

1 **Electronic Supplementary Information (ESI)**

2 **Life cycle assessment and techno-economic analysis of the utilization**
3 **of bio-oil components for the production of three chemicals**

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37 1 The procedures of the techno-economic-environmental analysis

38 1.1 Methodology for estimation of the total-capital investment

39 **Table S1** Methodology for total-capital investment for nth plant

Item	Percent of TDEC
Total purchased equipment-delivered cost	100%
Purchased equipment installation	39%
Instrumentation and controls (installed)	13%
Piping (installed)	31%
Electrical systems (installed)	10%
Buildings (including services)	29%
Yard improvements	10%
Service facilities (installed)	55%
Total installed cost (TIC)	287%
Land (if purchase is required)	6%
Engineering and supervision	32%
Construction expenses	34%
Total direct and indirect plant costs (TDIC)	359%
Contractor's fee (CF)	5% of TDIC
Contingency (CO)	10% of TDIC
Fixed-capital investment (FCI)	TDIC+CF+CO
Working capital	15% of FCI
Total capital investment	475%

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41 The total installed equipment cost is part of the total capital investment. The total
42 capital investment for all processes consists of fixed-capital investment for physical
43 equipment and facilities in the plant plus working capital which must be available to
44 pay salaries, keep raw materials and products on hand, and handle other special items
45 requiring a direct cash outlay. This method for estimating the total-capital investment
46 is based on the percentage of delivered-equipment cost. Namely, the determination of
47 the delivered-equipment cost is required firstly. The other items included in the fixed-
48 capital investment are estimated as percentages of the delivered-equipment cost , and
49 the working capital amounts to 15 percent of the fixed-capital investment.¹ The items
50 included in the total-capital investment and the corresponding ratio factors based on
51 delivered equipment cost are listed in Table S1. Unit process principles are used to
52 determine the equipment specifications,^{1, 2} and then the delivered-equipment cost of
53 each piece of the process equipments can be estimated from appropriate
54 manufacturers' bulletins, published cost data, empirical rules¹⁻³ or e-commerce
55 websites (such as Alibaba) as listed in Table S2.

56 **Table S2** The delivered-equipment cost of each piece of the process equipments

Equipments	Specification	Delivered-equipment cost
<i>Sub 1</i>		
Chopper	50 kw/ton	\$44,137
Biomass Chopping Screen	60 ton/day	\$3,286
Grinding Hammer Mill	50 kw/ton	\$44,137
Biomass Grinding Screen	60 ton/day	\$3,359
Belt Press	5.5 kw	\$19,425
Bale Moving Forklift*4	1.25 ton/h	\$14,021
Concrete Storage Slab	30 m*29 m*3.5 m	\$87,631
Discharge Conveyor	0.75 kw/ton	\$9,785
Bale Transport Conveyor	90 w/ton	\$77,845
Bale Unwrapping Conveyor	5.5 kw	\$29,210
Continuous Spray Rotary Drum	2.2 kw, 2.5 ton/h	\$185,089
Rotary Dryer	2.2 kw	\$99,519
Biomass Feeding Bin	Φ1.5*4.3 m	\$6,047
Screw Feeder	0.75 kw/ton	\$23,733
Pyrolysis Fluid Bed	Φ1.2 m*2 m	\$122,099
Non-condensable Gas Blower	90 kw	\$31,357
Pyrolysis Vapor Cyclones*2	3600 m ³ of gas per hour	\$184,316
Bio-oil Condenser*2	600 m ² of heat transfer area	\$291,722
Electro-Static Precipitator	30 kw	\$42,705
Condenser Water Pump*3	90 kw	\$62,527
Ice making machine	53 /kw, 592 kg of ice per hour	\$20,000
Condenser Oil Pump	5 kw	\$6,952
Cooling Tower	Φ 8.8m*6.5m	\$438,898
Wash Percolater	4 m ³	\$31,459
Solids Combustor	Φ0.3 m*0.8 m	\$35,680
Combustor Cyclones	3360 m ³ of gas per hour	\$161,343
Combustion Gas Blower	85 kw	\$9,084
<i>Sub 2</i>		
Settling Tank	3 m ³	\$35,965
Filter, vacuum rotary drum	3 kw, 600 kg of filtrate /(m ² .h)	\$185,089
Vacuum pump	10 kw	\$28,655
Settling Tank	3 m ³	\$35,965
Filter, vacuum rotary drum	3 kw, 600 kg of filtrate /(m ² .h)	\$185,089
Vacuum pump	10 kw	\$28,655
Mixer	10 kw, 3m ³	\$73,805
Vacuum freeze dryer	130 kw, 1.2 ton water per hour	\$365,261
Mixer	10 kw, 3 m ³	\$73,805
Filter, vacuum rotary drum	3 kw, 600 kg of filtrate /(m ² .h)	\$185,089
Evaporation crystallizer	1000 kg of acetic ether per	\$452,879
Settling Tank	3 m ³	\$35,965

Filter, vacuum rotary drum	3 kw, 600 kg of filtrate /(m ² .h)	\$185,089
Vacuum pump	10 kw	\$28,655
<i>Sub 3</i>		
Mixer*2	10 kw, 3 m ³	\$147,610
<i>Sub 4</i>		
Evaporator	600 kg of water per hour	\$349,285
Mixer	10 kw, 3 m ³	\$73,805
Evaporator	600 kg of water per hour	\$349,285
Mixer*4	3 kw, 0.8 m ³	\$104,268
Filter, vacuum rotary drum*4	3 kw, 75 kg of filtrate /(m ² .h)	\$212,611
Vacuum pump*4	10 kw	\$114,620
Evaporator*2	50 kg of methanol per hour	\$190,110

57 **1.2 Methodology for estimation of the operating cost and direct production cost**

58 **Table S3** Variable costs employed in the estimation of the direct production costs

59 (Source: www.alibaba.com and refs).⁴⁻⁶

Item	Value
Cotton straw	\$83/metric ton
Fertilizer	\$400/metric ton
Transport	\$0.71/(ton.mile)
Sulfuric acid 98 wt.%	\$300/metric ton
Process water	\$1.0/metric ton
Activated carbon	\$1500/metric ton
Calcium hydroxide	\$110/metric ton
Hydrochloric acid 32 wt.%	\$190/metric ton
Ethyl acetate	\$1200/metric ton
Calcium oxide	\$160/metric ton
Methanol	\$700/metric ton
Sodium hydroxide	\$500/metric ton
Phenol	\$1300/metric ton
Formaldehyde 37 wt.%	\$400/metric ton
Cooling water from river	\$0.15/metric ton
Average hourly wage	\$21/h
Electricity	\$0.061/kwh
Steam (6 bar)	\$20/metric ton
Solids disposal cost	\$22.23/metric
Waste water disposal cost	\$1.30/metric ton

60 The operating cost is divided into three classifications as follows: (1) direct
61 production costs, which mainly involve expenditures for raw materials, direct
62 operating labor, supervisory and clerical labor directly connected to the
63 manufacturing operation, utilities, plant maintenance and repairs. Some variable cost
64 parameters, such as the prices of cotton straw, phenol, and utilities, average hourly

65 wage and water treatment cost, are listed on the Table S3; (2) fixed charges,
 66 essentially include expenses directly associated with depreciation, property taxes,
 67 insurance. Some assumptions for the estimation of fixed charges, such as depreciation
 68 period, type of depreciation and property tax rate, are listed on the Table S4; (3)
 69 plant-overhead costs, which are used for medical services, warehouses, safety services,
 70 warehouses and so on. The estimation of fixed charges and plant-overhead costs can
 71 be based on the method of 'Percentage of total-capital investment'.⁷ However the
 72 estimation of direct production costs is slightly complex. Chemical engineering
 73 principles, such as material balance and energy balance, and the methodology
 74 proposed by Overcash et.al are used for calculation of the expenditures for raw
 75 materials and utilities.⁸ The method of estimating labor requirements is based on
 76 adding up the various principal processing steps on the flow sheet and plant capacity,
 77 and the cost for direct supervisory and clerical labor averages about 15 percent of the
 78 cost for operating labor.¹ The method for estimation of the expenditures for plant
 79 maintenance and repairs is the same as that for estimation of fixed charges.

