Electronic Supplementary Material (ESI) for Green Chemistry.

System-level integrative analysis for production of Lignin hydrogels

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Supplementary material

Economic parameters and assumptions

Table S1 Economic parameters and assumptions

Kraft lignin price ($/ton) [1]	500.0
Dimethyl sulfoxide ($/ton) [2]	1600.0
DMAP ($/ton) [3]	13870.0
MAAH ($/ton) [3]	10240.0
Methanol ($/ton) [3]	330.0
SBMA ($/ton) [4]	10000.0
PEGDMA ($/ton) [5]	1000.0
ACVA ($/ton) [6]	3800.0
CNF ($/ton) [7]	3500.0
MBAAm ($/ton)[8]	2300.0
NIPAAm ($/ton)[9]	5000.0
AIBN ($/ton)[3]	7000.0
H_2SO_4 ($/ton)[10]	95.0
Water ($/ton)[1]	0.66
Wastewater treatment nutrients ($/ton)[11]	7953.4
Disposal of ash ($/ton)[12]	35.4
Boiler chemicals ($/ton)[11]	1260.4
Natural gas ($/ton)[13]	239
Cooling tower chemicals ($/ton)[10]	3933.5
Boiler efficiency (%)[11]	71.0
Turbo-generator efficiency (%)[11]	24.0
Plant financing by equity (%) [11]	40.0
Plant life (years) [11]	30.0
Income tax rate (%) [10]	21.0
Discount rate (%)	10.0
Interest rate for debt financing (%) [11]	8.0
Term for debt financing (years) [11]	10.0
General plant depreciation (years) [11]	7.0
Steam plant depreciation (years) [11]	20.0
Working capital (% of fixed capital investment) [11]	5.0
On-stream percentage after startup (%) [11]	90.0
Startup time (years) [11]	0.5
Revenue and costs during startup	
Revenue (% of normal) [11]	50.0
Variable costs (% of normal) [11]	75.0
Fixed costs (% of normal) [11]	100.0
Construction period (years) [11]	3.0
First 12 months' expenditures (%) [11]	8.0
Next 12 months' expenditures (%) [11]	60.0
Last 12 months' expenditures (%) [11]	32.0

Assumption:

■ 10 % of the catalyst is refurbished every 6 months at a cost equivalent to 20 % of its original value. [14]

■ Cost of Methacryloxyethyl sulfobetaine was used for SBMA. [15]

Important stream information

Table S2 Process stream information for grade A hydrogel

	5	10	13	14	15	22	24	25	29
Components mass fraction									
MAAH	0.01	0	0	0	0	0	0	0	0
Lignin	0.07	0	0.001	0	0	0	0	0	0
DMSO	0.76	0.12	0.89	0.002	0	0.10	0.006	0.12	0.12
DMAP	0.00	0	0.001	0	0	0	0	0	0
Lignin-MA	0.01	0.002	0.01	0	0	0.02	0	0	0
Methanol	0.07	0.86	0.01	0.99	1	0.73	0.04	0.87	0.87
PEGDMA	0.00	0	0	0	0	0.003	0	0	0
SBMA	0.002	0	0.002	0	0	0.03	0	0	0
CNF	0	0	0	0	0	0	0	0	0
ACVA	0	0	0	0	0	0	0	0	0
Hydrogel	0.06	0.01	0.07	0	0	0	0.40	0.001	0.001
Water	0.002	0.001	0.002	0.001	0	0.09	0.54	0.001	0.001
Total mass flow (ton/hr)	259.3	1630	219.5	1410.4	5.4	188.9	122.6	595	0.18
Temperature (°C)	90	61.6	168.5	60	25	72.2	70	70	70
Pressure (atm)	1	1	1	1	1	1	1	1	1

