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Supplementary Material

Performance and Economic Analysis of Organosolv Softwood and Herbaceous Lignins to Activated Carbons as Electrode Materials in Supercapacitors

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Table S1. Supercapacitor performance of activated carbons produced by various biomass materials.

Precursors	Activation method	Surface area (m^2 g^{-1})	Electrolyte	Specific capacitance	References
Coffee endocarp	CO_2	709	1 M H_2SO_4	176 F g^{-1} at 10 mA	[1]
Corn husk	KOH	771	0.5 M H_2SO_4	314.83 F g^{-1} at 1 mV s^{-1}	[2]
Corn syrup	Physical self-activation	1473	6 M KOH	168 F g^{-1} at 0.2 A g^{-1}	[3]
Peanut shell	$ZnCl_2$	1565	6 M KOH	245 F g^{-1} at 0.05 A g^{-1}	[4]
Kraft lignin	KOH	1148	6 M KOH	91.7 F g^{-1} at 2 mV s^{-1}	[5]
Kraft lignin	steam & CO_2	591.7	2 M H_2SO_4	125.8 F g^{-1} at 0.15A g^{-1}	[6]
Sugarcane bagasse	K_2CO_3	725	2 M KOH	265 F g^{-1} at 0.2 A g^{-1}	[7]
GVL Lignin	steam & CO_2	1070	1 M H_2SO_4	367 at 0.1 mA cm^{-2}	this work

Table S2. Composition and elemental analysis of YP and SG lignin.

Lignin		**YP**	**SG**
Purity analysis (%)	ASL[a]+AIL[b]	96.60	94.04
	Ash	0.02	0.03
Molecular weight	M_n	2583	2238
	M_w	7747	6625
Molar-mass dispersity ($Đ_M$)	M_w/M_n	3.00	2.96
Ultimate analysis (at.%)	C	64.8	62.1
	H	6.3	6.1
	N	0.2	0.5
	O	28.7	31.3

[a] Acid-soluble lignin.

[b]Acid-insoluble lignin.

Table S3. Relative abundance of lignin linkages using ^{13}C-^{1}H NMR analysis.

	δC/δH (ppm)	**Label**	**Assignment**	**integral**	
				SG	**YP**
Lignin aromatic	2.49/39.5	DMSO	Solvent	1.00	1.00
	103.9/6.65	$S_{2/6}$	C_2/H_2 and C_6/H_6 in etherified syringyl units (S)	0.849	--
	110.9/7.00	G_2	C_2/H_2 in guaiacyl units (G)	0.370	1.046
	115.1/6.72&6.98 and118.7/6.77	G_5/G_6	C_5/H_5 and C_6/H_6 in guaiacyl units (G)	1.832	2.741
	114.8/6.73	$H_{3,5}$	$C_{3,5}/H_{3,5}$ in *p*-hydroxyphenyl units (H)	0.130	0.089
	127.8/7.20	$H_{2,6}$	$C_{2,6}/H_{2,6}$ in *p*-hydroxyphenyl units (H)	0.109	--
	115.5/6.72	$PCA_{3,5}$	C_3/H_3 and C_5/H_5 in p-coumarate (PCA)	1.030	0.259
	130.0/7.48	$PCA_{2,6}$	C_2/H_2 and C_6/H_6 in p-coumarate (PCA)	0.637	--
	113.5/6.27	PCA_β and FA_β	C_β/H_β in p-coumarate (PCA) and ferulate (FA)	0.273	0.033
	111.0/7.32	FA_2	C_2/H_2 in ferulic acid units (FA)	0.123	--
	123.0/7.10	FA_6	C_6/H_6 in ferulic acid units (FA)	0.040	0.134
Lignin aliphatic	53.2/3.47	B_β	C_β/H_β in *β*-5' phenylcoumaran substructures (B)	0.045	0.145
	53.6/3.07	C_β	C_β/H_β in *β*-*β* ' resinol substructures (C)	0.011	--
	55.5/3.75	OMe	C/H in methoxyls	8.233	8.202
	59.8/3.36 & 3.72	A_γ	C_γ/H_γ in normal (γ-hydroxylated) *β*-O-4' substructures (A)	1.142	0.862
	62.5/3.75	B_γ	C_γ/H_γ in β-5' phenylcoumaran substructures (B)	0.251	0.782
	71.2/3.80 & 4.17	C_γ	C_γ/H_γ in β-β' resinol substructures (C)	0.028	--
	71.5/4.75	A_α/A'_α	C_α/H_α in *β*-O-4' substructures (A, A′) –G & -S	0.257	0.156

Table S4. Pore structures of activated carbons prepared from YP and SG lignin precursors.