80 **Table S4** Assumptions for the estimation of the fixed charges

Item	Value/method
Equipment depreciation period	20 years
Building depreciation period	40 years
Amortization period	5 years
Type of depreciation or amortization	Straight-line
Property tax rate	2% of FCI
Insurance rate	1% of FCI

81 **1.3 Methodology for estimation of cash flow and IRR**

82 **Table S5** Assumptions or parameters for the calculation of IRR

Item	Value
Service life	20 years
Construction period	1 years
Income tax rate	39%
Annual capacity in the first year	30%
Annual capacity in the second year	50%
Annual capacity in the third year	80%
Salvage value at end of service life	Working capital+land+salvage value of buildings
Levogluosan	15\$/kg
Renewable phenol resin	2800\$/metric ton
Road de-icer	700\$/metric ton

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84 The 20-year facility IRR is calculated on the basis of a cash flow sheet in order
 85 to perform a profitability evaluation.¹ The determination or estimation of the market
 86 prices for the three chemicals is important for calculation of IRR. Levoglucosan is
 87 advertised for sale at \$1500/kg and \$20~90/kg on the carbosynth's Web site and the
 88 Alibaba Web site, respectively.^{9, 10} The purity of the levoglucosan sold at the
 89 carbosynth's Web site is 3% higher than that of the levoglucosan produced via the
 90 process. Moreover, from an economic perspective, mass production will lower the
 91 cost. Therefore, the price of the levoglucosan produced via the process is set at \$15/kg
 92 in this analysis. The phenolic resins from America are priced around \$4000/ton
 93 (¥25.5/kg) on the Guidechem Web site.¹¹ Considering that about 50wt% of the phenol
 94 used in the renewable phenol resin produced via the process is replaced and the
 95 phenolic resin is not as good as those phenolic resins based on petrochemical
 96 synthesis in quality and performance, the renewable phenol resin was valued at
 97 \$2800/ton. Food grade calcium acetate is priced at about \$1200/ton on the Alibaba
 98 Web site.¹² The deicer produced via the process is, at best, an industrial grade mixture
 99 of calcium salts. Hence the mixture is pegged at \$700/ton. Some necessary parameters
 100 for the calculation of the cash flow sheet, such as construction period, income tax rate
 101 and product prices, are showed in Table S5.

102 Moreover, the cash flow sheet also involves so-called general expenses. The
 103 general expenses, including research and development, administrative, distribution,
 104 marketing expenses etc, are estimated at about 4% of the operating costs per year.⁸
 105 The cash flow sheet is listed in Table S6.

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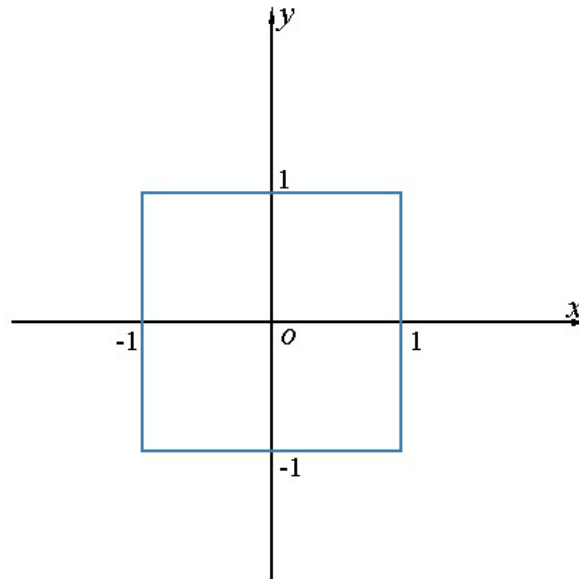
Table S6 The cash flow sheet

Year	Annual capacity	Cash flow
0	0	-\$26,240,599
1	30%	-\$12,199,189
2	50%	\$2,381,781
3	80%	\$13,413,186
4	100%	\$15,232,873
5	100%	\$15,232,873
6	100%	\$20,350,000
7	100%	\$20,350,000
8	100%	\$20,350,000
9	100%	\$20,350,000
10	100%	\$20,350,000
11	100%	\$20,350,000
12	100%	\$20,350,000
13	100%	\$20,350,000
14	100%	\$20,350,000
15	100%	\$20,350,000
16	100%	\$20,350,000

17	100%	\$20,350,000
18	100%	\$20,350,000
19	100%	\$20,350,000
20	100%	\$26,701,958

107 1.4 The average delivery distance

108 Since the biorefinery plant is located at the center of a square rural area, where
 109 cotton straw is uniformly distributed, the distance traveled by a truck delivering the
 110 cotton straw is uncertain and should be a random variable. Therefore, the average
 111 transportation distance to this plant, namely the random variable expectation, will be
 112 supposed to be the actual distance traveled by trucks delivering all the cotton straw. A
 113 formula of computation of the average delivery distance was given by Brown et al,
 114 but the deduced method and details of this formula was not provided.¹³ We give a
 115 following deduced method and steps of this formula.



131 **Fig. S1** A square with a side of length 2

132 Firstly, if F is the feedstock delivered annually to the plant, Y is the annual yield
 133 of cotton straw and f is the fraction of the acreage around the plant devoted to
 134 feedstock production, the square rural area should have a side of length $(F/(Y*f))^{0.5}$.
 135 Suppose that the average distance from a random point in the square to the center of
 136 the square is r_{ave} if the horizontal and vertical ordinate of the point all follow U (-1, 1).

137 Secondly, a square with a side of length 2 is considered as depicted in Fig. S1.

138 The average distance from a random point in the square to the center of the
 139 square (I) can be calculated as following if the horizontal and vertical ordinate of the
 140 point all follow U (-1, 1):

$$141 \quad I = \int_{-1}^1 \int_{-1}^1 \sqrt{x^2 + y^2} * \frac{1}{2} * \frac{1}{2} dx dy = \int_0^1 \int_0^1 \sqrt{x^2 + y^2} dx dy$$

$$142 \quad \text{Let : } x = r \cos \varphi, y = r \sin \varphi$$

143 So :

$$144 \quad I = \int_0^{\frac{\pi}{4}} d\varphi \int_0^{\sec \varphi} r^2 dr + \int_{\frac{\pi}{4}}^{\frac{\pi}{2}} d\varphi \int_0^{\csc \varphi} r^2 dr$$

$$I = \frac{1}{3}(\sqrt{2} + Ln(1 + \sqrt{2}))$$

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150 Finally, the two squares are similar.

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$$Q \frac{r_{ave}}{I} = \frac{\sqrt{\frac{F}{Yf}}}{2}$$

$$\therefore r_{ave} = \frac{1}{6} \sqrt{\frac{F}{Yf}} (\sqrt{2} + Ln(1 + \sqrt{2}))$$

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157 A ‘tortuosity factor’ τ is defined as the ratio of actual distance to the straight-line
158 distance from the plant. Therefore, the average delivery distance, which is expressed
159 as r_{square} in this following formula, should be:

160

$$r_{square} = \frac{1}{6} \tau \sqrt{\frac{F}{Yf}} (\sqrt{2} + Ln(1 + \sqrt{2}))$$

161

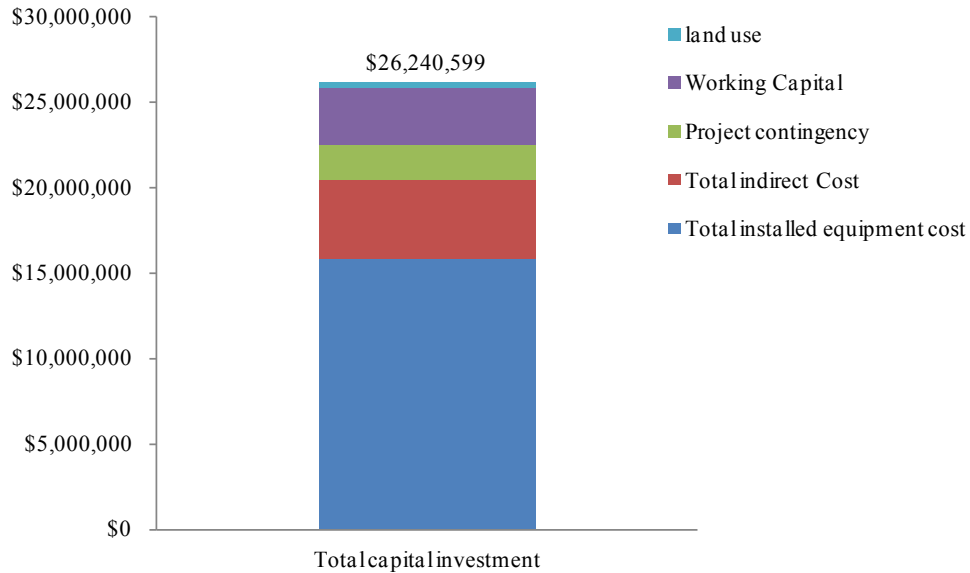
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163 In this study, F, Y, f and τ are assumed to be 18000 ton/year, 5 ton/acre per year,
164 60% and 1.5, respectively. Therefore, the average delivery distance is 1.76 miles.

