HP steam	↙	398.9	267.3	15.20
MP steam	↙	184.2	183.7	3552.88
LP steam	↙	159.0	158.1	2292.91

Fig. S.6. Composite curve for the basic design.

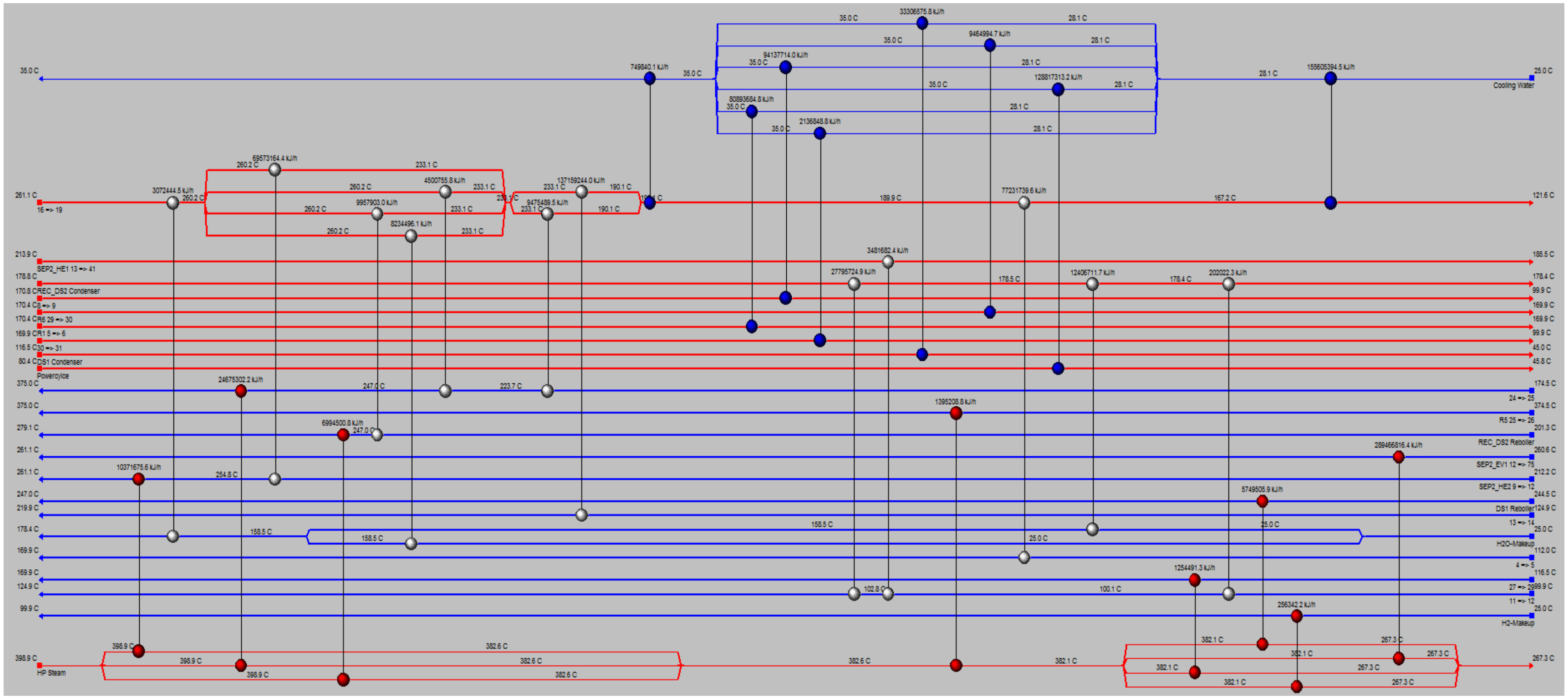


Fig. S.7. Grid diagram for the basic design.