Table S3 Process stream information for grade B hydrogel

	7	8	9	10	11	12	15	16	17
Components mass fraction									
Lignin	0.003	0.001	0	0.03	0	0	0	0.03	0.03
NIPAAm	0.04	0.01	0	0.44	0	0.002	0	0.44	0.44
MBAAm	0.001	0	0	0.01	0	0	0	0.01	0.01
Water	0.94	0.94	0.95	0.43	0.95	0.12	1	0.43	0.43
AIBN	0.002	0	0	0.02	0	0	0	0.02	0.02
Hydrogel	0	0.04	0.04	0	0.04	0.87	0	0	0
H_2SO_4	0.001	0.001	0	0.05	0	0	0	0.05	0.05
Total mass flow (ton/hr)	7252.6	7252.6	7093.8	158.7	7093.8	332.4	6761.4	157.1	1.58
Temperature (°C)	83.6	65.0	65.0	65.0	80.0	110.0	85.0	65.0	65.0
Pressure (atm)	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0

Heat integration results

Table S4 Energy requirements of different sub-systems for grade A lignin hydrogel

	Heating		Cooling		Electricity	
	After (MW)	Before (MW)	After (MW)	Before (MW)	After (MW)	Before (MW)
Recovery of solvents	74.7	459.4	124.8	486.2	28.4	28.4
Hydrogel production	0	3.5	0	24.1	0	0
Lignin methacrylate production	0	0	0	2.7	0	0
Total	74.7	462.9	124.8	513	28.4	28.4

Table S5 Energy requirements of different sub-systems for grade B lignin hydrogel

	Heating		Cooling		Electricity	
	After (MW)	Before (MW)	After (MW)	Before (MW)	After (MW)	Before (MW)
Recovery of solvents	16.2	4571.5	403.5	4669	263.9	263.9
Hydrogel production	0	2.1	0	292.1	0	0
Total	16.2	4573.6	403.5	4961.1	263.9	263.9

Project cost, Discounted cash flow and Uncertainty analysis

Table S6 Project cost worksheet for grade A hydrogel

Subsystems			Installed cost
Lignin methacrylate production			$ 15,308,179
Separation of lignin methacrylate			$ 12,553,121
Recovery of solvents			$ 350,085,042
Hydrogel production			$ 18,229,149
Wastewater treatment			$ 2,335,412
Storage			$ 8,040,849
Heat and power generation			$ 43,877,930
Utilities			$ 1,085,163
Total installed equipment cost			**$ 451,514,844**
Warehouse	4.0%	of ISBL†	$ 15,847,020
Site development	9.0%	of ISBL†	$ 35,655,794
Additional piping	4.5%	of ISBL†	$ 17,827,897
Total direct cost (TDC)			$ **520,845,555**
Prorateable expenses	10.0%	of TDC	$ 52,084,556
Field expenses	10.0%	of TDC	$ 52,084,556
Home office & construction fee	20.0%	of TDC	$ 104,169,111
Project contingency	10.0%	of TDC	$ 52,084,556
Other costs (start-up, permits, etc.)	10.0%	of TDC	$ 52,084,556
Total indirect cost			**$ 312,507,333**
Fixed capital investment (FCI)			**$ 833,352,888**
Land	2.0%	of FCI	$ 16,667,058
Working capital	5.0%	of FCI	$ 41,667,644
Total capital investment (TCI)			**$ 891,687,591**

† Inside battery limits (ISBL): Lignin methacrylate production, Separation of lignin methacrylate, Recovery of solvents, and Hydrogel production. All values are represented in 2016 US $.

Table S7 Project cost worksheet for grade B hydrogel

Subsystems				Installed cost
Hydrogel production			$	39,206,866
Recovery of solvents			$	1,240,033,721
Wastewater treatment			$	6,751,703
Storage			$	15,700,207
Heat and power generation			$	136,736,468
Utilities			$	2,382,025
Total installed equipment cost			**$**	**1,440,810,991**
Warehouse	4.0%	of ISBL†	$	51,169,623
Site development	9.0%	of ISBL†	$	115,131,653
Additional piping	4.5%	of ISBL†	$	57,565,826
Total direct cost (TDC)			$	**1,664,678,093**
Prorateable expenses	10.0%	of TDC	$	166,467,809
Field expenses	10.0%	of TDC	$	166,467,809
Home office & construction fee	20.0%	of TDC	$	332,935,619
Project contingency	10.0%	of TDC	$	166,467,809
Other costs (start-up, permits, etc.)	10.0%	of TDC	$	166,467,809
Total indirect cost			**$**	**998,806,856**
Fixed capital investment (FCI)			**$**	**2,663,484,950**
Land	2.0%	of FCI	$	53,269,699
Working capital	5.0%	of FCI	$	133,174,247
Total capital investment (TCI)			**$**	**2,849,928,896**