165 2 Investment and production cost

166 2.1 The investment

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182 **Fig. S2** Total capital investment of the process

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184 As showed in Fig. S2, which represents total capital investment as the
185 summation of total installed equipment cost, total indirect cost, project contingency,

186 working capital cost, and land use, the total capital investment for the biorefinery
187 process amounts to \$26.2 million, while the total installed equipment cost of the
188 whole process is \$15.7 million. Such a scale of investment is one order smaller than
189 the investment scale of biofuel plants.^{5, 14, 15} However, Chemicals have normally
190 higher added value than fuels. And this allows chemical plants can be operated with
191 smaller scale of economies than fuel plants when the two kinds of plants have the
192 same profit margin. Since the biorefinery process consists of four sub-processes, it is
193 important to know the percentage of the total installed equipment cost for each sub-
194 process.

195 Fig. S3 shows the relative weightings (percentage) of the four sub-processes
196 represented in the total installed equipment cost of the whole process. Bio-oil
197 preparation and separation (sub 1), extraction of levoglucosan (sub 2) and preparation
198 of deicer (sub 4) separately contribute 38%, 34% and 25% of the total installed
199 equipment cost, respectively. The really amazing thing about this figure is that
200 production of renewable phenol resin (sub 3) is the smallest (only 3%) contributor to
201 the total installed equipment cost. The reason is that the production of renewable
202 phenol resin requires a minimum number of unit operations or equipments in
203 comparison with other three sub-processes. From an economic point of view, the sub-
204 process 4, the preparation of deicer, seemingly is not feasible or cost-effective
205 because the total installed cost for the sub-process 4 accounts for 25% of the total but
206 the selling price (\$700/ton) and the production rate (37kg/h) of the deicer are all
207 comparatively low. On the other hand, it can be expected that the extraction of
208 levoglucosan and the production of renewable phenol resin are all cost-effective
209 because levoglucosan is a high added-value product and the production of renewable
210 phenol resin needs relatively small equipment investment.

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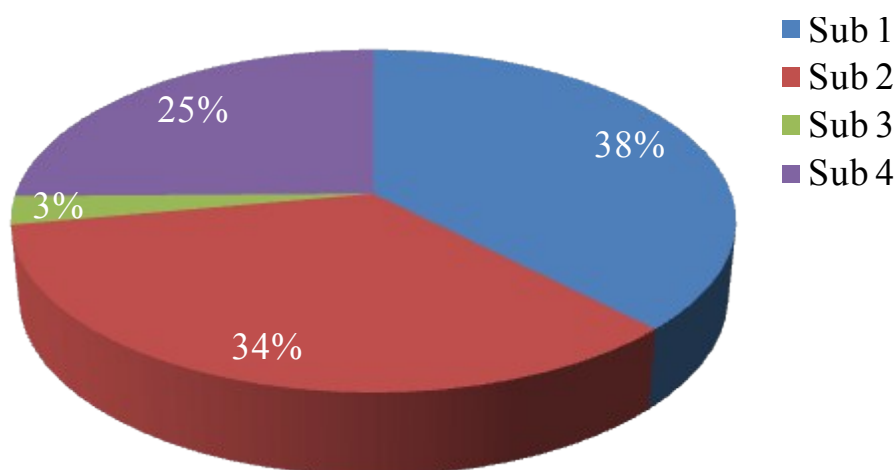
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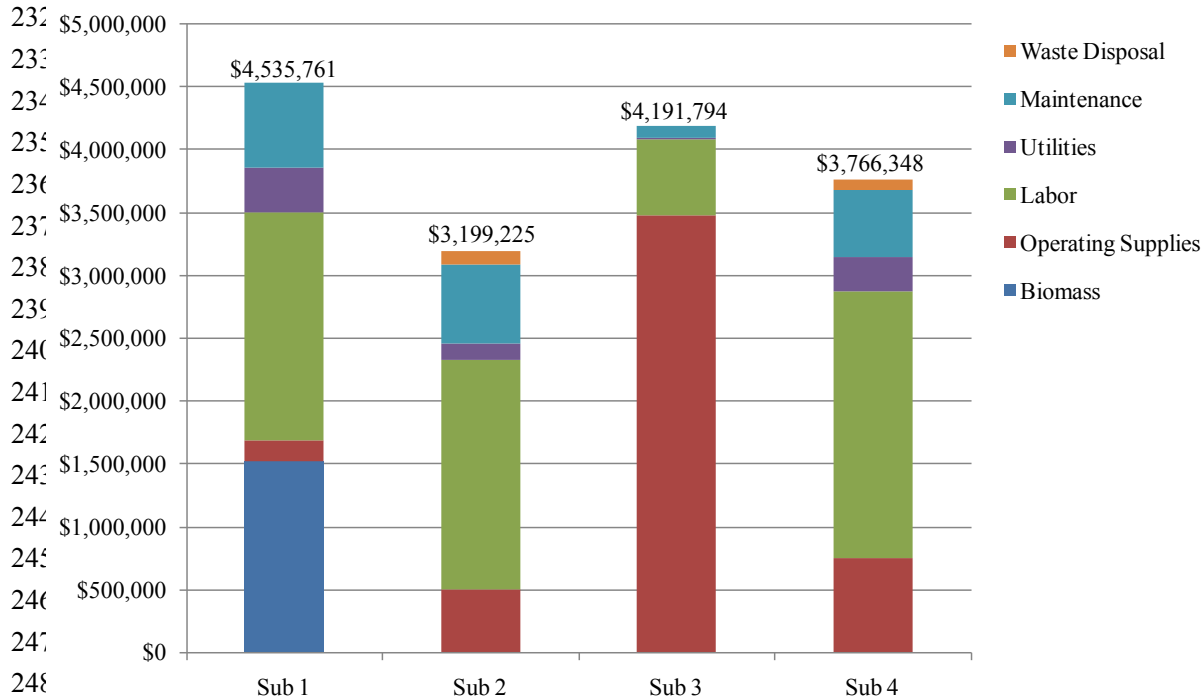


224 **Fig. S3** The percentage of the total installed equipment cost for each sub-process

225 2.2 The production cost

226 Determination of the necessary capital investment is only one part of a complete

227 cost estimate. Another equally important part is the estimation of costs for operating
 228 the plant or process. Fig. S4 shows the annual direct production costs for cotton straw
 229 to levoglucosan, renewable phenol resin and deicer. Similar to Fig. S3, the direct
 230 production cost of the whole process is breakdown to each sub-process area in Fig. S4.
 231



249 **Fig. S4** The annual direct production costs

250 The direct production costs of the four sub-processes vary from around \$3.2
 251 million/year to \$4.5 million/year, and total up to \$15.7 million/year. There is not
 252 much difference between the annual direct production cost of sub 4 (preparation of
 253 deicer) and the annual direct production cost of sub 2 (extraction of levoglucosan) or
 254 sub 3 (production of renewable phenol resin). However, in consideration of the yearly
 255 outputs and product prices of the three chemicals, it can be also inferred that sub 4
 256 (preparation of deicer) is not cost-effective. The labor costs of sub 1 (bio-oil
 257 preparation and separation), 2 (extraction of levoglucosan) and 4 (preparation of
 258 deicer) are the largest contributors to the annual direct production costs of the three
 259 sub-processes, respectively. This is because each of the three sub-processes contains
 260 quite a number of unit operations or equipments, which require a number of operating
 261 labor and a certain amount of direct supervisory and clerical labor for operation. On
 262 the basis of the same reason, the maintenance costs of the three sub-processes account
 263 for the certain proportion of the annual direct production costs of the three sub-
 264 processes. The operating supplies of sub 3 (production of renewable phenol resin)
 265 comprise the vast majority of the annual direct production cost of this sub-process
 266 because a substantial number of phenol and formaldehyde are used in the sub-process.
 267 Direct production cost is only part of operating cost. The operating cost includes all
 268 expenses directly connected with the manufacturing operation or the physical
 269 equipment of a process plant itself. However, unlike direct production cost, operating

270 cost is not appropriate for being breakdown to process area because it includes plant-
 271 overhead costs, which are reserved for hospital and medical services, safety services,
 272 salvage services and warehouse facilities, etc.