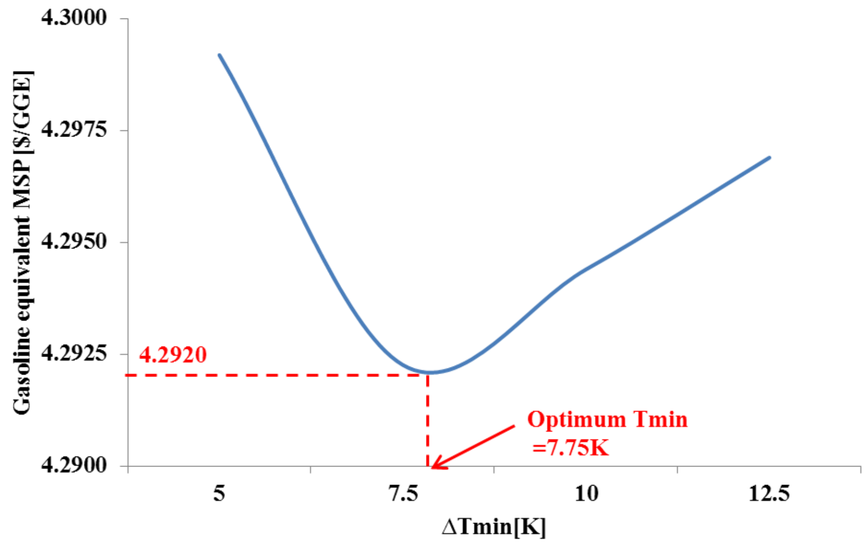


Fig. S.8. Effect of a minimum temperature difference (ΔT_{min}) on the MSP.

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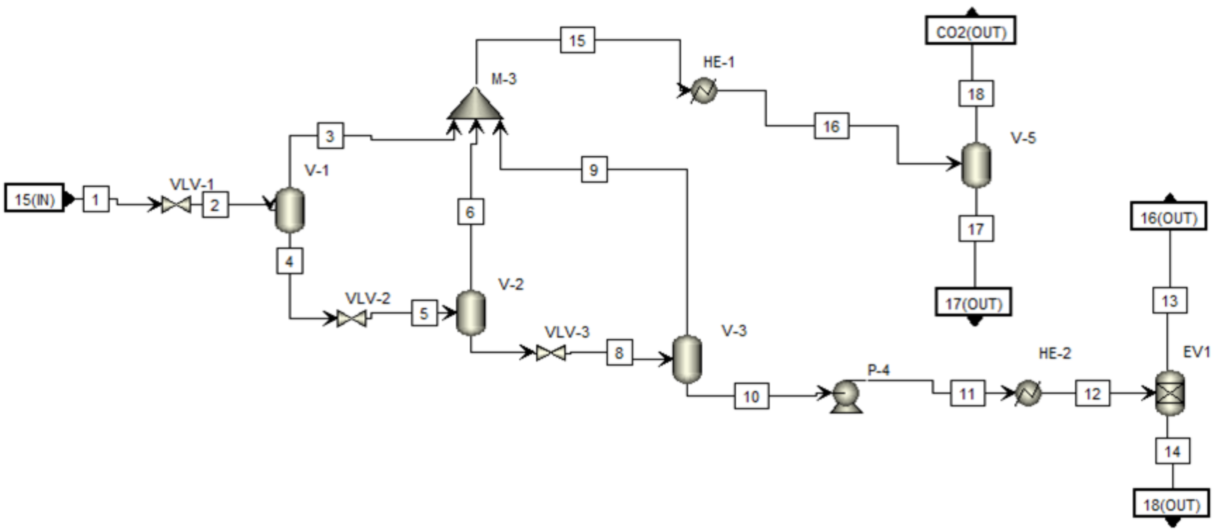
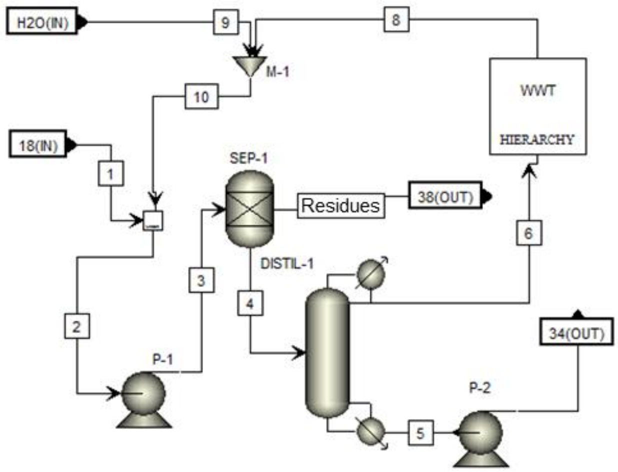
4. Process flow diagrams of other processing sections

The process flow diagrams of other processing sections (CO_2 and biomass residues separation, GVL recovery and Boiler/Turbogenerator) are developed using ASPEN Plus Process Simulator[3]. The flows and installed equipment costs of biomass handling and wastewater treatment are scaled based on the NREL report[4].