Carbon type	Specific surface area		Pore volume		
	S_{BET} ($m^2\ g^{-1}$)	S_{BJH} ($m^2\ g^{-1}$)	V_t ($cm^3\ g^{-1}$)	V_{micro} (%)	V_{meso} (%)
YP-AC	1070	467	1.27	56	44
SG-AC	507	56	0.29	89	11

S_{BET}: Specific surface area computed using BET equation.

S_{BJH}: Specific surface area computed using BJH equation.

V_t: Total pore volume estimated at a relative pressure of 0.98.

V_{micro}: Micropore volume determined from *t*-plot method.

V_{meso}: Mesopore volume determined from the subtraction of micropore volume from total pore volume.

Table S5. Material flow rate of the main streams based on the process flow diagram shown in Figure 10 and the energy consumption of the process areas.

Areas	Streams	Temperature (°C)	Pressure (atm)	Flow rate (tonne/h)		Energy requirement (MW)	
				YP bioref.	SG bioref.	YP bioref.	SG bioref.
	1	25	1	0.31	0.2		
	2	25	1	9.5	6.9		
	3	25	1	17.5	12.7		
	4	144.8	3.4	34.1	24.8		
A100	5	144.8	3.4	53.6	38.9	Electricity:	
	6	125	3.4	41.8	30.4	0.004	0.003
	7	153.6	1	33.9	24.7		
	25	194.7	1	9.1	5.2		
	8	149.8	4.5	215.7	157.0	Cooling:	
	9	149.8	4.5	212.1	154.4	7.4	5.3
A200	10	149.8	4.5	34.9	25.4	Electricity:	
	14	25	1	0.4	0.3	3.1	2.2
	17	138.5	3.4	4.9	3.6		
	18	138.5	3.4	0.4	0.3		
	11	25	1	0.1	0.1	Heating:	
	12	167.7	1.2	0.9	1.9	8.5	6.2
A300	13	25	1	0.09	0.07	Cooling:	
	15	208	1	24.9	18.1	9.7	7.1
	16	208	1	3.8	1.5	Electricity:	
	19	25	1	0.6	0.4	0.021	0.015
	20	800	1	3.6	2.6		
	21	800	1	0.2	0.1	Heating:	
A400	22	25	1	0.06	0.04	2.3	1.8
	23	800	1.5	0.2	0.1	Electricity:	
	24	800	1.5	0.1	0.1	0.4	0.3

Table S6. Detailed capital costs of the equipment in A400.

Equipment	Quantity	Equipment installed costs (Million $)		Source
		YP biorefinery	SG biorefinery	
Air separation unit	1	2.2	28.2	[8]
Fluidized bed reactor	3	2.9	30.1	[9]
Cyclone	3	0.1	5.5	Aspen Plus
Ball Mill	1	0.07	4.6	Aspen Plus
Compressor	3	0.6	20.6	[10]

Table S7. A summary of equipment installed costs of different process areas.

Area	Capital costs (Million $)	
	YP biorefinery	SG biorefinery
A100	34.2	28.2
A200	36.4	30.1
A300	6.7	5.5
A400	5.9	4.6
A500	24.9	20.6
A600	8.0	6.6
A700	2.7	2.3
A800	1.9	1.5

Table S8. Summary of cost components for YP- and SG-based biorefineries.

