

**Supporting Information (SI) for**

**Life Cycle Carbon Footprint of Ethanol and Potassium Acetate Produced from a Forest Product Wastewater Stream by a Co-located Biorefinery**

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## 1. Introduction

### 1.1 Ethanol potential from hardboard wastewater as feedstock

In the process of hardboard production, a large quantity of water is utilized to pre-treat the wood chips. The effluent water from the pre-treatment step, containing wood fibers, soluble sugar and extractives, is treated in wastewater treatment plants (WWTPs) in the U.S. It has been estimated recently that the annual capacity of U.S. hardboard production is 1.5 million tons in the 16 plants all over the country.<sup>1</sup> The amount of water needed for hardboard production is 18.3 L/kg hardboard (12 L/kg for smooth-one-side hardboard and 24.6 L/kg for smooth two-side-hardboard).<sup>1</sup> According to the characterization results of a hardboard wastewater,<sup>2</sup> the solid percentage is 1.42%, and 60% of the solid can be converted to sugar, and with 40% of sugar fermented to ethanol. Annual ethanol production from wastewater in U.S. hardboard facilities are calculated in equation (1) below.

$$\begin{aligned} & \text{Annual ethanol production from wastewater in hardboard facilities} \\ &= 1.5 \text{ million tons} \times 18.3 \text{ L/kg (million m}^3\text{/million tons)} \\ & \times 1 \text{ million ton/million m}^3 \times 1.42\% \times 60\% \times 40\% = 0.09 \text{ million tons} \\ &= 0.09 \text{ million tons} \times 1000 \text{ (kg/ton)} / 0.789 \text{ (kg/l)} / 3.785 \text{ (l/gallon)} = 31 \text{ million gallons} \end{aligned} \quad (1)$$

### 1.2 Biorefineries and biorefineries co-located with industrial facilities

Biorefineries are designed to produce biomass-derived products to replace petroleum-refinery energy products as well as other chemical by-products.<sup>3-5</sup> Previously, most biorefineries were designed as stand-alone facilities. However, integrating a co-located biorefinery into an existing manufacturing facility has been more and more discussed.<sup>6, 7</sup> In some cases, co-located biorefinery can not only minimize the waste materials discharged to the environment, but could also support the original facility with its by-products (steam, electricity etc.) to make all of the processes more efficient. Some candidate facilities with this potential include sawmill facilities, pulp and paper facilities, wood panel facilities, biochemical facilities, energy facilities and pellet facilities.<sup>6</sup> This paper focuses on biofuels production facility co-located with an existing forest

products manufacturing site, and sharing material and energy flows with that facility. Beyond the normal allocation issues of biorefinery co-products, the sharing of material and energy flows with the existing manufacturing facility must also be considered.

### 1.3 Attributional versus Consequential approaches

Attributional and consequential approaches are two main frameworks to perform LCA.<sup>8</sup> Attributional LCA (ALCA) is used to estimate the life cycle impact of a product including the processes and materials used to produce the product, whereas consequential LCA (CLCA) is used to perform the consequence of changes brought by a potential decision, including not only the changes in the processes and materials used to produce the product, but also the changes outside of the life cycle of the product.<sup>8,9</sup> Another obvious difference exists in the allocation methods, ALCA allocates the emissions based on the mass, energy content or market value of different products, whereas CLCA uses only system expansion (also known as displacement method or substitution method). Both approaches have advantages and disadvantages, however the uncertainty of CLCA is much higher compared to ALCA because of the need to model external technical and ecosystem processes. Regulatory development of biofuel has employed both approaches, for example, the GREET (Greenhouse gases, Regulated Emissions and Energy use in Transportation) model is an ALCA (except for land use changes caused by the production of biofuels which is included as a consequence of biofuels production), while the U.S. renewable fuel standards under the 2007 U.S. Energy Independence and Security Act (RFS2) by EPA is consistent with a CLCA methodology.<sup>10</sup>, however GHG emissions credits and debits are allocated to RINs-generating products using energy allocation. The EU's Renewable Energy Directive (RED) employs energy allocation in general, but system expansion for excess electricity from co-generation.<sup>9</sup> Therefore, both the RFS2 and RED has the option to employ "hybrid" allocation which includes both ALCA and CLCA elements.