STREAMS:	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Mass Flow [ton/hr]																		
C6SUGARS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5SUGARS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LIGNIN	15.0	15.0	0.0	15.0	15.0	0.0	15.0	15.0	0.0	15.0	15.0	15.0	0.0	15.0	0.0	0.0	0.0	0.0
GVL	359.3	359.3	0.9	358.5	358.5	0.4	358.1	358.1	0.3	357.8	357.8	357.8	352.3	5.5	1.5	1.5	1.2	0.3
SA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER	94.6	94.6	3.9	90.7	90.7	1.7	89.0	89.0	1.1	87.8	87.8	87.8	87.8	0.1	6.7	6.7	1.2	5.6
LA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURFURAL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURFURYL-ALCOHOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MTHF	0.1	0.1	0.0	0.1	0.1	0.0	0.1	0.1	0.0	0.1	0.1	0.1	0.1	0.0	0.0	0.0	0.0	0.0
C4H8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	5.1	5.1	3.3	1.7	1.7	0.8	0.9	0.9	0.3	0.6	0.6	0.6	0.6	0.0	4.5	4.5	0.0	4.5
C8H16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C12H2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C16H3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C20H4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HUMINS	24.8	24.8	0.0	24.7	24.7	0.0	24.7	24.7	0.0	24.7	24.7	24.7	0.0	24.7	0.1	0.1	0.0	0.1
Total Flow [ton/hr]	498.9	498.9	8.2	490.7	490.7	2.9	487.8	487.8	1.7	486.1	486.1	486.1	440.8	45.3	12.8	12.8	2.4	10.4
Temperature [C]	220	215	215	215	213	213	213	212	211	211	212	261	261	261	214	185	185	185
Pressure [bar]	34	17	17	17	14	14	14	13	13	13	30	30	2	2	13	13	13	13
Enthalpy [MW]	-870	-870	-24	-846	-846	-9	-837	-837	-6	-834	-834	-810	-687	-42	-36	-39	-6	-33

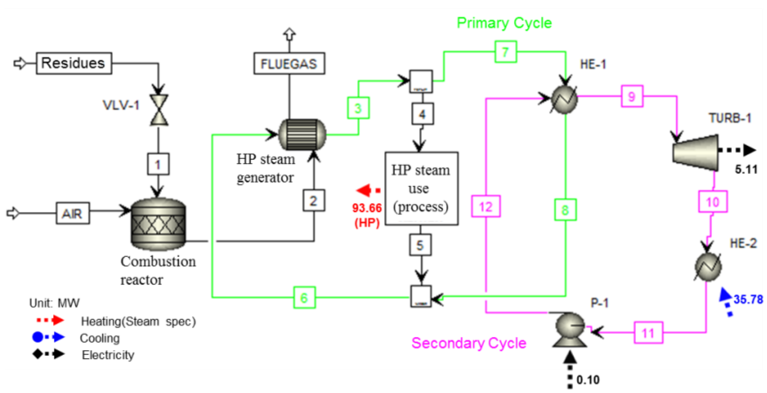
Fig. S.9. Detailed process flow diagram of the CO_2 and biomass residues separation section.



STREAMS:	1	4	5	6	7	8	9	10	Residues
Mass Flow [ton/hr]									
C6SUGARS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C5SUGARS	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
LIGNIN	15.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	15.0
GVL	5.5	5.3	5.3	0.1	5.3	0.0	0.0	0.0	0.2
SA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
WATER	0.1	20.0	1.3	18.7	1.3	18.7	33.9	52.5	32.6
LA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURFURAL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FA	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FURFURYL-ALCOHOL	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MTHF	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C4H8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C8H16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C12H2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C16H3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C20H4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HUMINS	24.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	24.7
Total Flow [ton/hr]	45.3	25.3	6.6	18.7	6.6	18.7	33.9	52.5	72.5
Temperature [C]	261	183	201	178	202	178	178	178	183
Pressure [bar]	2	10	10	10	16	1	1	1	10
Enthalpy [MW]	-42	-84	-12	-78	-12	-78	-144	-222	-200

Fig. S.10. Detailed process flow diagram of the GVL recovery section.

