

Inverse Molecular Design Techniques for Green Chemical Design in Integrated Biorefineries

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Supplementary material

The application of the developed two-stage optimization approach is demonstrated by reworking the design and production problem of biobased fuel taken from Ng et al. [1]. Information in Table A1, A2 and A3 are obtained by referring to the work published by Ng et al. [1], while potency factor in Table A4 is identified through incremental environmental burden assessment presented by Andiappan et al. [2].

Table S1. List of Conversion Pathway to produce Alkane from Biomass

Pathway	Feed	Process	Product	Conversion (%)	Selectivity (%)
1	Biomass	Ammonia Explosion	Sugars, Lignin	98	-
2	Biomass	Steam Explosion	Sugars, Lignin	49.2	-
3	L, C, H	Organosolv Separation	Lignin	79.0*	-
4	L, C, H	Organosolv Separation	Sugars	97.0*	-
5	Sugars	Autohydrolysis	HMF	90.9	-
6	Sugars	Dehydration of Sugars	Furfural	40.9	-
7	Sugars	Yeast Fermentation	Ethanol	61.9	-
8	Sugars	Bacterial Fermentation	Ethanol	41	-
9	Furfural	Hydrogenation of Furfural	THFA	98.2	-
10	THFA	Hydrogenation of THFA 1	1,5-PeD	99.0	95.0
			PeOH		4.0
11	THFA	Hydrogenation of THFA 2	1,5-PeD	60.0	51.0
			PeOH		22.0
12	Biomass	Pyrolysis	Syngas	94	-
13	Biomass	Gasification	Syngas	90	-
14	Biomass	Anaerobic Digestion	Methane	40	-
15	Biomass	Water Gas Shift Reaction	Syngas	100	-

Table S1 (continued). List of Conversion Pathway to produce Alkane from Biomass

16	Syngas	Fischer-Tropsch 1	Hydrocarb on C ₂ -C ₄	40.0	16.0
			Hydrocarb on C ₅ -C ₉		27.0
			Hydrocarb on C ₁₀ -C ₁₃		26.0
17	Syngas	Fischer Tropsch 2	Hydrocarb on C ₂ -C ₄	75.0	23.0
			Hydrocarb on C ₅ -C ₉		19.0
			Hydrocarb on C ₁₀ -C ₁₃		9.7
18	Syngas	Conversion of Syngas 1	Methanol	25.1	2.6
			Ethanol		61.4
19	Syngas	Conversion of Syngas 2	Methanol	24.6	3.9
			Ethanol		56.1
20	Syngas	Hydrogenation of CO	Methanol	28.8	20.7
			Ethanol		23.8
			Propanol		14.1
			Butanol		7.5
21	Alcohols	Monsanto Process	Ethanoic Acid	99	-
22	Alcohols	Dehydration of Alcohols 1	Ethane	67.0	1.0
23	Alcohols	Dehydration of Alcohols 2	Propane	59.0	40.0
			Butane		13.0
24	Alcohols	Dehydration of Alcohols 3	Pentane	64.0	50.0
			Hexane		6.0
			Heptane		8.0
			Hydrocarb on C ₁₀ - C ₁₂		48.0
25	Acids	Decarboxylation of Acids	Ethane	62.0	21.3
26	Alkanes	Fractional Distillation of Alkanes	Hydrocarb on C ₈	99.0*	-
			Hydrocarb on C ₂ - C ₉ ,C ₁₀ - C ₁₃	99.0*	-

Table S2. Price List for Product and Feedstock

Category	Component	Price (USD/tonne)
Feedstock	Biomass	170
Alkane Product	Ethane	490
	Propane	750
	Butane	1000
	Pentane	1200
	Hexane	1600
	Heptane	1800
	Octane	2000
	Nonane	2100
	Decane	2300
	Undecane	2500
Alcohol Product	Methanol	450
	Ethanol	770
	Propanol	950
	Butanol	1120
	Pentanol	1770
	Pentanediol	3000