273 As shown in Fig. S5, the operating cost of the whole process is around \$22.2
 274 million/year. The annual direct production cost, fixed charge and plant-overhead cost
 275 of the whole process account for about 71%, 12% and 17% of the operating cost,
 276 respectively. These percents are basically similar to other techno-economic analyses
 277 of some biorefinery processes via fast paralysis.^{5, 6} However, the labor cost of the
 278 whole process occupies about 29% of the operating cost; In comparison with
 279 production of biofuels,^{5, 6, 15} this percent is remarkably higher. There could be three
 280 reasons to explain this. Firstly, production of chemicals usually needs more
 281 purification steps or equipments than production of fuels. Secondly, not one chemical
 282 but three chemicals are produced in this birefinery process. Finally, mass production
 283 of biofuels usually is a continuous process, while the production of the three
 284 chemicals contains some batch steps. These reasons could result in more labor
 285 requirement in this birefinery process.

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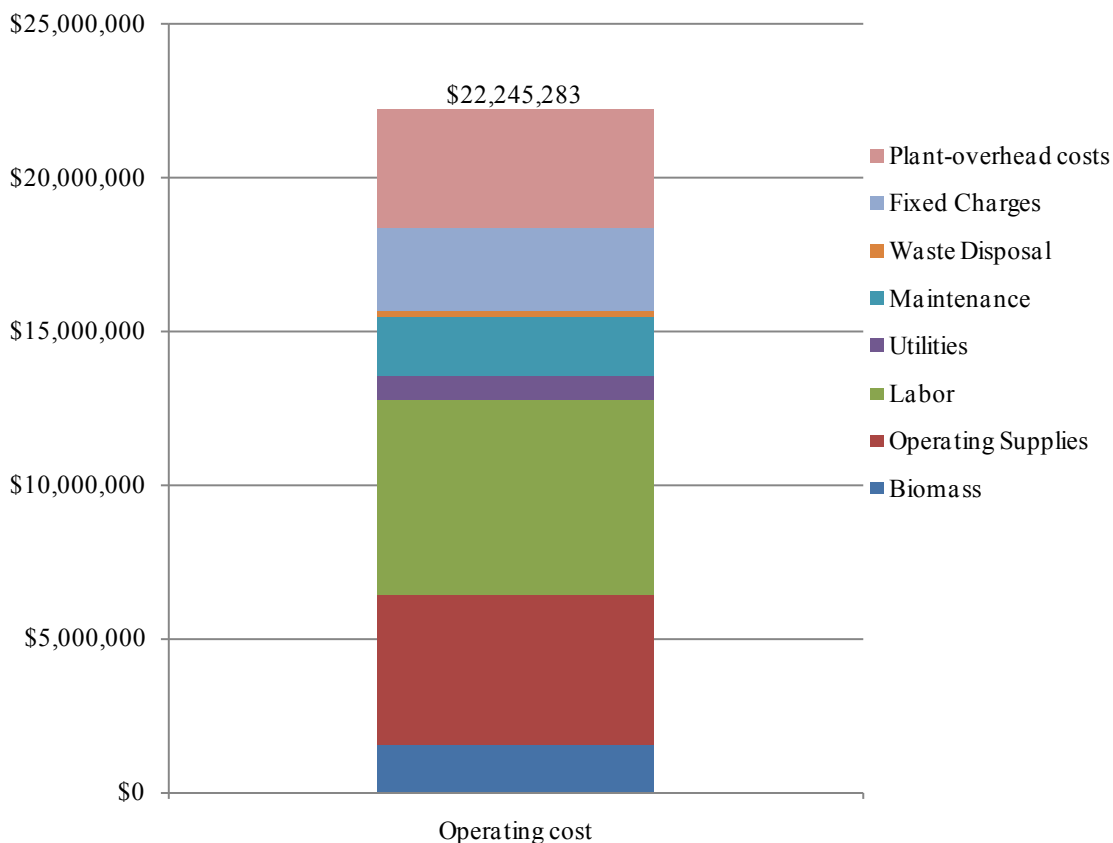


Fig. S5 The operating cost of the whole process

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317 **3 Some background data for this LCA study**

318 **3.1 LCI data for petrochemical production of phenol - formaldehyde resins (PF)**

319 Wilson et al. has developed an life-cycle inventory of formaldehyde-base resins
320 used in wood composites in terms of resources, emissions, energy and carbon.¹⁶ The
321 LCI for the production of PF is shown in Table S7, in which the environmental
322 burdens of the delivery of chemicals to the resin plants are ignored.

323 **Table S7** LCI data for conventional PF production route

Materials, Energy and Emissions	Value	Units
Phenol	2.44E-01	kg /kg _{PF}
Methanol	2.09E-01	kg /kg _{PF}
Sodium hydroxide	6.10E-02	kg /kg _{PF}
Process water	3.34E-01	kg /kg _{PF}
Cooling water from river (20°C)	1.56E-02	kg /kg _{PF}
Electricity	3.56E-02	kWh /kg _{PF}
Natural gas	8.21E-03	Nm ³ /kg _{PF}
Propane	2.93E-06	L /kg _{PF}
Carbon dioxide	1.76E-02	kg /kg _{PF}
Carbon monoxide	3.81E-05	kg /kg _{PF}

324 **3.2 LCI data for petrochemical production of calcium acetate**

325 Overcash et al has presented gate-to-gate process energy use for a calcium
326 acetate manufacturing process, in which calcium hydroxide and acetic acid were used
327 as raw materials.¹⁷ On the basis of the work of Overcash et al, LCI data for
328 petrochemical production of calcium acetate is shown in Table S8.

329 **Table S8** LCI data for petrochemical production of calcium acetate

Materials, Energy and Emissions	Value	Units
Calcium hydroxide	4.69E-01	kg /kg _{Calcium acetate}
Acetic acid	7.59E-01	kg /kg _{Calcium acetate}
Steam (6bar)	1.53E+00	MJ /kg _{Calcium acetate}
Electricity	1.05E-03	MJ /kg _{Calcium acetate}
Natural gas	9.32E-01	MJ /kg _{Calcium acetate}
Carbon dioxide	5.22E-02	kg /kg _{Calcium acetate}

330 **3.3 The GWP100a, CED, EI-99 metric for some chemicals and utilities**

331 Cradle-to-gate LCIA results according to the GWP100a, CED, EI-99 metric for
 332 some chemicals and utilities used in this process are listed in Table S9. All the data is
 333 mainly based on ecoinvent 2.2 database, and a few of the data is derived from some
 334 LCA documents. These LCA documents are listed in the last row in Table S9.

335 **Table S9** The GWP100a, CED, EI-99 metric for some chemicals and utilities

Substance	GWP100a (kg _{CO2-eq} /kg)	CED _{non-renewable} (MJ _{eq} /kg)	EI-99 (Points/kg)
<i>Materials</i>			
Fertilizer^a	1.66E+00	2.93E+01	1.66E-01
Sulfuric acid (98 wt. %)	1.20E-01	2.02E+00	4.00E-02
Process water	2.45E-05	2.79E-04	1.83E-06
Activated carbon ^b	2.94E-01	5.92E+00	1.76E-02
Calcium hydroxide	9.90E-01	5.50E+00	3.00E-02
Hydrochloric acid (32 wt. %)	8.53E-01	1.75E+01	6.00E-02
Ethyl acetate ^c	3.14E+00	9.63E+01	3.36E-01
Sodium hydroxide	1.10E+00	2.14E+01	6.00E-01
Phenol	3.48E+00	1.21E+02	4.40E-01
Formaldehyde (37 wt.%) ^c	4.14E-01	1.82E+01	6.25E-02
Calcium oxide ^d	1.31E+00	7.30E+00	2.80E-02
Methanol ^c	7.64E-01	4.08E+01	1.35E-01
<i>Energy</i>			
Diesel ^e	1.29E-02	1.20E+00	6.43E-03
Electricity ^e	4.90E-01	9.87E+00	2.00E-02
Steam (6 bar) ^e	1.00E-01	1.56E+00	5.77E-03
Cooling water from river (20°C)	0.00E+00	0.00E+00	0.00E+00
<i>Waste treatment</i>			
Waste liquid ^f	2.19E-02	2.42E-01	5.00E-04
Solid waste ^f	1.34E-02	6.52E-01	4.22E-02