The design of the boiler/turbogenerator system (Fig. S.11) is modified from the NREL report[4] that includes an extraction turbine, in which low-pressure (LP) steam is extracted for use in the process. To generate maximum electricity in the proposed process, a condensing turbine is used instead of an extraction turbine for power-only generation. The design of boiler/turbogenerator comprises a binary Rankine cycle system including two heat exchangers, a condensing turbine, and a pump (Fig. S.11). First, hot gases produced from the combustion of solid residues are used to generate high-pressure steam in the boiler, and then the high-pressure steam passes through the first heat exchanger in the primary cycle to provide heat to secondary cycle. The low-pressure steam in the secondary cycle enters into a turbine, in which it is expanded to a pressure of 0.1 bar, to generate power. The wet steam is cooled in the second heat exchanger (condenser) and pumped back to the first heat exchanger, and hence heat transmission from the primary cycle to the secondary cycle starts again.



STREAMS:	Residues	1	2	3	4	5	6	7	8	9	10	11	12
Mass Flow [ton/hr]													
CO2	0.0	0.0	71.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
H2O	32.6	32.6	54.7	255.5	168.6	168.6	255.5	87.0	87.0	52.4	52.4	52.4	52.4
N2	0.0	0.0	278.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O2	0.0	0.0	31.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
GVL	0.2	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Lignin	15.0	15.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HUMINS	24.7	24.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Flow [ton/hr]	72.5	72.5	436.0	255.5	168.6	168.6	255.5	87.0	87.0	52.4	52.4	52.4	52.4
Temperature [C]	183	105	1237	399	399	267	267	399	267	263	80	46	46
Pressure [bar]	10	1	1	52.7	52.7	52.7	52.7	52.7	52.7	6	0.1	0.1	6
Enthalpy [MW]	-200	-200	-142	-908	-599	-693	-1050	-278	-348	-189	-194	-230	-230

Fig. S.11. Detailed process flow diagram of the boiler/turbogenerator section (the basic design).

5. Economic Parameters

Table S.1. List of economic parameters.

Corn stover price ($ per ton)[a]	83.0
Sulfuric acid price ($ per ton)[a]	35.0
Lime price ($ per ton)[a]	99.0
Water price ($ per ton)[a]	0.2
Hydrogen price ($ per ton)[a]	7.1
Waste water treatment cost ($ per ton)[a]	36.0
Electricity price ($ per kW h)[a]	5.4
Equipment life span (years)[a]	20.0
Internal Rate of Return (%)[a]	10.0
Tax rate (%)[a]	39.0
Depreciation period (years)[b]	7.0
Pt_3Sn/SiO_2 ($ per kg)[c]	243.3
Amberlyst 70 ($ per kg)[c]	312.0
RuSn(1 : 4)/C catalyst ($ kg per)[c]	540.0

[a] Taken from study by Kazi *et al.*[5]
[b] Power generation unit depreciates over a 20-year period.[6]
[c] 10% of the catalyst is refurbished every 6 months at a cost equivalent to 20% of its original value.[6]
[*] Other parameters [5]

- Contingency factor is 20% of total project investment.
- Capital investment is spread over 3 years at a rate of 8%, 60%, and 32% in the first, second, and third years, respectively
- Working capital is 15% of fixed capital investment.

Table S.2. Capital and operating costs of the dryer unit for dry residues sale case.

	Flow [kg/hr] Input	Flow [kg/hr] Output	Heat required [MW]	Operating cost [MM$/yr]	Capital cost [MM$]
Biomass residues	13823	13121	7.07	3.02	0.28
Water	11310	687			

[*]Capital cost per kg/hr of water evaporated ($26/kg/h) for a single-pass rotary dryer[7]

6. Equipment List and Costs

The installed equipment costs are estimated using Aspen Process Economic Analyzer[8].