Cost components		Costs (Million $)	
		YP biorefinery	SG biorefinery
Inside-battery-limits (ISBL) equipment costs (A100-A400)		83.1	68.4
Outside-battery-limits (OSBL) equipment costs (A500-A800)		37.5	31.0
Warehouse	4.0% of ISBL	3.3	2.7
Site development	9.0% of ISBL	7.5	6.2
Additional piping	4.5% of ISBL	3.8	3.1
Total direct costs (TDC)		**135.2**	**111.4**
Prorateable expenses	10.0% of TDC	13.5	11.1
Field expenses	10.0% of TDC	13.5	11.1
Home office and construction fee	20.0% of TDC	27.0	22.3
Project contingency	40.0% of TDC	13.5	11.1
Other costs (start-up, permits, etc.)	10.0% of TDC	13.5	11.1
Total indirect costs		**81.0**	**66.9**
Fixed capital investment (FCI)		**216.2**	**178.3**
Land		1.9	1.9
Working capital	5.0% of FCI	10.8	8.9
Total capital investment (TCI)		**228.9**	**189.1**

Table S9. Summary of material prices and sources.

Component	Price ($/ton)	Source
YP	70	[4]
SG	80	[4]
H_2SO_4	86	[5]
GVL	1000	[6]
NaCl	182	USGS
Heavy oil	330	Baytex energy
Lime	237	[4]
CO_2	70	[7]
Boiler chemicals	5950	[4]
Cooling tower chemicals	3565	[4]
WWT nutrients	5251	[4]

Table S10. Financial assumptions.

Plant life	30 years
Capacity factor	90% (7884 hr/year)
Internal rate of return	30%
Plant depreciation	7 years
Loan terms	10-year loan at 8% APR
Construction time	3 years
Financing	40% equity
Federal tax rate	21%
First 12 months' expenditure	8%
Second 12 months' expenditure	60%
Last 12 months' expenditure	32%
Start-up time	6 months
Working capital	5% of fixed capital investment
Revenue during start-up	50%
Variable operating costs during start-up	75%
Fixed operating costs during start-up	100%

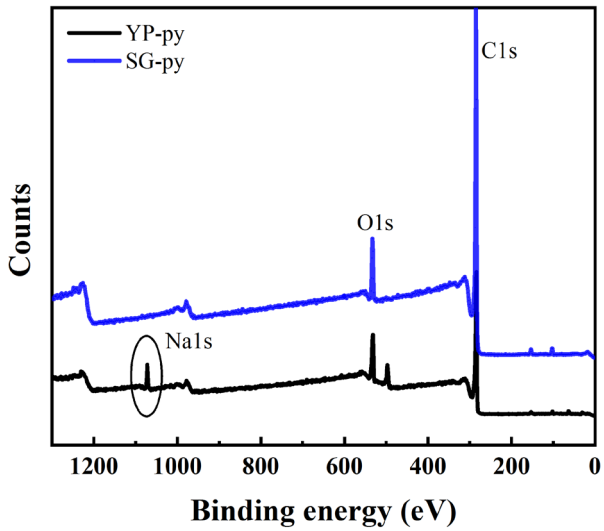

Figure S1. Survey-scan XPS spectra of YP-py and SG-py samples.

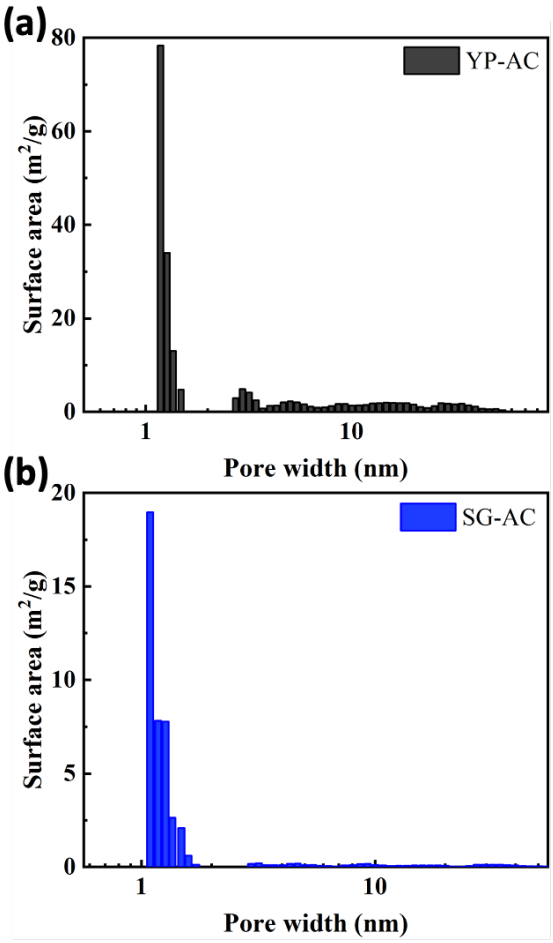

Figure S2. Pore size distributions of activated carbons prepared from (a) YP and (b) SG lignin precursors.

