Supplementary Information

Lignin Fractionation from Laboratory to Commercialization: Chemistry, Scalability and Techno-economic Analysis

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Table S 1 Factors for estimation of capital expenditure

	Item	Percent
Direct cost as a percentage of bare equipment cost	Purchased Equipment	100%
	Purchased Equipment Erection	25%
	Instrumentation and Controls	8%
	Piping	16%
	Electrical Systems	15%
	Buildings	15%
	Yard Improvements	10%
	Service Facilities	30%
	Land	4%
	Sub-Total Direct Cost	223%
Indirect cost as a percentage of direct costs	Engineering	4.7%
	Construction Expenses	12.5%
	Legal Expenses	1.6%
	Contractor Fee	1.6%
	Contingency	7.8%
	Sub-Total Indirect Cost	28.1%

Table S 2 Mass balance of industrial-scale lignin fractionation using ethanol (t/day, stream numbers refer to Figure 8)

Stream	Description	Lignin	Solvent	Total
1	Lignin	150.0	-	150.0
2	Fresh solvent	-	6.6	6.6
3	Recovered solvent	-	1171.0	1171.0
4	Slurry to filter	150.0	1177.7	1327.7
5	Solution to evaporator	58.2	1138.3	1196.5
6	Wet filter cake to dryer	91.8	39.3	131.1
7	Lignin fraction I (high MW)	91.8	0.5	92.3
8	Solvent vapor to condenser	-	38.9	38.9
9	Solvent vapor to condenser	-	1123.8	1123.8
10	Solution to drum dryer	58.2	14.6	72.8
11	Lignin fraction II (low MW)	58.2	0.3	58.5
12	Solvent vapor to condenser	-	14.3	14.3
13	Solvent losses	-	5.9	5.9

Table S 3 Mass balance of industrial-scale lignin fractionation using methanol (t/day, stream numbers refer to Figure 8)

Stream	**Description**	**Lignin**	**Solvent**	**Total**
1	Lignin	150.0	-	150.0
2	Fresh solvent	-	12.6	12.6
3	Recovered solvent	-	2360.4	2360.4
4	Slurry to filter	150.0	2373.0	2523.0
5	Solution to evaporator	81.3	2343.6	2424.9
6	Wet filter cake to dryer	68.7	29.4	98.1
7	Lignin fraction I (high MW)	68.7	0.3	69.0
8	Solvent vapor to condenser	-	29.1	29.1
9	Solvent vapor to condenser	-	2323.2	2323.2
10	Solution to drum dryer	81.3	20.3	101.6
11	Lignin fraction II (low MW)	81.3	0.4	81.7
12	Solvent vapor to condenser	-	19.9	19.9
13	Solvent losses	-	11.9	11.9

Table S 4 Mass balance of industrial-scale lignin fractionation using methyl ethyl ketone (t/day, stream numbers refer to Figure 8)

Stream	**Description**	**Lignin**	**Solvent**	**Total**
1	Lignin	150.0	-	150.0
2	Fresh solvent	-	3.8	3.8
3	Recovered solvent	-	600.0	600.0
4	Slurry to filter	150.0	603.8	753.8
5	Solution to evaporator	42.2	557.5	599.7
6	Wet filter cake to dryer	107.9	46.2	154.1
7	Lignin fraction I (high MW)	107.9	0.5	108.4
8	Solvent vapor to condenser	-	45.7	45.7
9	Solvent vapor to condenser	-	547.0	547.0
10	Solution to drum dryer	42.2	10.5	52.7
11	Lignin fraction II (low MW)	42.2	0.2	42.4
12	Solvent vapor to condenser	-	10.3	10.3
13	Solvent losses	-	3.0	3.0