† Inside battery limits (ISBL): Hydrogel production, and Recovery of solvents. All values are represented in 2016 US $.

Table S8 Discounted cash flow analysis for grade A hydrogel

Year	-2	-1	0	1	2	3	4	5	6	7	8
Fixed capital investment	26,667,292	200,004,693	106,669,170								
Land	16,667,058										
Working capital			41,667,644								
Loan payment				74,516,493	74,516,493	74,516,493	74,516,493	74,516,493	74,516,493	74,516,493	74,516,493
Loan interest payment	3,200,075	27,200,638	40,000,939	40,000,939	37,239,694	34,257,550	31,036,835	27,558,462	23,801,820	19,744,646	15,362,898
Loan principal	40,000,939	340,007,978	500,011,733	465,496,179	428,219,380	387,960,438	344,480,780	297,522,749	246,808,076	192,036,229	132,882,635
Total annual hydrogel sales				2,012,489,767	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689
Annual manufacturing cost											
Feedstock				53,462,390	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186
Other variable costs				2,137,727,976	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687
Fixed operating costs				23,823,352	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352
Total product cost				2,215,013,717	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225
Annual depreciation											
General plant writedown				14.29%	24.49%	17.49%	12.49%	8.93%	8.92%	8.93%	4.46%
Depreciation charge				112,815,972	193,342,417	138,079,170	98,605,422	70,500,114	70,421,166	70,500,114	35,210,583
Remaining value				676,658,987	483,316,569	345,237,399	246,631,977	176,131,863	105,710,697	35,210,583	0
Steam plant writedown				3.75%	7.22%	6.68%	6.18%	5.71%	5.29%	4.89%	4.52%
Depreciation charge				1,645,422	3,167,548	2,929,729	2,710,340	2,506,746	2,318,949	2,144,753	1,984,160
Remaining value				42,232,508	39,064,960	36,135,231	33,424,891	30,918,145	28,599,196	26,454,443	24,470,283
Net revenue				-356,986,283	-88,654,195	-30,170,986	12,742,867	44,530,142	48,553,529	52,705,951	92,537,823
Losses forward					-356,986,283	-445,640,479	-475,811,464	-463,068,597	-418,538,456	-369,984,926	-317,278,975
Taxable income				-356,986,283	-445,640,479	-475,811,464	-463,068,597	-418,538,456	-369,984,926	-317,278,975	-224,741,153
Income tax				0	0	0	0	0	0	0	0
Annual cash income				-277,040,444	70,578,971	70,578,971	70,578,971	70,578,971	70,578,971	70,578,971	70,578,971
Discount factor	1.2100	1.1000	1.0000	0.9091	0.8264	0.7513	0.6830	0.6209	0.5645	0.5132	0.4665
Annual present value				-251,854,949	58,329,728	53,027,026	48,206,387	43,823,988	39,839,989	36,218,172	32,925,611
Total capital investment + interest	56,306,655	249,925,865	188,337,753								
Net present worth			0								