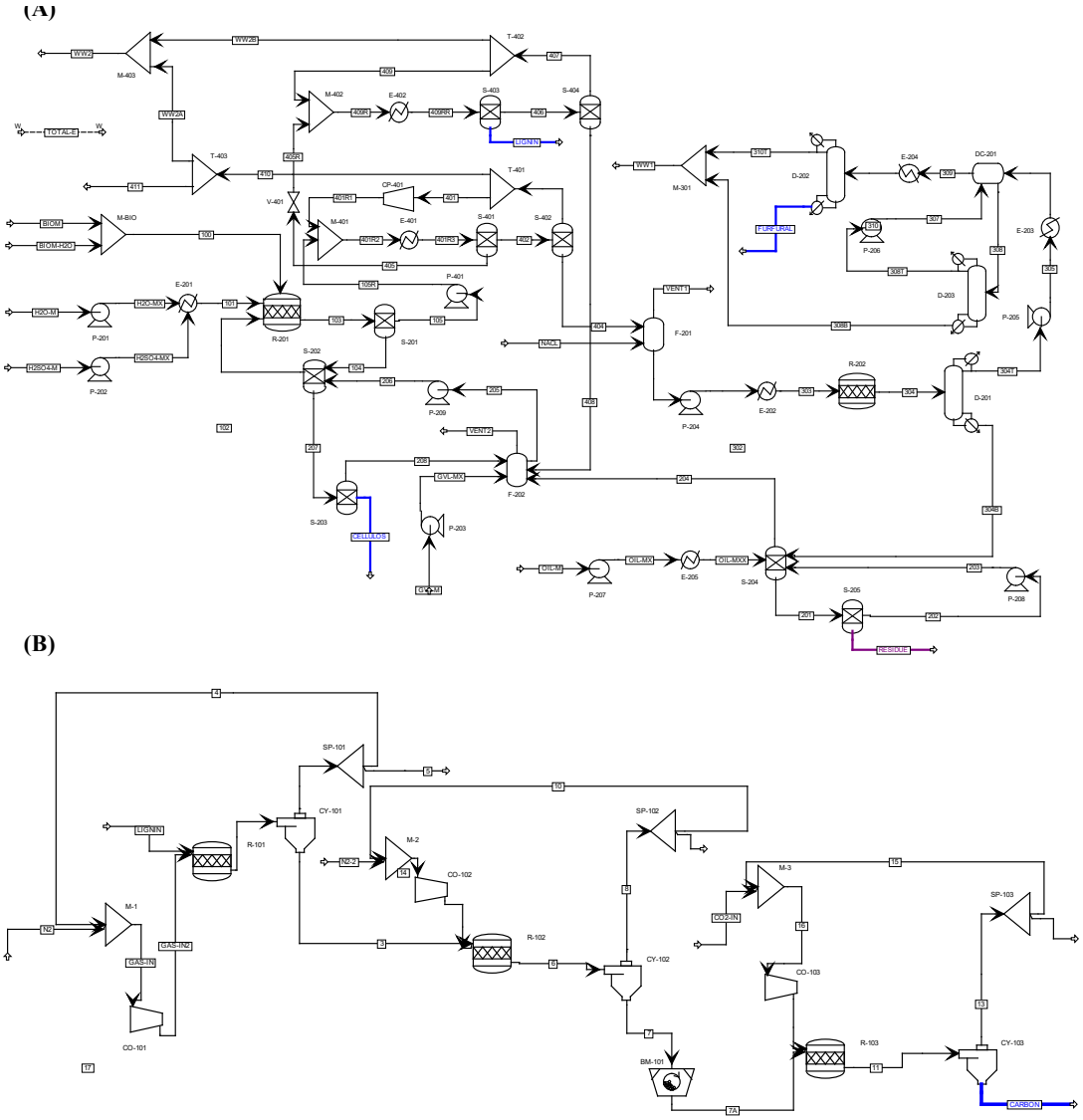

Figure S3. Aspen Plus model for (A) A100-A300 and (B) A400.

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