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337 ^a Values based on the work of Hasler et al.¹⁸

338 ^b Values based on the work of Arena et al.¹⁹

339 ^c Values based on the work of Amelio et al.²⁰

340 ^d Values based on the works of Huijbregts et al. and Alvarez-Gaitan et al.^{21, 22}

341 ^e Functional unit for diesel as well as steam is MJ and for electricity kWh

342 ^f Values based on the works of Rerat et al.²³

343 **Electronic Supplementary Information (ESI)**

344 **Life cycle assessment and techno-economic analysis of the utilization**
345 **of bio-oil components for the production of three chemicals**

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377 4 The procedures of the techno-economic-environmental analysis

378 4.1 Methodology for estimation of the total-capital investment

379 **Table S1** Methodology for total-capital investment for nth plant

Item	Percent of TDEC
Total purchased equipment-delivered cost	100%
Purchased equipment installation	39%
Instrumentation and controls (installed)	13%
Piping (installed)	31%
Electrical systems (installed)	10%
Buildings (including services)	29%
Yard improvements	10%
Service facilities (installed)	55%
Total installed cost (TIC)	287%
Land (if purchase is required)	6%
Engineering and supervision	32%
Construction expenses	34%
Total direct and indirect plant costs (TDIC)	359%
Contractor's fee (CF)	5% of TDIC
Contingency (CO)	10% of TDIC
Fixed-capital investment (FCI)	TDIC+CF+CO
Working capital	15% of FCI
Total capital investment	475%

380

381 The total installed equipment cost is part of the total capital investment. The total
382 capital investment for all processes consists of fixed-capital investment for physical
383 equipment and facilities in the plant plus working capital which must be available to
384 pay salaries, keep raw materials and products on hand, and handle other special items
385 requiring a direct cash outlay. This method for estimating the total-capital investment
386 is based on the percentage of delivered-equipment cost. Namely, the determination of
387 the delivered-equipment cost is required firstly. The other items included in the fixed-
388 capital investment are estimated as percentages of the delivered-equipment cost , and
389 the working capital amounts to 15 percent of the fixed-capital investment.¹ The items
390 included in the total-capital investment and the corresponding ratio factors based on
391 delivered equipment cost are listed in Table S1. Unit process principles are used to
392 determine the equipment specifications,^{1, 2} and then the delivered-equipment cost of
393 each piece of the process equipments can be estimated from appropriate
394 manufacturers' bulletins, published cost data, empirical rules¹⁻³ or e-commerce
395 websites (such as Alibaba) as listed in Table S2.

Table S2 The delivered-equipment cost of each piece of the process equipments

Equipments	Specification	Delivered-equipment cost
<i>Sub 1</i>		
Chopper	50 kw/ton	\$44,137
Biomass Chopping Screen	60 ton/day	\$3,286
Grinding Hammer Mill	50 kw/ton	\$44,137
Biomass Grinding Screen	60 ton/day	\$3,359
Belt Press	5.5 kw	\$19,425
Bale Moving Forklift*4	1.25 ton/h	\$14,021
Concrete Storage Slab	30 m*29 m*3.5 m	\$87,631
Discharge Conveyor	0.75 kw/ton	\$9,785
Bale Transport Conveyor	90 w/ton	\$77,845
Bale Unwrapping Conveyor	5.5 kw	\$29,210
Continuous Spray Rotary Drum	2.2 kw, 2.5 ton/h	\$185,089
Rotary Dryer	2.2 kw	\$99,519
Biomass Feeding Bin	Φ1.5*4.3 m	\$6,047
Screw Feeder	0.75 kw/ton	\$23,733
Pyrolysis Fluid Bed	Φ1.2 m*2 m	\$122,099
Non-condensable Gas Blower	90 kw	\$31,357
Pyrolysis Vapor Cyclones*2	3600 m ³ of gas per hour	\$184,316
Bio-oil Condenser*2	600 m ² of heat transfer area	\$291,722
Electro-Static Precipitator	30 kw	\$42,705
Condenser Water Pump*3	90 kw	\$62,527
Ice making machine	53 /kw, 592 kg of ice per hour	\$20,000
Condenser Oil Pump	5 kw	\$6,952
Cooling Tower	Φ 8.8m*6.5m	\$438,898
Wash Percolater	4 m ³	\$31,459
Solids Combustor	Φ0.3 m*0.8 m	\$35,680
Combustor Cyclones	3360 m ³ of gas per hour	\$161,343
Combustion Gas Blower	85 kw	\$9,084
<i>Sub 2</i>		
Settling Tank	3 m ³	\$35,965
Filter, vacuum rotary drum	3 kw, 600 kg of filtrate /(m ² .h)	\$185,089
Vacuum pump	10 kw	\$28,655
Settling Tank	3 m ³	\$35,965
Filter, vacuum rotary drum	3 kw, 600 kg of filtrate /(m ² .h)	\$185,089
Vacuum pump	10 kw	\$28,655
Mixer	10 kw, 3m ³	\$73,805
Vacuum freeze dryer	130 kw, 1.2 ton water per hour	\$365,261
Mixer	10 kw, 3 m ³	\$73,805
Filter, vacuum rotary drum	3 kw, 600 kg of filtrate /(m ² .h)	\$185,089
Evaporation crystallizer	1000 kg of acetic ether per	\$452,879
Settling Tank	3 m ³	\$35,965

Filter, vacuum rotary drum	3 kw, 600 kg of filtrate /(m ² .h)	\$185,089
Vacuum pump	10 kw	\$28,655
<i>Sub 3</i>		
Mixer*2	10 kw, 3 m ³	\$147,610
<i>Sub 4</i>		
Evaporator	600 kg of water per hour	\$349,285
Mixer	10 kw, 3 m ³	\$73,805
Evaporator	600 kg of water per hour	\$349,285
Mixer*4	3 kw, 0.8 m ³	\$104,268
Filter, vacuum rotary drum*4	3 kw, 75 kg of filtrate /(m ² .h)	\$212,611
Vacuum pump*4	10 kw	\$114,620
Evaporator*2	50 kg of methanol per hour	\$190,110

397 **4.2 Methodology for estimation of the operating cost and direct production**
398 **cost**

399 **Table S3** Variable costs employed in the estimation of the direct production costs

400 (Source: www.alibaba.com and refs). ⁶⁻⁸

Item	Value
Cotton straw	\$83/metric ton
Transport	\$0.71/(ton.mile)
Sulfuric acid 98 wt.%	\$300/metric ton
Process water	\$1.0/metric ton
Activated carbon	\$1500/metric ton
Calcium hydroxide	\$110/metric ton
Hydrochloric acid 32 wt.%	\$190/metric ton
Ethyl acetate	\$1200/metric ton
Calcium oxide	\$160/metric ton
Methanol	\$700/metric ton
Sodium hydroxide	\$500/metric ton
Phenol	\$1300/metric ton
Formaldehyde 37 wt.%	\$400/metric ton
Cooling water from river	\$0.15/metric ton
Average hourly wage	\$21/h
Electricity	\$0.061/kwh
Steam (6 bar)	\$20/metric ton
Solids disposal cost	\$22.23/metric
Waste water disposal cost	\$1.30/metric ton

401 The operating cost is divided into three classifications as follows: (1) direct
402 production costs, which mainly involve expenditures for raw materials, direct
403 operating labor, supervisory and clerical labor directly connected to the
404 manufacturing operation, utilities, plant maintenance and repairs. Some variable cost
405 parameters, such as the prices of cotton straw, phenol, and utilities, average hourly

406 wage and water treatment cost, are listed on the Table S3; (2) fixed charges,
 407 essentially include expenses directly associated with depreciation, property taxes,
 408 insurance. Some assumptions for the estimation of fixed charges, such as depreciation
 409 period, type of depreciation and property tax rate, are listed on the Table S4; (3)
 410 plant-overhead costs, which are used for medical services, warehouses, safety services,
 411 warehouses and so on. The estimation of fixed charges and plant-overhead costs can
 412 be based on the method of 'Percentage of total-capital investment'.⁴ However the
 413 estimation of direct production costs is slightly complex. Chemical engineering
 414 principles, such as material balance and energy balance, and the methodology
 415 proposed by Overcash et.al are used for calculation of the expenditures for raw
 416 materials and utilities.⁵ The method of estimating labor requirements is based on
 417 adding up the various principal processing steps on the flow sheet and plant capacity,
 418 and the cost for direct supervisory and clerical labor averages about 15 percent of the
 419 cost for operating labor.¹ The method for estimation of the expenditures for plant
 420 maintenance and repairs is the same as that for estimation of fixed charges.