Year	9	10	11	12	13	14	15	16	17	18	19
Fixed capital investment											
Land											
Working capital											
Loan payment	74,516,493	74,516,493	0	0	0	0	0	0	0	0	0
Loan interest payment	10,630,611	5,519,740	0	0	0	0	0	0	0	0	0
Loan principal	68,996,753	0	0	0	0	0	0	0	0	0	0
Total annual hydrogel sales	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689
Annual manufacturing cost											
Feedstock	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186
Other variable costs	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687
Fixed operating costs	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352
Total product cost	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225
Annual depreciation											
General plant writedown											
Depreciation charge											
Remaining value											
Steam plant writedown	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%
Depreciation charge	1,957,833	1,957,394	1,957,833	1,957,394	1,957,833	1,957,394	1,957,833	1,957,394	1,957,833	1,957,394	1,957,833
Remaining value	22,512,450	20,555,055	18,597,222	16,639,827	14,681,994	12,724,600	10,766,767	8,809,372	6,851,539	4,894,144	2,936,311
Net revenue	132,507,020	137,618,329	143,137,631	143,138,070	143,137,631	143,138,070	143,137,631	143,138,070	143,137,631	143,138,070	143,137,631
Losses forward	-224,741,153	-92,234,133	0	0	0	0	0	0	0	0	0
Taxable income	-92,234,133	45,384,197	143,137,631	143,138,070	143,137,631	143,138,070	143,137,631	143,138,070	143,137,631	143,138,070	143,137,631
Income tax	0	9,530,681	30,058,902	30,058,995	30,058,902	30,058,995	30,058,902	30,058,995	30,058,902	30,058,995	30,058,902
Annual cash income	70,578,971	61,048,290	115,036,562	115,036,469	115,036,562	115,036,469	115,036,562	115,036,469	115,036,562	115,036,469	115,036,562
Discount factor	0.4241	0.3855	0.3505	0.3186	0.2897	0.2633	0.2394	0.2176	0.1978	0.1799	0.1635
Annual present value	29,932,374	23,536,758	40,319,613	36,654,164	33,321,994	30,292,698	27,538,838	25,035,287	22,759,370	20,690,320	18,809,397
Total capital investment + interest											
Net present worth											

Year	20	21	22	23	24	25	26	27	28	29	30
Fixed capital investment											
Land											-16,667,058
Working capital											-41,667,644
Loan payment	0	0	0	0	0	0	0	0	0	0	0
Loan interest payment	0	0	0	0	0	0	0	0	0	0	0
Loan principal	0	0	0	0	0	0	0	0	0	0	0
Total annual hydrogel sales	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689	2,683,319,689
Annual manufacturing cost											
Feedstock	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186
Other variable costs	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687	2,443,117,687
Fixed operating costs	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352	23,823,352
Total product cost	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225	2,538,224,225
Annual depreciation											
General plant writedown											
Depreciation charge											
Remaining value											
Steam plant writedown	4.46%	2.23%									
Depreciation charge	1,957,394	978,917									
Remaining value	978,917	0									
Net revenue	143,138,070	144,116,547	145,095,464	145,095,464	145,095,464	145,095,464	145,095,464	145,095,464	145,095,464	145,095,464	145,095,464
Losses forward	0	0	0	0	0	0	0	0	0	0	0
Taxable income	143,138,070	144,116,547	145,095,464	145,095,464	145,095,464	145,095,464	145,095,464	145,095,464	145,095,464	145,095,464	145,095,464
Income tax	30,058,995	30,264,475	30,470,047	30,470,047	30,470,047	30,470,047	30,470,047	30,470,047	30,470,047	30,470,047	30,470,047
Annual cash income	115,036,469	114,830,989	114,625,417	114,625,417	114,625,417	114,625,417	114,625,417	114,625,417	114,625,417	114,625,417	114,625,417
Discount factor	0.1486	0.1351	0.1228	0.1117	0.1015	0.0923	0.0839	0.0763	0.0693	0.0630	0.0573
Annual present value	17,099,438	15,517,177	14,081,271	12,801,155	11,637,414	10,579,467	9,617,697	8,743,361	7,948,510	7,225,918	6,569,017
Total capital investment + interest											-3,343,077
Net present worth											

