

Supporting information

Table S1. Basic parameters used for evaluation of production cost

Project life time	20 years
Working capital	15% process capital cost
Labor	0.015 \$/kg product
Maintenance	6% process capital cost
Supplies	2% process capital cost
Property tax	3% process capital cost
Depreciation	Straight line

Table S2. Price of main utilities (estimated price of 2013\$)

Utility	Unit	Price
Electricity	\$/kW	1.00E-01
Steam	\$/kg	8.18E-03
Fuel oil	\$/kg	8.04E-01
Process water	\$/kg	1.00E-04

Table S3. Basic parameters of fossil-based processes used for comparing with bio-based processes

Fossil-based chemical	Price [\$/kg] ²⁰	GHG emissions [kg CO ₂ eqv./kg] ²²	Fossil energy consumption [MJ/kg] ²²
Acetic acid	5.30E-01	1.40E+00	6.52E+01
Ethylene	1.10E+00	2.50E+00	6.12E+01
Ethyl acetate	1.37E+00	2.84E+00	7.51E+01

Table S4. Basic parameters used for evaluation of transportation cost of bio-based feedstock (2013\$)

	Distance variable cost [\$/ton.km] ^{a)}	Distance fixed variable cost [\$/ton] ^{a)}
Sugarcane	1.30E-01	5.06E+00
Corn	1.30E-01	5.06E+00
Corn stover	1.30E-01	5.06E+00
Ethanol	6.00E-02	4.33E+00

a) Cost converted from data provided by Searcy et al. [24] in 2007

Table S5. Main input of bio-based ethylene production process^{a)}

Input	Unit [per kg]	Value
Bioethanol	kg	1.76E+00
Electricity	kW	9.73E-03
Steam	kg	1.63E-01
Fuel oil	kg	2.96E-02
Refrigeration	kg	1.26E+00

a) Calculated based on data provided by Cameron et al. [37]

Table S6. Main input and output of bio-based acetic acid production processes^{a)}

Input	Unit [per kg]	Alternative 1	Alternative 2
Bio-based ethylene	kg	0.00E+00	6.05E-01
Bioethanol	kg	7.93E-01	0.00E+00
Electricity	kW	8.40E-02	0.00E+00
Steam	kg	1.71E+00	4.22E+00
Fuel oil	kg	8.79E-02	1.18E-01
Steam production	kg	1.47E+00	1.59E+00

a) Obtained from simulation by using Aspen Plus [19]

Table S7. Main input and output of bio-based ethyl acetate production processes^{a)}

Input	Unit [per kg]	Alternative 1	Alternative 2	Alternative 3
Acetic acid	kg	0.00E+00	6.80E-01	0.00E+00
Ethylene	kg	0.00E+00	5.50E-01	0.00E+00
Ethanol	kg	1.07E+00	1.51E+00	1.24E+00
Electricity	kW	5.58E-02	5.45E-01	1.49E-01
Steam	kg	4.15E+00	5.13E+00	1.23E+01
Fuel oil	kg	0.00E+00	1.25E-01	9.46E-02
Steam production	kg	0.00E+00	2.84E+00	1.40E+00
Hydrogen production	kg	0.00E+00	0.00E+00	4.71E-02

Table S7 (Continued). Main input and output of bio-based ethyl acetate production processes^{a)}

Input	Unit [per kg]	Alternative 3A	alternative 3B	Alternative 3C	Alternative 3D	Alternative 3E
Acetic acid	kg	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ethylene	kg	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ethanol	kg	1.23E+00	1.22E+00	1.27E+00	1.13E+00	1.14E+00
Electricity	kW	1.47E-01	1.43E-01	1.53E-01	1.38E-01	1.38E-01
Steam	kg	5.94E+00	6.09E+00	4.93E+00	8.38E+00	8.38E+00
Fuel oil	kg	3.36E-02	5.63E-02	6.83E-02	2.42E-01	4.81E-02
Steam production	kg	4.98E-01	8.37E-01	1.01E+00	3.55E+00	7.11E-01
Hydrogen production	kg	4.98E-02	4.92E-02	5.10E-02	4.63E-02	4.71E-02

a) Obtained from simulation by using Aspen Plus [19]