421 **Table S4** Assumptions for the estimation of the fixed charges

Item	Value/method
Equipment depreciation period	20 years
Building depreciation period	40 years
Amortization period	5 years
Type of depreciation or amortization	Straight-line
Property tax rate	2% of FCI
Insurance rate	1% of FCI

422 **4.3 Methodology for estimation of the operating cost and direct production cost**

423 **Table S5** Assumptions or parameters for the calculation of IRR

Item	Value
Service life	20 years
Construction period	1 years
Income tax rate	39%
Annual capacity in the first year	30%
Annual capacity in the second year	50%
Annual capacity in the third year	80%
Salvage value at end of service life	Working capital+land+salvage value of buildings
Levogluconan	15\$/kg
Renewable phenol resin	2800\$/metric ton
Road de-icer	700\$/metric ton

424

425 The 20-year facility IRR is calculated on the basis of a cash flow sheet in order
 426 to perform a profitability evaluation.¹ The determination or estimation of the market
 427 prices for the three chemicals is important for calculation of IRR. Levoglucosan is
 428 advertised for sale at \$1500/kg and \$20~90/kg on the carbosynth's Web site and the
 429 Alibaba Web site, respectively.^{9, 10} The purity of the levoglucosan sold at the
 430 carbosynth's Web site is 3% higher than that of the levoglucosan produced via the
 431 process. Moreover, from an economic perspective, mass production will lower the
 432 cost. Therefore, the price of the levoglucosan produced via the process is set at \$15/kg
 433 in this analysis. The phenolic resins from America are priced around \$4000/ton
 434 (¥25.5/kg) on the Guidechem Web site.¹¹ Considering that about 50wt% of the phenol
 435 used in the renewable phenol resin produced via the process is replaced and the
 436 phenolic resin is not as good as those phenolic resins based on petrochemical
 437 synthesis in quality and performance, the renewable phenol resin was valued at
 438 \$2800/ton. Food grade calcium acetate is priced at about \$1200/ton on the Alibaba
 439 Web site.¹² The deicer produced via the process is, at best, an industrial grade mixture
 440 of calcium salts. Hence the mixture is pegged at \$700/ton. Some necessary parameters
 441 for the calculation of the cash flow sheet, such as construction period, income tax rate
 442 and product prices, are showed in Table S5.

443 Moreover, the cash flow sheet also involves so-called general expenses. The
 444 general expenses, including research and development, administrative, distribution,
 445 marketing expenses etc, are estimated at about 4% of the operating costs per year.⁵
 446 The cash flow sheet is listed in Table S6.

447

Table S6 The cash flow sheet

Year	Annual capacity	Cash flow
0	0	-\$26,240,599
1	30%	-\$12,199,189
2	50%	\$2,381,781
3	80%	\$13,413,186
4	100%	\$15,232,873
5	100%	\$15,232,873
6	100%	\$20,350,000
7	100%	\$20,350,000
8	100%	\$20,350,000
9	100%	\$20,350,000
10	100%	\$20,350,000
11	100%	\$20,350,000
12	100%	\$20,350,000
13	100%	\$20,350,000
14	100%	\$20,350,000
15	100%	\$20,350,000
16	100%	\$20,350,000

17	100%	\$20,350,000
18	100%	\$20,350,000
19	100%	\$20,350,000
20	100%	\$26,701,958

448 4.4 The average delivery distance

449 Since the biorefinery plant is located at the center of a square rural area, where
450 cotton straw is uniformly distributed, the distance traveled by a truck delivering the
451 cotton straw is uncertain and should be a random variable. Therefore, the average
452 transportation distance to this plant, namely the random variable expectation, will be
453 supposed to be the actual distance traveled by trucks delivering all the cotton straw. A
454 formula of computation of the average delivery distance was given by Brown et al,
455 but the deduced method and details of this formula was not provided.¹³ We give a
456 following deduced method and steps of this formula.

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472 **Fig. S1** A square with a side of length 2

473 Firstly, if F is the feedstock delivered annually to the plant, Y is the annual yield
474 of cotton straw and f is the fraction of the acreage around the plant devoted to
475 feedstock production, the square rural area should have a side of length $(F/(Y*f))^{0.5}$.
476 Suppose that the average distance from a random point in the square to the center of
477 the square is r_{ave} if the horizontal and vertical ordinate of the point all follow U (-1, 1).

478 Secondly, a square with a side of length 2 is considered as depicted in Fig. S1.

479 The average distance from a random point in the square to the center of the
480 square (I) can be calculated as following if the horizontal and vertical ordinate of the
481 point all follow U (-1, 1):

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$$I = \int_{-1}^1 \int_{-1}^1 \sqrt{x^2 + y^2} * \frac{1}{2} * \frac{1}{2} dx dy = \int_0^1 \int_0^1 \sqrt{x^2 + y^2} dx dy$$

$$\text{Let : } x = r \cos \varphi, y = r \sin \varphi$$

So :

$$I = \int_0^{\frac{\pi}{4}} d\varphi \int_0^{\sec \varphi} r^2 dr + \int_{\frac{\pi}{4}}^{\frac{\pi}{2}} d\varphi \int_0^{\csc \varphi} r^2 dr$$

$$I = \frac{1}{3} (\sqrt{2} + \ln(1 + \sqrt{2}))$$

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491 Finally, the two squares are similar.

492

$$Q \frac{r_{ave}}{I} = \frac{\sqrt{\frac{F}{Yf}}}{2}$$

$$\therefore r_{ave} = \frac{1}{6} \sqrt{\frac{F}{Yf}} (\sqrt{2} + Ln(1 + \sqrt{2}))$$

498 A ‘tortuosity factor’ τ is defined as the ratio of actual distance to the straight-line
499 distance from the plant. Therefore, the average delivery distance, which is expressed
500 as r_{square} in this following formula, should be:

501

$$r_{square} = \frac{1}{6} \tau \sqrt{\frac{F}{Yf}} (\sqrt{2} + Ln(1 + \sqrt{2}))$$

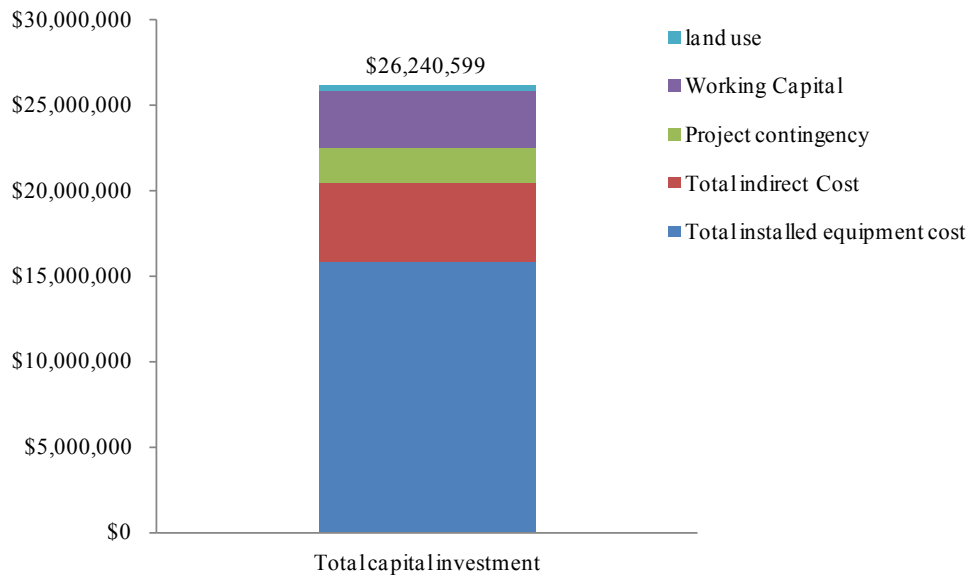
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503
504 In this study, F, Y, f and τ are assumed to be 18000 ton/year, 5 ton/acre per year,
505 60% and 1.5, respectively. Therefore, the average delivery distance is 1.76 miles.