Table S9 Discounted cash flow analysis for grade B hydrogel

Year	-2	-1	0	1	2	3	4	5	6	7	8
Fixed capital investment	85,231,518	639,236,388	340,926,074								
Land	53,269,699										
Working capital			133,174,247								
Loan payment				238,162,680	238,162,680	238,162,680	238,162,680	238,162,680	238,162,680	238,162,680	238,162,680
Loan interest payment	10,227,782	86,936,149	127,847,278	127,847,278	119,022,045	109,490,795	99,197,044	88,079,793	76,073,162	63,106,000	49,101,466
Loan principal	127,847,278	1,086,701,859	1,598,090,970	1,487,775,567	1,368,634,932	1,239,963,047	1,100,997,411	950,914,523	788,825,005	613,768,325	424,707,111
Total annual hydrogel sales				8,822,607,004	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005
Annual manufacturing cost											
Feedstock				53,462,390	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186
Other variable costs				9,731,108,304	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633
Fixed operating costs				63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229
Total product cost				9,847,696,923	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048
Annual depreciation											
General plant writedown				14.29%	24.49%	17.49%	12.49%	8.93%	8.92%	8.93%	4.46%
Depreciation charge				361,072,358	618,800,703	441,928,309	315,590,885	225,638,639	225,385,965	225,638,639	112,692,982
Remaining value				2,165,676,123	1,546,875,420	1,104,947,111	789,356,226	563,717,586	338,331,622	112,692,982	0
Steam plant writedown				3.75%	7.22%	6.68%	6.18%	5.71%	5.29%	4.89%	4.52%
Depreciation charge				5,127,618	9,871,006	9,129,894	8,446,212	7,811,754	7,226,522	6,683,679	6,183,223
Remaining value				131,608,851	121,737,845	112,607,951	104,161,739	96,349,985	89,123,463	82,439,784	76,256,561
Net revenue				-1,519,137,172	-239,893,797	-52,749,041	84,565,816	186,269,770	199,114,308	212,371,638	339,822,285
Losses forward					-1,519,137,172	-1,759,030,970	-1,811,780,011	-1,727,214,195	-1,540,944,425	-1,341,830,117	-1,129,458,479
Taxable income				-1,519,137,172	-1,759,030,970	-1,811,780,011	-1,727,214,195	-1,540,944,425	-1,341,830,117	-1,129,458,479	-789,636,193
Income tax				0	0	0	0	0	0	0	0
Annual cash income				-1,263,252,599	269,637,277	269,637,277	269,637,277	269,637,277	269,637,277	269,637,277	269,637,277
Discount factor	1.2100	1.1000	1.0000	0.9091	0.8264	0.7513	0.6830	0.6209	0.5645	0.5132	0.4665
Annual present value				-1,148,411,454	222,840,724	202,582,477	184,165,888	167,423,535	152,203,213	138,366,557	125,787,780
Total capital investment + interest	179,962,089	798,789,790	601,947,599								
Net present worth			0								

Year	9	10	11	12	13	14	15	16	17	18	19
Fixed capital investment											
Land											
Working capital											
Loan payment	238,162,680	238,162,680	0	0	0	0	0	0	0	0	0
Loan interest payment	33,976,569	17,641,680	0	0	0	0	0	0	0	0	0
Loan principal	220,521,000	0	0	0	0	0	0	0	0	0	0
Total annual hydrogel sales	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005
Annual manufacturing cost											
Feedstock	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186
Other variable costs	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633
Fixed operating costs	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229
Total product cost	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048
Annual depreciation											
General plant writedown											
Depreciation charge											
Remaining value											
Steam plant writedown	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%
Depreciation charge	6,101,181	6,099,814	6,101,181	6,099,814	6,101,181	6,099,814	6,101,181	6,099,814	6,101,181	6,099,814	6,101,181
Remaining value	70,155,380	64,055,566	57,954,385	51,854,571	45,753,390	39,653,576	33,552,395	27,452,581	21,351,399	15,251,586	9,150,404
Net revenue	467,722,207	484,058,463	501,698,775	501,700,143	501,698,775	501,700,143	501,698,775	501,700,143	501,698,775	501,700,143	501,698,775
Losses forward	-789,636,193	-321,913,987	0	0	0	0	0	0	0	0	0
Taxable income	-321,913,987	162,144,476	501,698,775	501,700,143	501,698,775	501,700,143	501,698,775	501,700,143	501,698,775	501,700,143	501,698,775
Income tax	0	34,050,340	105,356,743	105,357,030	105,356,743	105,357,030	105,356,743	105,357,030	105,356,743	105,357,030	105,356,743
Annual cash income	269,637,277	235,586,937	402,443,214	402,442,927	402,443,214	402,442,927	402,443,214	402,442,927	402,443,214	402,442,927	402,443,214
Discount factor	0.4241	0.3855	0.3505	0.3186	0.2897	0.2633	0.2394	0.2176	0.1978	0.1799	0.1635
Annual present value	114,352,527	90,828,962	141,053,891	128,230,719	116,573,464	105,975,801	96,341,706	87,583,306	79,621,244	72,382,898	65,802,681
Total capital investment + interest											
Net present worth											