Table S 5 Costs of each equipment of the fractionation process

Equipment	Quantity	Bare equipment cost				Description
		Acetone	Ethanol	Methanol	MEK	
Fresh solvent storage tank	1	$177,899	$147,532	$203,907	$127,213	Vertical, shop fabrication, stainless steel 304
Fresh solvent pump	1	$10,430	$9,207	$11,422	$7,532	Progressive cavity, stainless steel, Double mesh seal
Recovered solvent storage tank	1	$155,068	$131,645	$179,595	$121,054	Vertical, shop fabrication, SS304
Recovered solvent pump	1	$10.456	$10,454	$10,429	$10,371	Horizontal, 1 stage, vertical split case, stainless steel 304, double mesh seal
Fractionation tank	1	$289,398	$240,397	$331,304	$203,303	Vertical, shop fabrication, stainless steel 304
Lignin + solvent solution pump	1	$19,063	$16,962	$20,756	$14,055	Horizontal, 1 stage, vertical split case, stainless steel 304, double mesh seal
Filter	4/5/4/6	$361,574	$389,664	$376,374	$385,393	Plate and Frame, stainless steel 304
Drum dryer	1	$330,013	$283,781	$322,431	$250,874	Double, vacuum, stainless steel 304, Area 55 -480 ft2
Rotary Dryer	1	$126,732	$219,902	$184,080	$193,508	Indirect gas fired, stainless steel 304
Lignin + solvent solution pump in	1	$18,770	$16,410	$20,496	$13,069	Horizontal, 1 stage, vertical split case, stainless steel 304, double mesh seal
Evaporator	1	$669,993	$807,144	$1,232,360	$399,218	Shell/Tube, small (5 - 100 ft2) stainless steel 304 150 Psi
Lignin + solvent solution pump out	1	$7,638	$6,734	$7,472	$6,029	Horizontal, 1 stage, vertical split case, stainless steel 304, double mesh seal
Condenser	1	$1,139,724	$1,193,561	$2,006,253	$580,845	Shell/tube, fixed / U, medium, CS shell, stainless steel 304 tube
Incinerator	1	$512,693	$378,775	$508,585	$262,624	Heater, stainless steel, 1500 Psia
Cooling tower	1	$786,731	$828,209	$1,476,407	$371,499	Induced draft, between 10 and 600 MBTU/h, carbon steel
Cooling tower pumps	2	$27,121	$28,030	$40,614	$16,760	Horizontal, 1 stage, vertical split case, stainless steel 304, double mesh seal
Silos F1	3	$162,778	$185,089	$167,232	$195,827	Shop fabrication, cone roof, stainless steel 304
Silos F2	3	$181,203	$157,800	$177,385	$140,950	Shop fabrication, cone roof, stainless steel 304
Total		**$6,787,085**	**$7,323,760**	**$9,136,075**	**$5,917,396**	

Note: the number of filters vary with the solvent used.

Equation derivation S1 Relation of weight average molecular weights between BCL and fractionated lignins

The weight average molecular weight is calculated using the following equation:

$$M_w = \frac{n_1 M_1^2}{\sum n_i M_i} + \frac{n_2 M_2^2}{\sum n_i M_i} + \frac{n_3 M_3^2}{\sum n_i M_i} + \frac{n_4 M_4^2}{\sum n_i M_i} + \dots + \frac{n_i M_i^2}{\sum n_i M_i}$$

Assume

$$Fraction\ I = n_1 M_1 + n_2 M_2 + n_3 M_3 = Yield_I * \sum n_i M_i$$

$$Fraction\ II = n_4 M_4 + \dots + n_i M_i = Yield_{II} * \sum n_i M_i$$

Then,

$$M_{wI} = \frac{n_1 M_1^2}{Yield_I \times \sum n_i M_i} + \frac{n_2 M_2^2}{Yield_I \times \sum n_i M_i} + \frac{n_3 M_3^2}{Yield_I \times \sum n_i M_i}$$

$$Yield_I \times M_{wI} = \frac{n_1 M_1^2}{\sum n_i M_i} + \frac{n_2 M_2^2}{\sum n_i M_i} + \frac{n_3 M_3^2}{\sum n_i M_i}$$

In analogy,

$$Yield_{II} \times M_{wII} = \frac{n_4 M_4^2}{\sum n_i M_i} + \dots + \frac{n_i M_i^2}{\sum n_i M_i}$$

Hence,

$$Yield_I \times M_{wI} + Yield_{II} \times M_{wII} = \left(\frac{n_1 M_1^2}{\sum n_i M_i} + \frac{n_2 M_2^2}{\sum n_i M_i} + \frac{n_3 M_3^2}{\sum n_i M_i}\right) + \left(\frac{n_4 M_4^2}{\sum n_i M_i} + \dots + \frac{n_i M_i^2}{\sum n_i M_i}\right)$$

$$Yield_I \times M_{wI} + Yield_{II} \times M_{wII} = M_w$$

Based on above equations, theoretically,

$$Yield_{sol} \times M_{w-sol} + Yield_{ins} \times M_{w-ins} = M_{w-BCL}$$

However, the weight average molecular weight of insoluble fraction is much higher than expected. We speculated that the lignin aggregation caused over estimation of its molecular weight.