SUPPLEMENTARY MATERIAL

In-depth Exergy Analysis of the Thermochemical Conversion of Flax Straw via Pyrolysis

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Table S1. Chemical components used in Aspen Plus [31, 32].

Chemical compound	Component ID	Type	Component name	Formula
Biomass Components				
tannin	TANN	solid		$C_{15}H_{12}O_7$
C-rich lignin	LIGC	solid		$C_{15}H_{14}O_4$
O-rich lignin	LIGO	solid		$C_{20}H_{22}O_{10}$
H-rich lignin	LIGH	solid		$C_{22}H_{28}O_9$
Triglyceride	TGL	conventional		$C_{57}H_{100}O_7$
Hemicellulose-glucomannan	GMSW	solid		$C_5H_8O_4$
Hemicellulose-xylan	XYHW	solid		$C_5H_8O_4$
Cellulose	CELL	solid		$C_6H_{10}O_5$
Moisture	H2OL	conventional	Water	H_2O
Pyrolysis Intermediate Species				
Secondary lignin intermediate	LIG	solid		$C_{11}H_{12}O_4$
C-rich lignin intermediate	LIGCC	solid		$C_{15}H_{14}O_4$
H/O-rich lignin intermediate	LIGOH	solid		$C_{19}H_{22}O_8$
Activated hemicellulose 1	HCE1	solid		$C_5H_8O_4$

Activated hemicellulose 2	HCE2	solid		$C_5H_8O_4$
Activated cellulose	CELLA	solid		$C_6H_{10}O_5$
Tannin intermediate	ITANN	solid		$C_8H_4O_4$
Pyrolysis End-Products				
Char	CHAR	solid	Carbon	C
Sinapyl aldehyde	FE2MACR	conventional		$C_{11}H_{12}O_4$
Free fatty acid	FFA	conventional	Linoleic acid	$C_{18}H_{32}O_2$
High-molecular-weight lignin	HMWL	solid		$C_{24}H_{28}O_4$
Glyoxal	GLYOX		Glyoxal	$C_2H_2O_2$
Ethylene	C2H4	conventional	Ethylene	C_2H_4
Acetaldehyde	CH3CHO	conventional	Acetaldehyde	C_2H_4O
Acetic acid	ACAC	conventional	Acetic acid	$C_2H_4O_2$
Glycol aldehyde	HAA	conventional	Glycol-aldehyde	$C_2H_4O_2$
Ethanol	C2H5OH	conventional	Ethanol	C_2H_6O
Acrolein	ACROL	conventional	Acrolein	C_3H44O
N-propionaldehyde	ALD3	conventional	N-propionaldehyde	C_3H_6O
3-hydroxypropanal	C3H6O2	conventional		$C_3H_6O_2$
Furfural	FURF	conventional	Furfural	$C_5H_4O_2$
Xylosan	XYLAN	conventional		$C_5H_8O_4$
Levoglucosan	LVG	conventional	Levoglucosan	$C_6H_{10}O_5$
Phenol	PHENOL	conventional	Phenol	C_6H_6O

5-hydroXymethyl-furfural	HMFU	conventional	5-hydroXymethyl-furfural	$C_6H_6O_3$
Anisole	ANISOLE	conventional	Methyl-phenyl-ether	C_7H_8O
p-coumaryl alcohol	COUMARYL	conventional		$C_9H_{10}O_2$
Formaldehyde	CH2O	conventional	Formaldehyde	CH_2O
Formic acid	HCOOH	conventional	Formic acid	CH_2O_2
Methane	CH4	conventional	Methane	CH_4
Methanol	CH3OH	conventional	Methanol	CH_4O
Carbon monoxide	CO	conventional	Carbon monoxide	CO
Carbon dioxide	CO2	conventional	Carbon dioxide	CO_2
Hydrogen	H2	conventional	Hydrogen	H_2
Water	H2O	conventional	Water	H_2O

Table S2. Estimated Solid Property Model Parameters [31, 32].

Component ID	**Molecular weight (kg/kmol)**	**Standard solid enthalpy of formation (kJ/g mol)**	**Heat capacity model coefficients**		**Solid density ($kmol/m^3$)**
			C_1 (J/(g mol K))	C_2 (J/(g mol K^2))	
Lignins and Tannins					
LIG	208.213 88	−729.31	13.2251	0.828 34	7.3002
LIGC	258.273 76	−759.39	16.4048	1.027 49	5.8852
LIGCC	258.273 76	−759.39	16.4048	1.027 49	5.8852
LIGH	436.458 92	−1722.7	27.7226	1.736 36	3.4826
LIGO	422.388 68	−1847.5	26.8289	1.680 39	3.5986