Table S3. List of Capital and Operating Cost for Conversion Pathways

Pathway	Process	Capital Cost (USD/yr)	Operating Cost (USD/yr)
1	Ammonia Explosion	19.64	11.26
2	Steam Explosion	13.90	7.97
3	Organosolv Separation	40.68	23.31
4	Organosolv Separation	40.68	23.31
5	Autohydrolysis	63.46	36.37
6	Dehydration of Sugars	27.62	15.83
7	Yeast Fermentation	40.62	23.27
8	Bacterial Fermentation	31.43	18.01
9	Hydrogenation of Furfural	30.22	17.32
10	Hydrogenation of THFA 1	43.52	24.94
11	Hydrogenation of THFA 2	45.45	26.05
12	Pyrolysis	62.86	36.02
13	Gasification	86.43	55.00
14	Anaerobic Digestion	26.23	15.03
15	Water Gas Shift Reaction	15.11	8.66
16	Fischer-Tropsch 1	193.41	110.83
17	Fischer Tropsch 2	181.93	104.25
18	Conversion of Syngas 1	38.56	22.10
19	Conversion of Syngas 2	41.10	23.55
20	Hydrogenation of CO	40.19	23.03
21	Monsanto Process	40.68	23.31
22	Dehydration of Alcohols 1	40.50	23.21
23	Dehydration of Alcohols 2	37.47	21.47
24	Dehydration of Alcohols 3	34.45	19.74
25	Decarboxylation of Acids	45.94	26.32
26	Fractional Distillation of Alkanes	169.48	98.22

Table S4. List of Component with Heat of Formation and Potency Factor

Component	MW	Heat of Formation (kJ/mol)	Potency Factor
Lignin	151.50	-8124.62	0.00
Cellulose	162.14	-6603.33	0.00
Hemicellulose (xylan)	132.12	-5458.74	0.00
Ammonia	17.03	-45.94	2.45
Ethyl benzoate	150.17	-285.00	0.00
Water	18.02	-285.83	0.00
Furfural	96.08	-200.20	11.00
HMF	126.11	-277.20	11.00
Glucose	180.16	-1275.00	0.00
Ethanol	46.07	-234.00	11.45
Carbon dioxide	44.01	-393.52	1.00
Hydrogen	2.02	0.00	0.00
THFA	102.13	-505.59	11.00
Oxygen	32.00	0.00	0.00
Carbon monoxide	28.01	-110.53	3.03
methane	16.04	-74.87	32.03
Nitrogen	28.04	0.00	0.00
Methanol	32.04	-238.40	12.71
Acetic acid	60.05	-483.52	12.25
Ethane	30.07	-84.00	11.14
Propanol	60.09	-302.54	11.22
Propane	44.10	-104.70	11.41
Pentanol	88.15	-298.00	11.00
Pentane	72.15	-146.80	12.22

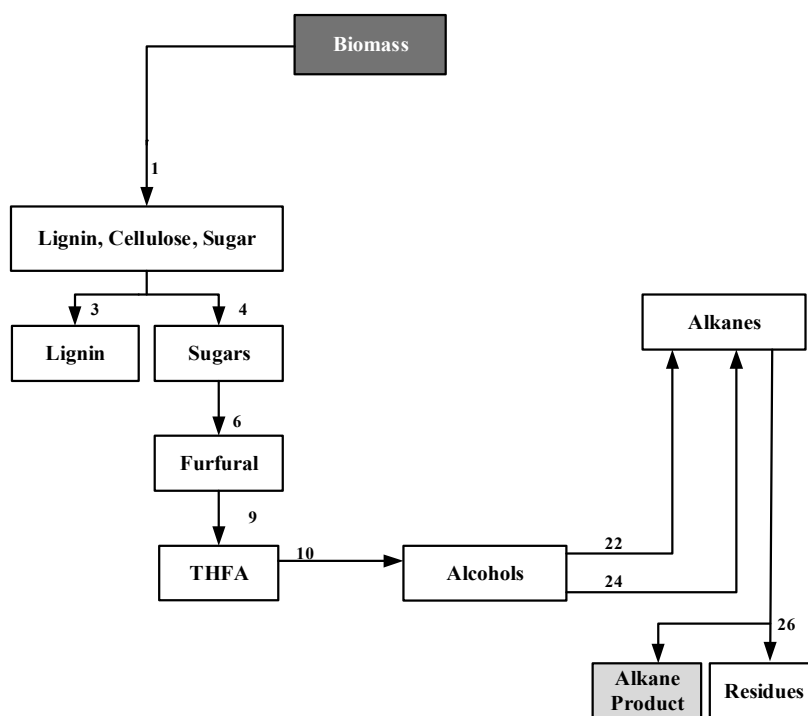


Figure S1. Conversion Pathway for Maximum Economic Performance, Minimum Environmental Burden and Minimum Energy Consumption

