processes

MDPI

Integrated Biorefinery of Empty Fruit Bunch from Palm Oil Industries to Produce Valuable Biochemicals

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Supplementary Information

This Supplementary Information has the following sections:

(A) sustainability assessment,

(B) multi-objective optimization code, and

(C) multi-criteria decision making.

A. Sustainability Assessment

The integrated biorefinery of empty fruit bunch (EFB) is modelled in Aspen Plus, and all information shown in this supplementary data is for the base case capacity of 75 ton/h of EFB

1. Techno-economic analysis

Tables S1 and S2 display the factors used for the estimation of capital investment and for the estimation of operating costs, respectively. Table S3 and S4 are a summary of raw material cost and selling price of products and economic results for all production processes involved.

Table S1. The estimation of capital investment

Component of investment	Factor
A. Total plant direct cost (TPDC)	
Equipment purchase cost	1
purchased equipment installation	0.39
instrumentations and control-installed	0.13
piping-installed	0.31
electrical installed	0.1
buildings-including services	0.29
yard improvement	0.1
service facilities-installed	0.55
B. Total plant indirect cost (TPIC)	
Engineering and supervision	0.32
Construction expenses	0.34
C. Total direct and indirect costs (TPC = TPDC + TPIC)	
D. Contractor's fee and contingency (CFC)	
contractor's fee	0.05
Contingency	0.1
E. Fixed Capital Investment (FCI = TPC + CFC)	
Working capital (30% of FCI) (WC)	0.3
Land use (6% of Equipment purchase cost)	0.06
Total Capital Investment (TCI = FCI + WC + LU)	

Table S2. The estimation of operating costs

Category	Feature	Value used in Text
Direct manufacturing costs (DMC)	Raw material cost	C_{RM}
	Utilities cost	C_{WT}
	Operating labor	C_{OL}
	Supervisory and clerical labor	0.2 C_{OL}
	Maintenance and repair	0.06 FCI
	Operating supplies	0.009 FCI
	Laboratory charges	0.15 C_{OL}
	Patent and royalties	0.03 C_{OM}
Fixed manufacturing costs (FMC)	Local taxes and insurance	0.03 FCI
	Plant overhead	0.708 C_{OL} + 0.036 FCI
General manufacturing costs (GMC)	Administration costs	0.177 C_{OL} + 0.009 FCI
	Distribution and selling costs	0.11 C_{OM}
	Research and development	0.05 C_{OM}

Table S3. Raw material and product selling price

Raw material	Price ($/kg)
Empty fruit bunch	0.005
Sulfuric acid	0.075
Ammonia	0.495
Hydrogen	10
Raney-nickel	2.6
Carbon dioxide	0.0098
$AlCl_3$	0.0006
Ionic liquid	$3.56x10^{-05}$
Ethyl acetate	0.7
NaOH	0.7
SO_2	0.0015
Glucose	0.0015
CNUTR	$1.267\ x10^{-05}$
Oil	6
Product	**Price ($/kg)**
Xylitol	4.05
Levulinic acid	8.28
Succinic acid	2.6
Guaiacol	1.6
Vanillin	20

Table S4. Economic results for 75 ton/hour of dry empty fruit bunch

Component	Process							
	Dilute acid	Enzyme	Saccharification	Xylitol	Levulinic acid	Succinic acid	Guaiacol	Vanillin
Capital investment (M$)	5.2	58.2	3.4	31.4	7.7	42.6	52.2	18.8
Operating cost (M$/year)	13.4	20.8	1.2	122.9	4.1	70.1	42.6	115.2
Sales Revenue (M$/year)	-	-	-	626.96	838.5	191.75	73.57	385.36
Profit (M$/year)	-	-	-	335	823	313	25	74

2. Life cycle assessment

Figure S1 reveals the global warming potential of each production process involved.