LIGOH	378.378 88	−1429.2	24.0335	1.505 30	4.0171
HMWL	380.483 92	−958.26	24.1672	1.513 68	3.9949
ITANN	164.117 36	−616.98	10.4242	0.652 91	9.2617
TANN	304.256 08	−1079.7	19.3254	1.210 42	4.9958
Cellulose species					
CELL	162.1424	−1019.0	−1.5328	0.675 27	9.3745
CELLA	162.1424	−1019.0	−1.5328	0.675 27	9.3745
Hemicellulose Species					
XYHW	132.116 12	−759.2	−1.2489	0.550 22	11.5050
GMSW	132.116 12	−759.2	−1.2489	0.550 22	11.5050
HCE1	132.116 12	−759.2	−1.2489	0.550 22	11.5050
HCE2	132.116 12	−759.2	−1.2489	0.550 22	11.5050

Table S3. Estimated Fluid Property Model Parameters [31, 32].

Parameters	**3-hydroxypropanal**	**Triglyceride**	**P-coumaryl alcohol**	**Sinapyl aldehyde**	**Xylosan**
Molecular weight (kg/kmol)	74.079 44	897.4168	150.1772	208.213 88	132.116 12
Ideal gas enthalpy of formation (kJ/g mol)	−345.3	−1546.3	−193.5	−483.8	−642.3
Critical temperature (K)	605.0	934.6	791.4	837.9	744.3
Critical pressure (bar)	56.36	2.027	56.90	29.25	2.134
Acentric factor	1.133	2.084 19	1.198	0.981	0.292

Ideal Gas Heat Capacity Estimates (J/g mol-K)					
$C_p^{*, ig}$(298 K)	91.46	1304.35	177.30	240.85	142.76
$C_p^{*, ig}$(400 K)	109.33	1648.81	225.11	302.37	179.06
$C_p^{*, ig}$(500 K)	126.37	1950.68	264.73	357.37	215.39
$C_p^{*, ig}$(600 K)	141.02	2194.89	296.16	402.54	240.55
$C_p^{*, ig}$(800 K)	164.75	2564.01	342.81	471.36	281.03
$C_p^{*, ig}$ (1000 K)	182.00	2840.98	374.75	520.31	307.48
Aly−Lee $C_p^{*,ig}$ Equation Coefficients					
$C_{CP,1}$, J/(kmol K)	77 793.84	1 008 344	128 972.6	190 226.6	115 298.4
$C_{CP,2}$, J/(kmol K)	106 997.7	1 979 396	342 667.4	491 979.1	224 458.5
$C_{CP,3}$, K	814.165	777.2196	1575.222	1728.691	824.2086
$C_{CP,4}$, J/(kmol K)	66 750.56	1 165 050	266 861.9	371 592.6	59 411.96
$C_{CP,5}$, K	2048.402	2438.886	728.2816	797.2112	2302.592
$C_{CP,6}$, K	298	298.15	298	298	298
$C_{CP,7}$, K	1000	1500	1000	1000	1000
Extended Antoine Equation Coefficients (K/Pa)					
$C_{PL,1}$	136.9781	234.71	286.7075	286.6149	135.2637
$C_{PL,2}$	−13 924.84	−34 699	−25 124.63	−25 391.53	−14 336.53
$C_{PL,3}$	−15.464 95	−27.25	−37.267 39	−37.287 66	−15.745 01
$C_{PL,4}$	$1.303\ 768 \times 10^{-17}$	1.5475×10^{-18}	$1.486\ 27 \times 10^{-5}$	$1.361\ 18 \times 10^{-5}$	$2.245\ 921 \times 10^{-18}$
$C_{PL,5}$	6	6	2	2	6
$C_{PL,6}$	261.15	262.15	406.15	406.15	455.4
$C_{PL,7}$	605	934.6	791.4	837.9	744.3

Table S4. Product yield from simulation in Aspen Plus and experimental results.

Temperature (°C)	Experimental results			Simulation results		
	Biochar (wt%)	**Bio-oil (wt%)**	**Biogas (wt%)**	**Biochar (wt%)**	**Bio-oil (wt%)**	**Biogas (wt%)**
400	42.8	35.8	21.4	41.34	37.56	21.23
500	34.8	40.3	24.9	34.52	39.76	25.61
600	29.5	31.9	38.6	27.78	32.86	39.26

Table S5. Gas composition in Aspen Plus.

Temperature (°C)/ Components (vol%)	**400**	**500**	**600**
	Slow pyrolysis		
CO	59.5	40.1	33.9
CO_2	15.1	20.2	24.2
H_2	10.2	17.3	24.9
CH_4	14.2	20.7	15.5
C2-C3*	1.0	1.7	1.5

* - stands for C_2H_4, C_2H_6, C_3H_8