Section	Equipment ID	Equipment cost [$]	Installed cost [$]
Biomass deconstruction	P-1	51,400	147,900
	R-1	9,835,000	11,841,500
	SEP-1	90,300	211,300
GVL production	P-2	65,200	206,100
	R-2	292,000	911,500
	R-3	502,000	1,279,000
	R-4	491,000	1,265,500
CO_2/Biomass residues separation	P-4	63,800	200,300
	V-1	346,600	599,600
	V-2	315,900	568,700
	V-3	288,800	541,500
	V-5	87,300	225,200
GVL recovery	EV1	1,369,000	1,667,300
	DISTIL-1	345,000	709,000
	P-1	6,600	57,400
	P-2	5,800	40,900
	SEP-1	540,700	1,074,400
Butene production	P-3	66,800	113,000
	R-5	868,000	1,813,500
	DISTIL-2	1,803,300	2,313,800
Butene oligomerization	R-6	1,240,500	1,777,800
	SEP-3	122,100	241,100

7. Discounted Cash Flow

Table S.3. Discounted cash flow for the base case.

Year	-2	-1	0	1	2	3	4	5	6	7	8	9	10
Capital Investment	27,176,427	203,823,199	108,705,706										
Working Capital			50,955,800										
Fuel Sales				105,352,464	140,469,952	140,469,952	140,469,952	140,469,952	140,469,952	140,469,952	140,469,952	140,469,952	140,469,952
Electricity Sales				1,705,679	2,274,239	2,274,239	2,274,239	2,274,239	2,274,239	2,274,239	2,274,239	2,274,239	2,274,239
Total Annual Sales				107,058,144	142,744,192	142,744,192	142,744,192	142,744,192	142,744,192	142,744,192	142,744,192	142,744,192	142,744,192
Feedstock Cost				50,662,500	57,900,000	57,900,000	57,900,000	57,900,000	57,900,000	57,900,000	57,900,000	57,900,000	57,900,000
Other Raw Materials				1,280,057	1,462,922	1,462,922	1,462,922	1,462,922	1,462,922	1,462,922	1,462,922	1,462,922	1,462,922
Catalyst Regeneration Cost				3,023,541	3,455,475	3,455,475	3,455,475	3,455,475	3,455,475	3,455,475	3,455,475	3,455,475	3,455,475
Other Variable Costs				4,225,079	4,828,662	4,828,662	4,828,662	4,828,662	4,828,662	4,828,662	4,828,662	4,828,662	4,828,662
Fixed Operating Costs				10,100,000	10,100,000	10,100,000	10,100,000	10,100,000	10,100,000	10,100,000	10,100,000	10,100,000	10,100,000
Total Product Cost				69,291,177	77,747,059	77,747,059	77,747,059	77,747,059	77,747,059	77,747,059	77,747,059	77,747,059	77,747,059
Annual Depreciation													
General Plant													
DDB				65,459,939	46,757,099	33,397,928	23,855,663	17,039,759	12,171,257	8,693,755			
SL				32,729,969	27,274,975	23,378,550	20,873,705	19,879,719	19,879,719	19,879,719			
Actual				65,459,939	46,757,099	33,397,928	23,855,663	19,879,719	19,879,719	19,879,719			
Remaining Value				163,649,847	116,892,748	83,494,820	59,639,157	39,759,438	19,879,719	0			
Power and Steam Plant													
DDB				8,294,666	7,672,566	7,097,124	6,564,839	6,072,476	5,617,041	5,195,763	4,806,080	4,445,624	4,112,203
SL				5,529,777	5,384,257	5,257,129	5,148,894	5,060,397	4,992,925	4,948,345	4,929,313	4,929,313	4,929,313
Actual				8,294,666	7,672,566	7,097,124	6,564,839	6,072,476	5,617,041	5,195,763	4,929,313	4,929,313	4,929,313
Remaining Value				102,300,880	94,628,314	87,531,190	80,966,351	74,893,875	69,276,834	64,081,072	59,151,758	54,222,445	49,293,132
Net Revenue				-35,833,006	10,773,643	24,708,257	34,782,806	39,251,113	39,706,549	40,127,827	60,273,995	60,273,995	60,273,995
Losses Forward					-35,833,006	-25,059,363	-351,106	0	0	0	0	0	0
Taxable Income				-35,833,006	-25,059,363	-351,106	34,431,700	39,251,113	39,706,549	40,127,827	60,273,995	60,273,995	60,273,995
Income Tax				0	0	0	13,428,363	15,307,934	15,485,554	15,649,852	23,506,858	23,506,858	23,506,858
Annual Cash Flow				37,921,599	65,203,308	65,203,308	51,774,945	49,895,374	49,717,754	49,553,456	41,696,450	41,696,450	41,696,450
Discount Factor	1.21	1.10	1.00	0.91	0.83	0.75	0.68	0.62	0.56	0.51	0.47	0.42	0.39
Annual Present Value				34,474,181	53,887,032	48,988,211	35,362,984	30,981,102	28,064,376	25,428,758	19,451,702	17,683,365	16,075,787
TPI + Interest	32,883,476	224,205,519	159,661,506										
NPV			0										