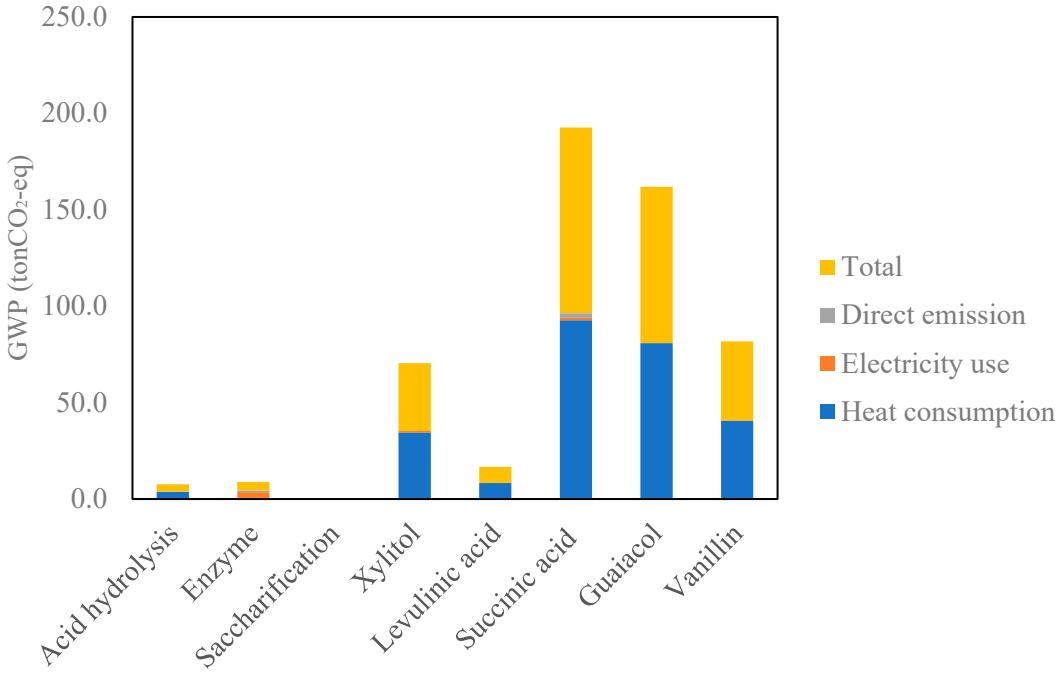

Figure S1. Total global warming potential

3. **Inherent safety**

Table S5 presents results of inherent safety assessment for five upgrading processes involved.

Table S5. Inherent safety results summary

Process	Chemicals	Type of hazards	FEDI	TDI
Xylitol	Hydrogen, xylitol	Flammable	118	87
Levulinic acid	Hydroxymethylfurfural, formic acid, levulinic acid	Toxic/corrosive	163	285
Succinic acid	Succinic acid	Toxic/corrosive	144	341
Guaiacol	Hibert kethon, guaiacol	Toxic/corrosive	172	325
Vanillin	Vanillin, sulfuric acid, ethyl acetate	Toxic/corrosive	195	204

B. **Multi-objective optimization code**

The developed model equations of all responses/outputs of all processes are given below. Interaction between the parameters were obtained and correlated with the output as shown in following Equations.

1. Objective function (@Biorefinery)

$$Max\ annual\ profit\ = -(11012.84 + 0.23x_1 - 226.11x_2 + 0.06x_1x_2 - 2.59x10^{-9}x_1^2 + 1.16x_2^2 - (x_3)(-204.03 + 0.304x_1 + 5.69x_4 + 0.14x_1x_4 - 1.1x10^{-11}x_1^2 - 0.039x_4^2) - (1 - (x_3)\big(1743.27 - 0.29x_1 - 46.15x_5 + 0.069x_1x_5 + 4.5x10^{-5}x_1^2 + 0.3x_5^2\big) - (x_6)(49.11 - 0.63x_1 - 1.402x_7 + 0.04x_1x_7) - (1 - (x_6)(547.12 + 0.063x_1 - 149.27x_8 + 0.32x_1x_8 + 9.13x10^{-7}x_1^2 + 10.17x_8^2) + (43.53 + 0.0039x_1 - 0.88x_2 + 1.18x10^{-4}x_1x_2 - 1.4x10^{-4}x_1^2 + 4.5x10^{-3}x_2^2) + (x_3)(0.27 + 5.24x10^{-3}x_1 - 1.24x10^{-4}x_4 + 4.11x10^{-5}x_1x_4) + (1 - (x_3)\big(15.46 - 0.032x_1 - 0.37x_5 + 3.74x10^{-4}x_1x_5 + 5.63x10^{-4}x_1^2 + 2.85x10^{-3}x_5^2\big) + (x_6)(6.11 + 0.073x_1 - 0.32x_7 + 3.73x10^{-4}x_1x_7 - 1.43x10^{-4}x_1^2 + 4.42x10^{-3}x_7^2) - \big(1 - (x_6)\big)(-3.11 + 0.025x_1 + 1.02x_8 + 1.3x10^{-4}x_1x_8 - 7.95x10^{-5}x_1^2 - 0.068x_8^2) + 0.32 + 0.038 - 1.0563x_1 + 0.123x_1 + (62.53 + 1.63x_1 - 1.25x_2 + 1.8x10^{-4}x_1x_2 - 3.13x10^{-4}x_1^2 + 6.42x10^{-3}x_2^2 + (x_3)(0.77 + 0.037x_1 - 2.32x10^{-4}x_4 + 9.58x10^{-5}x_1x_4) + (1 - (x_3)(-3.22 + 0.69x_1 + 0.21x_5 + 1.34x10^{-3}x_1x_5 + 8.88x10^{-4}x_1^2 + (x_6)(3.09 + 0.58x_1 + 0.057x_7) + (1 - (x_6))(-7.23 + 1.59x_1 + 1.38x_8 + 1.76x10^{-4}x_1x_8 - 3.12x10^{-4}x_1^2 - 0.086x_8^2) + 0.968 + 0.1662x_1 - 0.667 + 0.32x_1$$