Year	20	21	22	23	24	25	26	27	28	29	30
Fixed capital investment											
Land											-53,269,699
Working capital											-133,174,247
Loan payment	0	0	0	0	0	0	0	0	0	0	0
Loan interest payment	0	0	0	0	0	0	0	0	0	0	0
Loan principal	0	0	0	0	0	0	0	0	0	0	0
Total annual hydrogel sales	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005	11,763,476,005
Annual manufacturing cost											
Feedstock	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186	71,283,186
Other variable costs	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633	11,121,266,633
Fixed operating costs	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229	63,126,229
Total product cost	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048	11,255,676,048
Annual depreciation											
General plant writedown											
Depreciation charge											
Remaining value											
Steam plant writedown	4.46%	2.23%									
Depreciation charge	6,099,814	3,050,591									
Remaining value	3,050,591	0									
Net revenue	501,700,143	504,749,366	507,799,957	507,799,957	507,799,957	507,799,957	507,799,957	507,799,957	507,799,957	507,799,957	507,799,957	507,799,957
Losses forward	0	0	0	0	0	0	0	0	0	0	0	0
Taxable income	501,700,143	504,749,366	507,799,957	507,799,957	507,799,957	507,799,957	507,799,957	507,799,957	507,799,957	507,799,957	507,799,957	507,799,957
Income tax	105,357,030	105,997,367	106,637,991	106,637,991	106,637,991	106,637,991	106,637,991	106,637,991	106,637,991	106,637,991	106,637,991	106,637,991
Annual cash income	402,442,927	401,802,590	401,161,966	401,161,966	401,161,966	401,161,966	401,161,966	401,161,966	401,161,966	401,161,966	401,161,966	401,161,966
Discount factor	0.1486	0.1351	0.1228	0.1117	0.1015	0.0923	0.0839	0.0763	0.0693	0.0630	0.0573	
Annual present value	59,820,577	54,295,813	49,281,132	44,801,029	40,728,208	37,025,644	33,659,676	30,599,706	27,817,914	25,289,013	22,990,012	
Total capital investment + interest											-10,684,833	
Net present worth												

Procedure adopted for Uncertainty analysis

Uncertainty analysis was studied through Monte Carlo simulation in which the cumulative probability curves have been generated by following the protocol as suggested by Turton et al.[16] In this analysis, it has been assumed that the parameters follow a triangular distribution by maintaining same range of variation.[17]

Procedure

(1) Selection of influential parameters and the range of their variation

(2) Generation of random numbers based on triangular distribution and range of variation

(3) Assigning random numbers to the influential parameters

(4) Calculation of cumulative probability

(5) Iteration of steps (1-3) for 10,000 times

(6) Construction of a cumulative probability curve from the generated data.