Year	11	12	13	14	15	16	17	18	19	20
Capital Investment										
Working Capital										-50,955,800
Fuel Sales	140,469,952	140,469,952	140,469,952	140,469,952	140,469,952	140,469,952	140,469,952	140,469,952	140,469,952	140,469,952
Electricity Sales	2,274,239	2,274,239	2,274,239	2,274,239	2,274,239	2,274,239	2,274,239	2,274,239	2,274,239	2,274,239
Total Annual Sales	142,744,192	142,744,192	142,744,192	142,744,192	142,744,192	142,744,192	142,744,192	142,744,192	142,744,192	142,744,192
Feedstock Cost	57,900,000	57,900,000	57,900,000	57,900,000	57,900,000	57,900,000	57,900,000	57,900,000	57,900,000	57,900,000
Other Raw Materials	1,462,922	1,462,922	1,462,922	1,462,922	1,462,922	1,462,922	1,462,922	1,462,922	1,462,922	1,462,922
Catalyst Regeneration Cost	3,455,475	3,455,475	3,455,475	3,455,475	3,455,475	3,455,475	3,455,475	3,455,475	3,455,475	3,455,475
Other Variable Costs	4,828,662	4,828,662	4,828,662	4,828,662	4,828,662	4,828,662	4,828,662	4,828,662	4,828,662	4,828,662
Fixed Operating Costs	10,100,000	10,100,000	10,100,000	10,100,000	10,100,000	10,100,000	10,100,000	10,100,000	10,100,000	10,100,000
Total Product Cost	77,747,059	77,747,059	77,747,059	77,747,059	77,747,059	77,747,059	77,747,059	77,747,059	77,747,059	77,747,059
Annual Depreciation										
General Plant										
DDB										
SL										
Actual										
Remaining Value										
Power and Steam Plant										
DDB	3,803,787	3,518,503	3,254,616	3,010,519	2,784,730	2,575,876	2,382,685	2,203,984	2,038,685	1,885,783
SL	4,929,313	4,929,313	4,929,313	4,929,313	4,929,313	4,929,313	4,929,313	4,929,313	4,929,313	4,929,313
Actual	4,929,313	4,929,313	4,929,313	4,929,313	4,929,313	4,929,313	4,929,313	4,929,313	4,929,313	4,929,313
Remaining Value	44,363,819	39,434,506	34,505,192	29,575,879	24,646,566	19,717,253	14,787,940	9,858,626	4,929,313	0
Net Revenue	60,273,995	60,273,995	60,273,995	60,273,995	60,273,995	60,273,995	60,273,995	60,273,995	60,273,995	60,273,995
Losses Forward	0	0	0	0	0	0	0	0	0	0
Taxable Income	60,273,995	60,273,995	60,273,995	60,273,995	60,273,995	60,273,995	60,273,995	60,273,995	60,273,995	60,273,995
Income Tax	23,506,858	23,506,858	23,506,858	23,506,858	23,506,858	23,506,858	23,506,858	23,506,858	23,506,858	23,506,858
Annual Cash Flow	41,696,450	41,696,450	41,696,450	41,696,450	41,696,450	41,696,450	41,696,450	41,696,450	41,696,450	41,696,450
Discount Factor	0.35	0.32	0.29	0.26	0.24	0.22	0.20	0.18	0.16	0.15
Annual Present Value	14,614,351	13,285,774	12,077,976	10,979,979	9,981,799	9,074,362	8,249,420	7,499,473	6,817,703	6,197,912
TPI + Interest										-7,574,255
NPV										

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