$$Min\ GWP = 6.99 + 0.48x_1 - 0.15x_2 + 4.22x10^{-5}x_1x_2 - 1.06x10^{-4}x_1^2 + 7.92x10^{-4}x_2^2 + (x_3)\left(-1.58 + 0.064x_1 + 0.044x_4 + 6.05x10^{-4}x_1x_4 + 8.87x10^{-7}x_1^2 - 3.03x10^{-4}x_4^2\right) + \left(1 - (x_3)\right)\left(-375.55 + 1.61x_1 + 10.2x_5 + 7.16x10^{-3}x_1x_5 - 3.27x10^{-4}x_1^2 - 0.069x_5^2\right) + (x_6)\left(11.31 + 0.72x_1 - 0.32x_7 + 9.8x10^{-3}x_1x_7\right) + \left(1 - (x_6)\right)\left(0.37 + 0.54x_1 - 0.1x_8 + 2.25x10^{-4}x_1x_8 - 4.96x10^{-6}x_1^2 + 7.09x10^{-3}x_8^2\right) + 0.0083 + 0.051x_1 + 0.705 + 0.2694x_1$$

$$Min\ FEDI = 724.22 + 0.78x_1 - 13.73x_2 + 1.2x10^{-3}x_1x_2 - 2.43x10^{-3}x_1^2 + 0.071x_2^2 + (x_3)\left(58.44 + 1.13x_1 + 0.59x_4 + 1.51x10^{-3}x_1x_4 - 3.29x10^{-3}x_1^2 - 2.67x10^{-3}x_4^2\right) + (1 - (x_3))(232.03 + 0.85x_1 - 4.53x_5 + 3.12x10^{-3}x_1x_5 - 2.9x10^{-3}x_1^2 + 0.033x_5^2 + (x_6)(399.28 + 0.52x_1 - 17.46x_7 + 0.025x_1x_7 - 4.18x10^{-3}x_1^2 + 0.24x_7^2 + (1 - (x_6))(171.76 + 0.96x_1 - 12.59x_8 + 0.012x_1x_8 - 2.95x10^{-3}x_1^2 + 0.97x_8^2 + 62.943 + 0.4396x_1$$

$$Min\ TDI = 909.22 + 0.59x_1 - 18.10x_2 + 2.16x10^{-3}x_1x_2 - 1.95x10^{-3}x_1^2 + 0.094x_2^2 + (x_3)\left(46.54 + 2.18x_1 + 1.57x_4 + 5.56x10^{-3}x_1x_4 - 6.34x10^{-3}x_1^2 - 7.21x10^{-3}x_4^2\right) + (1 - (x_3))(635.56 + 2.2x_1 - 14.1x_5 + 0.012x_1x_5 - 7.54x10^{-3}x_1^2 + 0.101x_5^2 + (x_6)(61.04 + 1.87x_1 + 3.33x_7 + (1 - (x_6))(122.95 + 1.84x_1 - 12.53x_8 + 0.015x_1x_8 - 5.14x10^{-3}x_1^2 + 0.95x_8^2) + 77.893 + 0.8216x_1$$