LCA inventory data and results

Table S10 Data set derived from EcoInvent 3 database

Materials	Name of data set	Database
Ash	Dummy_Disposal, fly ash, to unspecified landfill/kg/RNA	Ecoinvent 3
Biomass	Wood chips, wet, measured as dry mass {RoW} | market for | Cut-off, U	Ecoinvent 3
CO_2	Carbon dioxide	Ecoinvent 3
Electricity	Electricity, high voltage {GLO} | market for | Cut-off, U	Ecoinvent 3
H_2O	Water/m3	Ecoinvent 3
Natural gas	Heat, district or industrial, natural gas {GLO} | market for | Cut-off, U	Ecoinvent 3
Sulfuric acid	Sulfuric acid {GLO} | market for | Cut-off, U	Ecoinvent 3
SBMA	Methyl methacrylate {GLO}| market for | Cut-off, U	Ecoinvent 3
ACVA	Cyanoacetic acid {GLO}| market for | Cut-off, U	Ecoinvent 3
MBAAm	Polyacrylamide {GLO}| market for | Cut-off, U	Ecoinvent 3
AIBN	Acrylonitrile {GLO}| market for | Cut-off, U	Ecoinvent 3
DMSO	Dimethyl sulfoxide {GLO}| market for | Cut-off, U	Ecoinvent 3
Methacrylic acid	Methacrylic acid {GLO}| market for | Cut-off, U	Ecoinvent 3
Acetic anhydride	Acetic anhydride {RoW}| market for | Cut-off, U	Ecoinvent 3
Polyethylene glycol	Triethylene glycol {GLO}| market for | Cut-off, U	Ecoinvent 3
CNF	Carboxymethyl cellulose, powder {GLO}| market for | Cut-off, U	Ecoinvent 3
Water	Water, process, unspecified natural origin	Ecoinvent 3
Methanol	Methanol {GLO}| market for | Cut-off, U	Ecoinvent 3
Acrylonitrile	Acrylonitrile {GLO}| market for | Cut-off, U	Ecoinvent 3
Isopropanol	Isopropanol {GLO}| market for| Cut-off, U	Ecoinvent 3
NaOH	Neutralising agent, sodium hydroxide-equivalent {GLO}| market for| Cut-off, U	Ecoinvent 3
CaO	Quicklime, milled, loose {RoW}| market for quicklime, milled, loose | Cut-off, U	Ecoinvent 3
H_2O_2 (50%)	Hydrogen peroxide, without water, in 50% solution state {GLO} market for | Cut-off, U	Ecoinvent 3
$NaClO_3$	Sodium hypochlorite, without water, in 15% solution state {GLO}| market for | Cut-off, U	Ecoinvent 3
CH_3OH	Methanol {GLO}| market for | Cut-off, U	Ecoinvent 3
CO_2 (liquid)	Carbon dioxide, liquid {RoW}| market for | Cut-off, U	Ecoinvent 3
SO_2	Sulfur dioxide	Ecoinvent 3

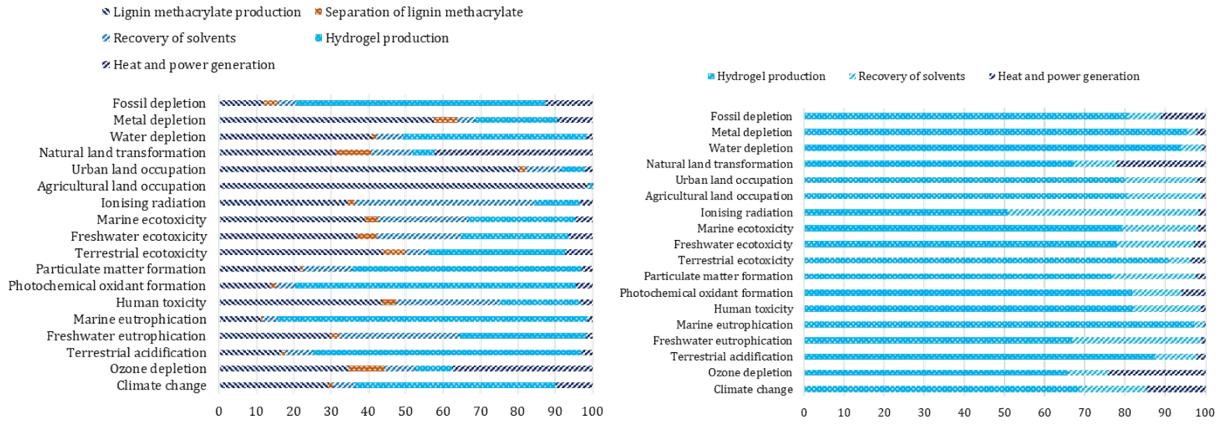

Fig. S1 Contribution of different sub-systems (represented in %) involved in lignin hydrogel production towards 18 different categories summarizing environmental impact