Table S8. Bioethanol production cost (2013\$) [\$/kg ethanol]

Bioethanol from sugarcane ³³	Cost
Feedstock	3.06E-01
Labor	3.89E-02
Other inputs	1.86E-02
Energy	2.53E-02
Maintenance	8.00E-02
Administration	7.73E-02
Depreciation	4.90E-02
Cost of capital	3.45E-02
Total	6.29E-01
Bioethanol from corn ³⁴	Cost
Feedstock	7.28E-01
Enzymes	1.11E-02
Yeasts	1.13E-03
Chemicals	1.07E-02
Denaturants	1.54E-02
Repairs and maintenance	8.28E-03
Transportation	2.48E-03
Water	4.07E-03
Electricity	1.27E-02
Natural gas	5.30E-02
Other	6.62E-03
Depreciation	3.63E-02
Interest	2.10E-02
Labor and management	1.26E-02
Property taxes	7.61E-04
Revenue (DDGS)	-2.38E-01
Total	6.86E-01

(DDGS: Distillers Dried Grains with Solubles)

Table S8 (Continued). Bioethanol production cost (2013\$) [\$/kg ethanol]

Bioethanol from corn stover ^{a)}	Cost
Depreciation	7.00E-02
Feedstock + Handling	2.80E-01
Sulfuric Acid	1.00E-02
Ammonia	2.00E-02
Glucose (enzyme production)	7.00E-02
Other Raw Materials	4.00E-02
Waste Disposal	1.00E-02
Net Electricity	-4.00E-02
Capital Depreciation	8.00E-02
Fixed Costs	7.00E-02
Average Income Tax	4.00E-02
Average Return on Investment	2.10E-01
Total	8.60E-01

a) Cost converted from data provided by Humbird et al. [35] in 2007

Table S9. Capital cost of alternative bioethanol-based chemical processes (2013\$)

(Plant size: 150,000 tons/year)

Alternative Process	Capital cost
Bioethanol-based ethylene process ^{a)}	\$9,578,807
Bioethanol-based acetic acid process ^{b)}	
Alternative 1	\$9,491,484
Alternative 2	\$9,490,726
Bioethanol-based ethyl acetate ^{b)}	
Alternative 1	\$19,575,505
Alternative 2	\$17,595,879
Alternative 3	\$18,632,996
Alternative 3A	\$17,289,085
Alternative 3B	\$17,154,329
Alternative 3C	\$15,054,724
Alternative 3D	\$22,202,364
Alternative 3E	\$22,152,364

a) Cost calculated based on data provided by Cameron et al. [37] in 2012

b) Cost calculated by Aspen Icarus [19] in 2006 and converted to 2013\$

Table S10. Demand and transportation distance of bio-based feedstocks used in potential process alternatives producing ethyl acetate

	Alternative 1	Alternative 3A	Alternative 3B	Alternative 3C	Alternative 3E
Demand of feedstock [tons/year]					
Sugarcane	2,267,095	2,597,741	2,574,338	2,684,534	2,418,657
Corn	483,432	553,938	548,947	572,446	515,750
Corn stover	674,578	772,962	765,999	798,788	719,675
Centralized plant scenario					
Number of plant	1	1	1	1	1
Total transportation distance [km]					
Sugarcane process	1,404	3,996	3,996	3,996	3,996
Corn process	265	780	780	780	416
Corn stover process	104	246	246	416	246
Decentralized plant scenario for sugarcane utilizing process					
Number of plant	3	3	3	3	3
Transportation distance of biomass [km]	180	642	642	642	180
Transportation distance of bioethanol [km]	1,140	1,140	1,140	1,140	1,140