2. Demand constraint (@Bconstraint)

$$xylitol\ demand = -(339.902 + 0.00713x_1 - 6.979x_2 + 0.00184x_1x_2 - 7.99x10^{-3}x_1^2 + 0.0358x_2^2) + 19;$$

$$levulinic\ acid\ demand = -(x_3)(-3.08 + 0.0459x_1 + 0.0858x_4 + 0.0021x_1x_4 - 1.66x10^{-13}x_1^2 - 0.000596x_4^2) + 1.9;$$

$$succinic\ acid\ demand = -(1 - (x_3))(-1.1344 + 0.00169x_1 + 0.0144x_5 + 0.0031x_1x_5) + 88.75;$$

$$guaiacol\ demand = -(x_6)(-0.1344 - 0.0556x_1 + 0.000304x_7 + 0.0022x_1x_7) + 5.6;$$

$$evulinic\ acid\ demand = -(1 - (x_6)3.419 + 0.00039x_1 - 0.9329x_8 + 0.0021x_1x_8 + 5.71x10^{-9}x_1^2 + 0.0635x_8^2) + 4.7;$$

3. Solver

```
options = optimoptions('gamultiobj','Display','iter',...
        'MaxGeneration',1000,...
        'PopulationSize',100,...
        'CrossoverFraction',0.8,...
        'MigrationFraction',0.2,...
        'PlotFcn',@gaplotpareto);

        fitness = @Biorefinery;
        nvars = 8 ;
        ConsFcn = @Bconstraint;
        LB = [50 96 0 67 73 0 33 7];
        UB = [100 99 1 77 80 1 37 7.7];
        [x,fval] = gamultiobj(fitness,nvars,[],[],[],[],LB,UB,[],options);

        %pareto front
        figure(1);
        scatter3(fval(:,1),fval(:,2),fval(:3).'o');
        xlabel('Annual profit($Million/year');
        ylabel('GWP (kg CO2 eq)');
        zlabel('FEDI');
        view(40,35)
```

C. Multi-criteria decision making

1. Fuzzy Analytical Hierarchy Process

Table S6. Decision maker attribute

Decision maker 1									
	Economic Viability			Environmental Performance			Safety Index		
Economic Viability	**1**	**1**	**1**	1	1	1	1	1	1
Environmental Performance	1	1	1	**1**	**1**	**1**	1	1	1
Safety Index	1	1	1	1	1	1	**1**	**1**	**1**

Decision maker 2

	Economic Viability			Environmental Performance			Safety Index		
Economic Viability	**1**	**1**	**1**	1	1	1	0.179	0.333	0.667
Environmental Performance	1	1	1	**1**	**1**	**1**	0.179	0.333	0.667
Safety Index	1.5	3	5.6	1.5	3	5.6	**1**	**1**	**1**

Decision maker 3									
	Economic Viability			Environmental Performance			Safety Index		
Economic Viability	**1**	**1**	**1**	3	5	7.9	3	5	7.9
Environmental Performance	0.127	0.2	0.333	**1**	**1**	**1**	0.179	0.333	0.667
Safety Index	0.127	0.2	0.333	1.5	3	5.6	**1**	**1**	**1**

Decision maker 4									
	Economic Viability			Environmental Performance			Safety Index		
Economic Viability	**1**	**1**	**1**	3	5	7.9	1.5	3	5.6
Environmental Performance	0.127	0.2	0.333	**1**	**1**	**1**	0.179	0.333	0.667
Safety Index	0.179	0.333	0.667	1.5	3	5.6	**1**	**1**	**1**

Decision maker 5									
	Economic Viability			Environmental Performance			Safety Index		
Economic Viability	**1**	**1**	**1**	0.313	0.5	0.833	1.5	3	5.6
Environmental Performance	1.2	2	3,2	**1**	**1**	**1**	1.5	3	5.6
Safety Index	0.179	0.333	0.667	0.179	0.333	0.667	**1**	**1**	**1**