Table S11 Comparison of environmental impact in terms of different sub-systems involved in lignin hydrogel production (Grade A hydrogel)

		Lignin methacrylate production	Separation of lignin methacrylate	Recovery of solvents	Hydrogel production	Heat and power generation
Climate change	kg CO2 eq.	0.848	0.029	0.177	1.544	0.286
Ozone depletion	kg CFC-11 eq	0.000	0.000	0.000	0.000	0.000
Terrestrial acidification	kg SO2 eq.	0.002	0.000	0.001	0.007	0.000
Freshwater eutrophication	kg P eq.	0.000	0.000	0.000	0.000	0.000

Marine eutrophication	kg N eq.	0.000	0.000	0.000	0.001	0.000
Human toxicity	kg 1,4-DB eq.	0.097	0.009	0.061	0.048	0.008
Photochemical oxidant formation	kg NMVOC	0.001	0.000	0.000	0.006	0.000
Particulate matter formation	kg PM10 eq.	0.001	0.000	0.000	0.002	0.000
Terrestrial ecotoxicity	kg 1,4-DB eq.	0.000	0.000	0.000	0.000	0.000
Freshwater ecotoxicity	kg 1,4-DB eq.	0.003	0.000	0.002	0.002	0.000
Marine ecotoxicity	kg 1,4-DB eq.	0.003	0.000	0.002	0.002	0.000
Ionising radiation	kBq U235 eq	0.017	0.001	0.024	0.006	0.002
Agricultural land occupation	m^2a	0.547	0.000	0.004	0.004	0.000
Urban land occupation	m^2a	0.009	0.000	0.001	0.001	0.000
Natural land transformation	m^2	0.000	0.000	0.000	0.000	0.000
Water depletion	m^3	0.006	0.000	0.001	0.008	0.000
Metal depletion	kg Fe eq.	0.013	0.001	0.001	0.005	0.002
Fossil depletion	kg oil eq.	0.104	0.033	0.044	0.586	0.110

Table S12 Comparison of environmental impact in terms of different sub-systems involved in lignin hydrogel production (Grade B hydrogel)

		Hydrogel production	Solvent recovery	Heat and power generation
Climate change	kg CO2 eq	2.483	0.605	0.530
Ozone depletion	kg CFC-11 eq	0.000	0.000	0.000
Terrestrial acidification	kg SO2 eq	0.021	0.002	0.001
Freshwater eutrophication	kg P eq	0.001	0.000	0.000
Marine eutrophication	kg N eq	0.005	0.000	0.000
Human toxicity	kg 1,4-DB eq	1.026	0.210	0.014
Photochemical oxidant formation	kg NMVOC	0.009	0.001	0.001
Particulate matter formation	kg PM10 eq	0.006	0.002	0.000
Terrestrial ecotoxicity	kg 1,4-DB eq	0.000	0.000	0.000
Freshwater ecotoxicity	kg 1,4-DB eq	0.023	0.006	0.001
Marine ecotoxicity	kg 1,4-DB eq	0.022	0.005	0.001
Ionising radiation	kBq U235 eq	0.090	0.084	0.003
Agricultural land occupation	m^2a	0.058	0.013	0.001

Urban land occupation	m^2a	0.017	0.004	0.000
Natural land transformation	m^2	0.000	0.000	0.000
Water depletion	m^3	0.064	0.004	0.000
Metal depletion	kg Fe eq.	0.182	0.004	0.004
Fossil depletion	kg oil eq.	1.483	0.151	0.204

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