Table S11. Environmental impact caused by bioethanol production

Process	Production of feedstock/ bioethanol	Global warming [kg CO ₂ eqv. /kg ethanol]	Photochemical ozone depletion [kg CFC-11 eqv. /kg ethanol]	Acidification [kg SO ₂ eqv. /kg ethanol]	Eutrophication [kg PO ₄ eqv. /kg ethanol]	Photo-oxidant formation [kg C ₂ H ₄ eqv. /kg ethanol]	Energy consumption [MJ/ kg ethanol]
Sugarcane	Feedstock ²²	3.10E-01	3.26E-08	3.61E-03	1.33E-03	6.77E-05	2.27E+00
process	Bioethanol ²²	4.08E-01	4.19E-08	6.03E-03	1.95E-03	1.11E-04	3.15E+00
Corn	Feedstock ³¹	6.93E-01	1.07E-07	3.79E-03	7.97E-03	6.58E-05	6.28E+00
process	Bioethanol ²²	1.91E+00	1.71E-07	1.33E-02	1.40E-02	2.30E-04	1.90E+01
Corn stover	Feedstock ³¹	3.86E-01	1.82E-08	2.11E-03	4.44E-03	1.12E-05	3.50E+00
process	Bioethanol ^{31,32}	9.42E-01	3.20E-08	3.96E-02	1.73E-03	1.01E-04	1.28E+01

Table S12. The amount of CO₂ absorbed by bio-based feedstock used for bio-based chemical production

Bio-based chemical production	Unit	Value
Bio-based ethylene	kg CO ₂ /kg ethylene	3.14E+00
Bio-based acetic acid	kg CO ₂ /kg acetic acid	1.47E+00
Bio-based ethyl acetate	kg CO ₂ /kg ethyl acetate	2.00E+00

Table S13. Environmental impact caused by potential process alternatives producing ethyl acetate

Alternative process	Utilized feedstock	Global warming [kg CO ₂ eqv. /kg ethanol]	Photochemical ozone depletion [kg CFC-11 eqv. /kg ethanol]	Acidification [kg SO ₂ eqv. /kg ethanol]	Eutrophication [kg PO ₄ eqv. /kg ethanol]	Photo-oxidant formation [kg C ₂ H ₄ eqv. /kg ethanol]	Energy consumption [MJ/ kg ethanol]
Alternative 1	Sugarcane	1.42E+00	8.14E-08	2.46E-02	4.06E-03	8.29E-04	1.11E+01
	Corn	3.44E+00	2.99E-07	3.26E-02	2.41E-02	9.55E-04	3.24E+01
	Corn stover	2.07E+00	5.54E-08	5.91E-02	7.18E-03	7.57E-04	2.28E+01
Alternative 3A	Sugarcane	1.79E+00	1.19E-07	3.13E-02	4.86E-03	1.08E-03	1.59E+01
	Corn	4.11E+00	3.68E-07	4.05E-02	2.79E-02	1.23E-03	4.03E+01
	Corn stover	2.54E+00	8.95E-08	7.08E-02	8.44E-03	1.00E-03	2.93E+01
Alternative 3B	Sugarcane	1.77E+00	1.35E-07	3.10E-02	4.84E-03	1.07E-03	1.68E+01
	Corn	4.06E+00	3.82E-07	4.01E-02	2.76E-02	1.21E-03	4.10E+01
	Corn stover	2.51E+00	1.05E-07	7.01E-02	8.38E-03	9.86E-04	3.00E+01
Alternative 3C	Sugarcane	1.62E+00	1.48E-07	2.71E-02	4.88E-03	8.80E-04	1.62E+01
	Corn	4.01E+00	4.05E-07	3.66E-02	2.87E-02	1.03E-03	4.14E+01
	Corn stover	2.39E+00	1.17E-07	6.79E-02	8.57E-03	7.96E-04	3.00E+01
Alternative 3E	Sugarcane	2.06E+00	1.24E-07	3.83E-02	4.87E-03	1.41E-03	1.87E+01
	Corn	4.22E+00	3.56E-07	4.69E-02	2.63E-02	1.55E-03	4.15E+01
	Corn stover	2.76E+00	9.58E-08	7.51E-02	8.20E-03	1.34E-03	3.12E+01