GROUP (GEOMETRIC MEAN)									
	Economic Viability			Environmental Performance			Safety Index		
Economic Viability	1	1	1	1.23	1.66	2.20	1.04	1.72	2.78
Environmental Performance	0.45	0.60	0.81	1	1	1	0.39	0.64	1.11
Safety Index	0.36	0.58	0.96	0.90	1.55	2.59	1	1	1

2. Technique for Order Preference

Table S7. TOPSIS key calculation information for profit, GWP, and FEDI

Profit (F1)	**GWP (F2)**	**FEDI (F3)**	**Normalized Weighted F1**	**Normalized Weighted F2**	**Normalized Weighted F3**	**S**	**S -**	**Relative Closeness**
931.8	284.0	594.7	0.09289	0.03296	0.05194	0.00233	0.01660	0.8771
925.4	285.3	594.1	0.09226	0.03312	0.05189	0.00240	0.01595	0.8693
918.7	287.7	592.1	0.09159	0.03339	0.05172	0.00258	0.01526	0.8553
915.7	285.3	592.3	0.09129	0.03311	0.05174	0.00269	0.01499	0.8478
914.0	288.9	591.4	0.09111	0.03353	0.05165	0.00285	0.01477	0.8382
905.7	290.0	590.2	0.09029	0.03366	0.05155	0.00340	0.01395	0.8038
896.2	285.7	589.9	0.08934	0.03316	0.05152	0.00406	0.01306	0.7628
894.3	283.0	589.1	0.08915	0.03284	0.05145	0.00416	0.01292	0.7562
887.9	296.9	586.0	0.08851	0.03446	0.05118	0.00502	0.01214	0.7075
884.5	286.9	588.4	0.08818	0.03329	0.05139	0.00508	0.01189	0.7007
882.3	280.4	586.8	0.08796	0.03255	0.05125	0.00519	0.01181	0.6948
875.9	297.6	583.7	0.08732	0.03454	0.05098	0.00607	0.01096	0.6436
870.1	296.2	579.3	0.08674	0.03437	0.05060	0.00649	0.01044	0.6168
866.4	283.4	584.3	0.08637	0.03289	0.05103	0.00668	0.01020	0.6043
860.8	281.6	584.0	0.08581	0.03268	0.05101	0.00721	0.00970	0.5738
855.3	287.3	581.4	0.08526	0.03334	0.05078	0.00776	0.00906	0.5388
851.4	290.2	580.3	0.08488	0.03368	0.05068	0.00816	0.00865	0.5144
842.3	288.5	579.5	0.08397	0.03349	0.05061	0.00902	0.00781	0.4640
839.0	289.7	579.5	0.08364	0.03362	0.05061	0.00936	0.00746	0.4435

836.1	299.4	577.5	0.08335	0.03475	0.05044	0.00983	0.00711	0.4196
831.2	291.6	576.7	0.08286	0.03384	0.05037	0.01015	0.00672	0.3985
825.9	287.6	580.2	0.08234	0.03338	0.05067	0.01064	0.00625	0.3700
821.5	292.7	575.1	0.08190	0.03398	0.05023	0.01111	0.00582	0.3440
816.7	292.5	575.5	0.08141	0.03395	0.05026	0.01158	0.00537	0.3166
815.5	294.1	573.9	0.08129	0.03413	0.05013	0.01172	0.00527	0.3101
809.8	289.2	576.5	0.08073	0.03356	0.05035	0.01223	0.00479	0.2814
803.2	294.4	572.7	0.08007	0.03417	0.05002	0.01293	0.00420	0.2453
803.2	294.4	572.7	0.08007	0.03417	0.05002	0.01293	0.00420	0.2452
793.5	298.6	571.1	0.07910	0.03465	0.04988	0.01395	0.00341	0.1964
786.6	297.3	571.5	0.07841	0.03450	0.04992	0.01461	0.00288	0.1645
781.4	296.4	571.0	0.07790	0.03440	0.04987	0.01511	0.00260	0.1466
775.7	297.9	570.2	0.07733	0.03458	0.04980	0.01569	0.00235	0.1302
771.1	298.0	570.0	0.07688	0.03459	0.04978	0.01615	0.00223	0.1213
766.4	300.2	568.5	0.07640	0.03484	0.04965	0.01665	0.00229	0.1209
766.4	300.2	568.5	0.07640	0.03484	0.04965	0.01665	0.00229	0.1209