506 5 Investment and production cost

507 5.1 The investment

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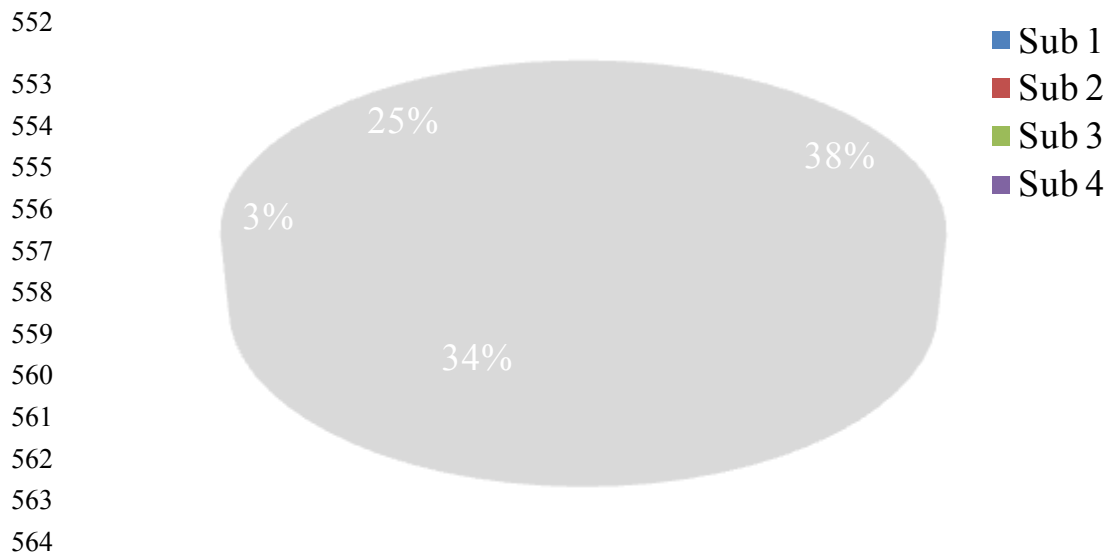
523 **Fig. S2** Total capital investment of the process

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525 As showed in Fig. S2, which represents total capital investment as the
526 summation of total installed equipment cost, total indirect cost, project contingency,

527 working capital cost, and land use, the total capital investment for the biorefinery
528 process amounts to \$26.2 million, while the total installed equipment cost of the
529 whole process is \$15.7 million. Such a scale of investment is one order smaller than
530 the investment scale of biofuel plants.^{7, 14, 15} However, Chemicals have normally
531 higher added value than fuels. And this allows chemical plants can be operated with
532 smaller scale of economies than fuel plants when the two kinds of plants have the
533 same profit margin. Since the biorefinery process consists of four sub-processes, it is
534 important to know the percentage of the total installed equipment cost for each sub-
535 process.

536 Fig. S3 shows the relative weightings (percentage) of the four sub-processes
537 represented in the total installed equipment cost of the whole process. Bio-oil
538 preparation and separation (sub 1), extraction of levoglucosan (sub 2) and preparation
539 of deicer (sub 4) separately contribute 38%, 34% and 25% of the total installed
540 equipment cost, respectively. The really amazing thing about this figure is that
541 production of renewable phenol resin (sub 3) is the smallest (only 3%) contributor to
542 the total installed equipment cost. The reason is that the production of renewable
543 phenol resin requires a minimum number of unit operations or equipments in
544 comparison with other three sub-processes. From an economic point of view, the sub-
545 process 4, the preparation of deicer, seemingly is not feasible or cost-effective
546 because the total installed cost for the sub-process 4 accounts for 25% of the total but
547 the selling price (\$700/ton) and the production rate (37kg/h) of the deicer are all
548 comparatively low. On the other hand, it can be expected that the extraction of
549 levoglucosan and the production of renewable phenol resin are all cost-effective
550 because levoglucosan is a high added-value product and the production of renewable
551 phenol resin needs relatively small equipment investment.

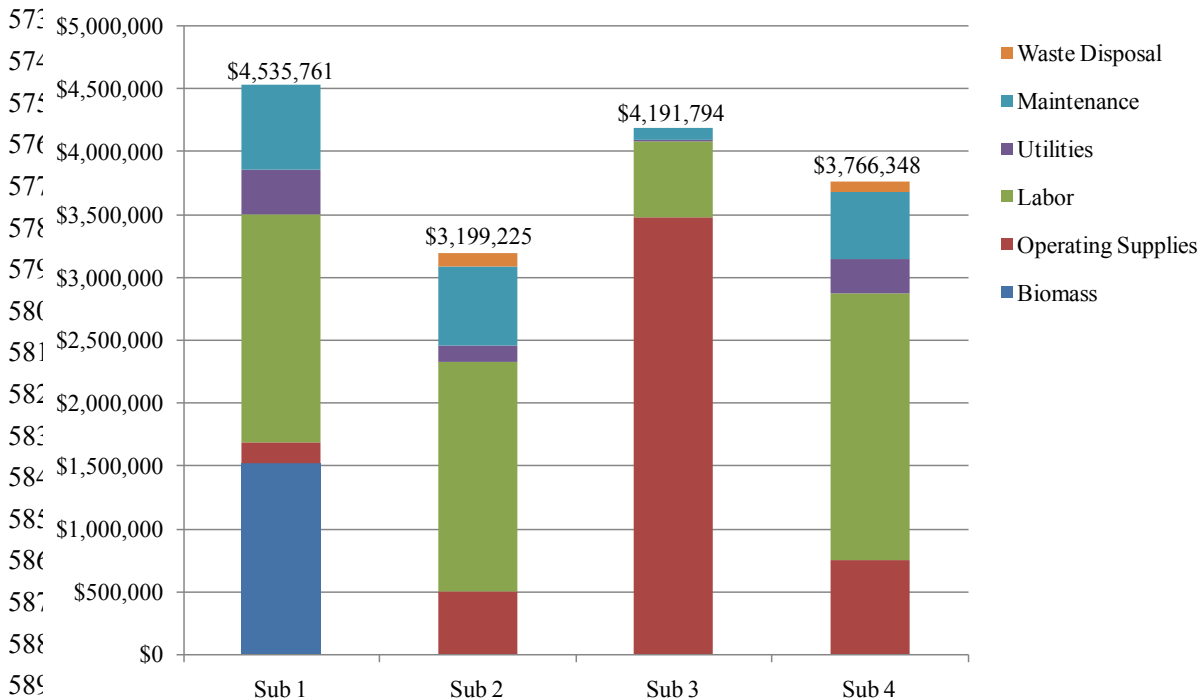


565 **Fig. S3 The percentage of the total installed equipment cost for each sub-process**

566 5.2 The production cost

567 Determination of the necessary capital investment is only one part of a complete

568 cost estimate. Another equally important part is the estimation of costs for operating
 569 the plant or process. Fig. S4 shows the annual direct production costs for cotton straw
 570 to levoglucosan, renewable phenol resin and deicer. Similar to Fig. S3, the direct
 571 production cost of the whole process is breakdown to each sub-process area in Fig. S4.
 572



590 **Fig. S4** The annual direct production costs

591 The direct production costs of the four sub-processes vary from around \$3.2
 592 million/year to \$4.5 million/year, and total up to \$15.7 million/year. There is not
 593 much difference between the annual direct production cost of sub 4 (preparation of
 594 deicer) and the annual direct production cost of sub 2 (extraction of levoglucosan) or
 595 sub 3 (production of renewable phenol resin). However, in consideration of the yearly
 596 outputs and product prices of the three chemicals, it can be also inferred that sub 4
 597 (preparation of deicer) is not cost-effective. The labor costs of sub 1 (bio-oil
 598 preparation and separation), 2 (extraction of levoglucosan) and 4 (preparation of
 599 deicer) are the largest contributors to the annual direct production costs of the three
 600 sub-processes, respectively. This is because each of the three sub-processes contains
 601 quite a number of unit operations or equipments, which require a number of operating
 602 labor and a certain amount of direct supervisory and clerical labor for operation. On
 603 the basis of the same reason, the maintenance costs of the three sub-processes account
 604 for the certain proportion of the annual direct production costs of the three sub-
 605 processes. The operating supplies of sub 3 (production of renewable phenol resin)
 606 comprise the vast majority of the annual direct production cost of this sub-process
 607 because a substantial number of phenol and formaldehyde are used in the sub-process.
 608 Direct production cost is only part of operating cost. The operating cost include all
 609 expenses directly connected with the manufacturing operation or the physical
 610 equipment of a process plant itself. However, unlike direct production cost, operating

611 cost is not appropriate for being breakdown to process area because it includes plant-
 612 overhead costs, which are reserved for hospital and medical services, safety services,
 613 salvage services and warehouse facilities, etc.