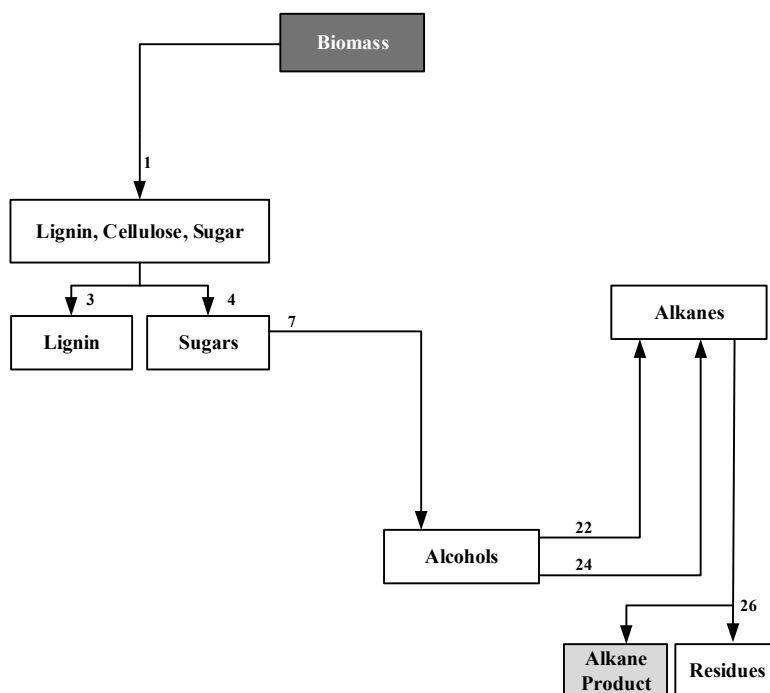


Figure S2. Conversion Pathway for Maximum Product C11 Yield

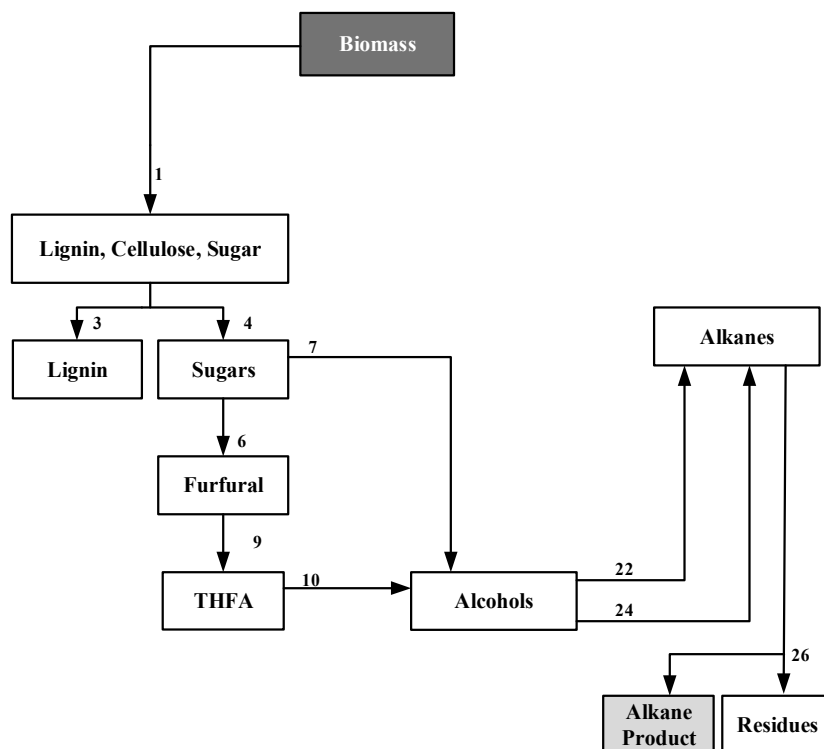


Figure S3. Conversion Pathway for Multi-objective Optimisation

References

1. Ng, L.Y.; Chemmangattuvalappil, N.G.; Ng, D.K.S. Robust chemical product design via fuzzy optimization approach. *Comput. Aided Chem. Eng.* **2014**, *34*, 387–392.
2. Andiappan, V.; Ko, A.S.Y.; Lau, V.W.S.; Ng, L.Y.; Ng, R.T.L.; Chemmangattuvalappil, N.G.; Ng, D.K.S. Synthesis of Sustainable Integrated Biorefinery via Reaction Pathway Synthesis: Economic, Incremental Environmental Burden and Energy Assessment with Multiobjective Optimization. *AIChE J.* **2015**, *61*, 132–146.