Positive Ideal	0.09289	0.03255	0.04965
Negative Ideal	0.07640	0.03484	0.05194

Table S8.: TOPSIS key calculation information for profit, GWP, and TDI

Profit (F1)	**GWP (F2)**	**TDI (F3)**	**Normalized Weighted F1**	**Normalized Weighted F2**	**Normalized Weighted F3**	**S**	**S -**	**Relative Closeness**
931.3	284.1	956.9	0.08721	0.03403	0.05096	0.00055	0.00538	0.9079
929.5	284.2	956.8	0.08704	0.03403	0.05095	0.00057	0.00521	0.9018
927.4	283.8	956.2	0.08684	0.03399	0.05092	0.00061	0.00502	0.8912
925.3	283.7	955.8	0.08664	0.03397	0.05089	0.00073	0.00482	0.8683
923.3	283.6	955.6	0.08646	0.03396	0.05089	0.00087	0.00463	0.8416
922.9	283.5	955.5	0.08642	0.03395	0.05088	0.00090	0.00460	0.8367
920.8	283.3	955.0	0.08622	0.03393	0.05085	0.00106	0.00440	0.8054

919.6	283.2	954.9	0.08611	0.03391	0.05085	0.00116	0.00429	0.7871
916.8	282.9	954.3	0.08585	0.03388	0.05082	0.00140	0.00403	0.7414
915.9	282.8	954.1	0.08577	0.03387	0.05081	0.00148	0.00395	0.7278
914.6	282.7	953.9	0.08564	0.03386	0.05079	0.00159	0.00383	0.7060
912.1	282.5	953.4	0.08540	0.03383	0.05077	0.00182	0.00359	0.6631
912.1	282.5	953.4	0.08540	0.03383	0.05077	0.00182	0.00359	0.6631
910.0	282.3	953.0	0.08521	0.03381	0.05075	0.00201	0.00340	0.6283
909.1	282.2	952.9	0.08513	0.03380	0.05074	0.00209	0.00332	0.6131
906.9	282.3	952.8	0.08492	0.03380	0.05074	0.00230	0.00311	0.5746
905.7	281.9	952.2	0.08481	0.03375	0.05070	0.00240	0.00301	0.5556
903.9	281.8	952.1	0.08464	0.03375	0.05070	0.00257	0.00284	0.5252
901.6	281.7	951.7	0.08442	0.03373	0.05068	0.00279	0.00263	0.4853
900.4	281.5	951.4	0.08432	0.03371	0.05066	0.00289	0.00253	0.4666
897.2	281.5	951.1	0.08401	0.03371	0.05065	0.00320	0.00223	0.4110
895.4	281.2	950.6	0.08384	0.03367	0.05062	0.00336	0.00208	0.3816
893.3	281.3	950.5	0.08365	0.03369	0.05062	0.00356	0.00189	0.3464
892.5	281.2	950.4	0.08357	0.03368	0.05061	0.00364	0.00181	0.3328
890.6	281.4	950.2	0.08339	0.03370	0.05060	0.00382	0.00164	0.3007
888.3	281.4	950.2	0.08318	0.03370	0.05060	0.00402	0.00144	0.2639
887.3	281.3	950.0	0.08309	0.03369	0.05059	0.00412	0.00136	0.2477
885.2	281.5	949.9	0.08289	0.03371	0.05058	0.00432	0.00117	0.2138
882.6	281.5	949.6	0.08265	0.03371	0.05056	0.00456	0.00096	0.1746
882.5	281.5	949.6	0.08263	0.03371	0.05056	0.00457	0.00096	0.1729
879.2	281.8	949.4	0.08233	0.03375	0.05056	0.00488	0.00070	0.1257
877.9	281.8	949.3	0.08221	0.03375	0.05055	0.00500	0.00063	0.1113
875.3	282.1	949.2	0.08196	0.03378	0.05055	0.00524	0.00050	0.0873
873.8	282.1	949.1	0.08183	0.03378	0.05054	0.00538	0.00049	0.0828
873.8	282.1	949.1	0.08183	0.03378	0.05054	0.00538	0.00049	0.0828

Positive Ideal	0.08721	0.03367	0.05054
Negative Ideal	0.08183	0.03403	0.05096