614 As shown in Fig. S5, the operating cost of the whole process is around \$22.2
 615 million/year. The annual direct production cost, fixed charge and plant-overhead cost
 616 of the whole process account for about 71%, 12% and 17% of the operating cost,
 617 respectively. These percents are basically similar to other techno-economic analyses
 618 of some biorefinery processes via fast paralysis.^{7, 8} However, the labor cost of the
 619 whole process occupies about 29% of the operating cost; In comparison with
 620 production of biofuels,^{7, 8, 15} this percent is remarkably higher. There could be three
 621 reasons to explain this. Firstly, production of chemicals usually needs more
 622 purification steps or equipments than production of fuels. Secondly, not one chemical
 623 but three chemicals are produced in this birefinery process. Finally, mass production
 624 of biofuels usually is a continuous process, while the production of the three
 625 chemicals contains some batch steps. These reasons could result in more labor
 626 requirement in this birefinery process.

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629 \$25,000,000

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631 \$22,245,283

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633 \$20,000,000

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635 \$15,000,000

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637 \$10,000,000

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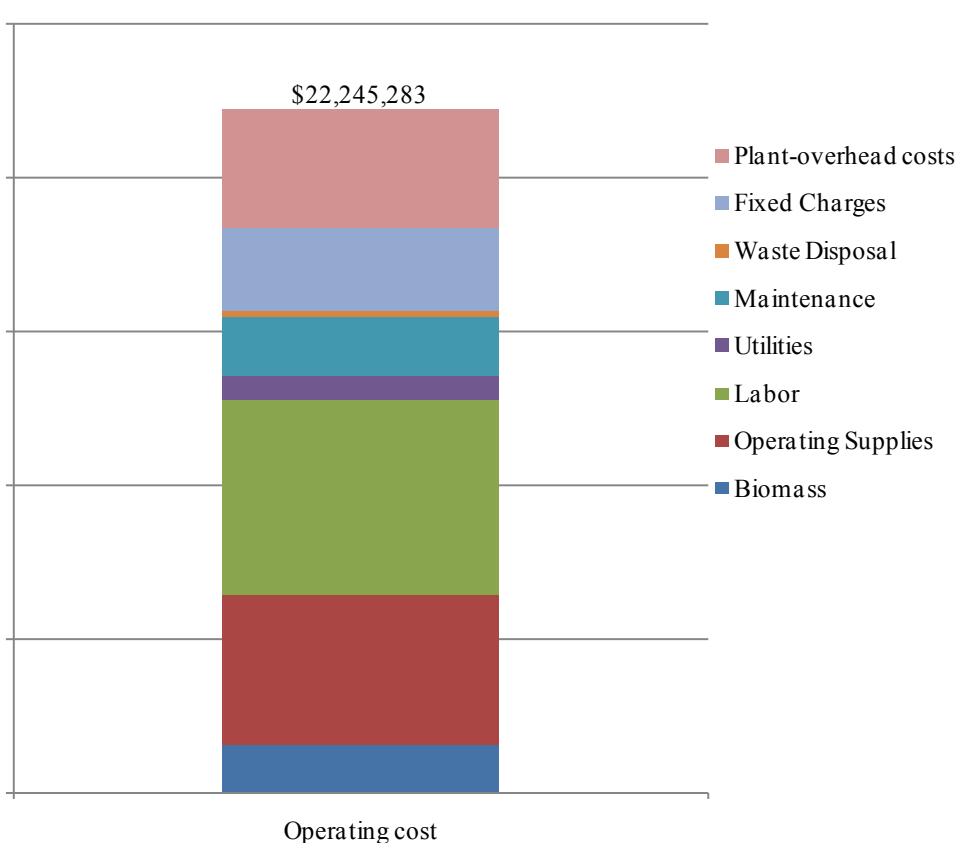


Fig. S5 The operating cost of the whole process

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658 **6 Some background data for this LCA study**

659 **6.1 LCI data for petrochemical production of phenol - formaldehyde resins (PF)**

660 Wilson et al. has developed an life-cycle inventory of formaldehyde-base resins
661 used in wood composites in terms of resources, emissions, energy and carbon.¹⁶ The
662 LCI for the production of PF is shown in Table S7, in which the environmental
663 burdens of the delivery of chemicals to the resin plants are ignored.

664 **Table S7** LCI data for conventional PF production route

Materials, Energy and Emissions	Value	Units
Phenol	2.44E-01	kg /kg _{PF}
Methanol	2.09E-01	kg /kg _{PF}
Sodium hydroxide	6.10E-02	kg /kg _{PF}
Process water	3.34E-01	kg /kg _{PF}
Cooling water from river (20°C)	1.56E-02	kg /kg _{PF}
Electricity	3.56E-02	kWh /kg _{PF}
Natural gas	8.21E-03	Nm ³ /kg _{PF}
Propane	2.93E-06	L /kg _{PF}
Carbon dioxide	1.76E-02	kg /kg _{PF}
Carbon monoxide	3.81E-05	kg /kg _{PF}

665 **6.2 LCI data for petrochemical production of calcium acetate**

666 Overcash et al has presented gate-to-gate process energy use for a calcium
667 acetate manufacturing process, in which calcium hydroxide and acetic acid were used
668 as raw materials.¹⁷ On the basis of the work of Overcash et al, LCI data for
669 petrochemical production of calcium acetate is shown in Table S8.

670 **Table S8** LCI data for petrochemical production of calcium acetate

Materials, Energy and Emissions	Value	Units
Calcium hydroxide	4.69E-01	kg /kg _{Calcium acetate}
Acetic acid	7.59E-01	kg /kg _{Calcium acetate}
Steam (6bar)	1.53E+00	MJ /kg _{Calcium acetate}
Electricity	1.05E-03	MJ /kg _{Calcium acetate}
Natural gas	9.32E-01	MJ /kg _{Calcium acetate}
Carbon dioxide	5.22E-02	kg /kg _{Calcium acetate}

671 **6.3 The GWP100a, CED, EI-99 metric for some chemicals and utilities**

672 Cradle-to-gate LCIA results according to the GWP100a, CED, EI-99 metric for
 673 some chemicals and utilities used in this process are listed in Table S9. All the data is
 674 mainly based on ecoinvent 2.2 database, and a few of the data is derived from some
 675 LCA documents. These LCA documents are listed in the last row in Table S9.

676 **Table S9** The GWP100a, CED, EI-99 metric for some chemicals and utilities

Substance	GWP100a (kgCO ₂ -eq/kg)	CED _{non-renewable} (MJ _{eq} /kg)	EI-99 (Points/kg)
<i>Materials</i>			
Sulfuric acid (98 wt. %)	1.20E-01	2.02E+00	4.00E-02
Process water	2.45E-05	2.79E-04	1.83E-06
Activated carbon ^a	2.94E-01	5.92E+00	1.76E-02
Calcium hydroxide	9.90E-01	5.50E+00	3.00E-02
Hydrochloric acid (32 wt. %)	8.53E-01	1.75E+01	6.00E-02
Ethyl acetate ^b	3.14E+00	9.63E+01	3.36E-01
Sodium hydroxide	1.10E+00	2.14E+01	6.00E-01
Phenol	3.48E+00	1.21E+02	4.40E-01
Formaldehyde (37 wt.%) ^b	4.14E-01	1.82E+01	6.25E-02
Calcium oxide ^c	1.31E+00	7.30E+00	2.80E-02
Methanol ^b	7.64E-01	4.08E+01	1.35E-01
<i>Energy</i>			
Diesel ^d	1.29E-02	1.20E+00	6.43E-03
Electricity ^d	4.90E-01	9.87E+00	2.00E-02
Steam (6 bar) ^d	1.00E-01	1.56E+00	5.77E-03
Cooling water from river (20°C)	0.00E+00	0.00E+00	0.00E+00
<i>Waste treatment</i>			
Waste liquid ^e	2.19E-02	2.42E-01	5.00E-04
Solid waste ^e	1.34E-02	6.52E-01	4.22E-02

677

678 ^a Values based on the work of Arena et al.¹⁸

679 ^b Values based on the work of Amelio et al.¹⁹

680 ^c Values based on the works of Huijbregts et al. and Alvarez-Gaitan et al.^{20, 21}

681 ^d Functional unit for diesel as well as steam is MJ and for electricity kWh

682 ^e Values based on the works of Rerat et al.²²

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