### 1.4 Scenario analysis, sensitivity analysis and uncertainty analysis

In LCA, the goals of scenario analysis, sensitivity analysis and uncertainty analysis are similar, and this section will focus on the differences among them. Simulations and models have been applied in many fields of sciences, engineering and in policy studies. In a simulation which is

related to future picturing and decision making, many uncertainties need to be taken into account.<sup>11, 12</sup> Scenario analysis is a method picturing several alternative outcomes instead of offering one exact prediction. The purpose of a scenario analysis is to understand the effect and interactions between variables on the results of a model, where the variables include not only model inputs but also any assumptions.<sup>13</sup> A standard scenario analysis should include the assumptions with least certainty, and there are usually an optimistic, a pessimistic and a most likely scenario.<sup>13, 14</sup>

A sensitivity analysis is a study evaluating how sensitive is the result of a model to the uncertainty of one variable. In another words, the purpose of a sensitivity analysis is to show how wide or narrow the range that one variable can be without significant change to the result of the model.<sup>12</sup> Uncertainty analysis studies the uncertainty of model conclusion quantitatively.<sup>12</sup> Uncertainty analysis requires that the inputs to the model (variables) be known with regard to their statistical uncertainty characteristics (average, variance, etc.). Therefore, sensitivity analysis and uncertainty analysis are usually conducted together; that is to identify the variables in the model to which the results are most sensitive to using sensitivity analysis, and to quantitatively evaluate the uncertainty by uncertainty analysis.

In a preliminary carbon footprint analysis such as the one conducted in this study, uncertainty characteristics for all important variables have not yet been established. In addition, key model assumptions and variables have not yet been identified. Therefore, our study uses scenario analysis as the initial approach to understand model uncertainty and effects of model assumptions. Future studies may investigate carbon footprint uncertainty after statistical properties of key inputs are established through research on the biofuel conversion processes.

## 2. Energy saving from hot water return

From our industrial partner, we know that the flow rate of the hot water returned from the biorefinery to the hardboard facility is 92455 lb/hr, and the temperature of hot water drops from 174 °F to 95 °F when used in the hardboard facility. The heat efficiency of 0.8 was applied in the assumption to estimate the energy and GHG savings. Therefore, the energy saving is

$$92455 \frac{\text{lb}}{\text{hr}} \times (174^\circ\text{F} - 95^\circ\text{F}) \times 24 \frac{\text{hr}}{\text{day}} \times 345 \frac{\text{day}}{\text{yr}} \times 1\text{btu} \div 0.8 = 7.56 \times 10^{10} \text{ BTU} = 7.98 \times 10^7 \text{ MJ/yr} \quad (2)$$

The hot water return can reduce  $7.98 \times 10^7$  MJ/yr energy generated from coal in the hardboard facility.

### 3. WWT burden

#### 3.1. N<sub>2</sub>O

In general wastewater treatment processes, emissions of N<sub>2</sub>O are between 0.96 g to 3.2 g per m<sup>3</sup>.

<sup>15</sup> Therefore, the emission factor of N<sub>2</sub>O in hardboard facilities is assumed to be 2 g N<sub>2</sub>O/m<sup>3</sup>, around the middle of the general range.

$$4. \text{ Emissions} = \text{Annual volume of wastewater treated} \times \text{N}_2\text{O emitted per m}^3 = 322 \frac{\text{gal}}{\text{min}} \times 60 \frac{\text{min}}{\text{hr}} \times 24 \frac{\text{hr}}{\text{day}} \times 345 \frac{\text{day}}{\text{yr}} \times 3.785 \frac{\text{l}}{\text{gal}} \times \frac{0.001\text{m}^3}{1} \times 2 \text{ g } \frac{\text{N}_2\text{O}}{\text{m}^3} = 1.21 \times 10^6 \text{ gN}_2\text{O/yr} \quad (3)$$

#### 4.1. CH<sub>4</sub>

The annual methane emission is assumed following equation (4), <sup>15</sup>

$$\begin{aligned} \text{Annual methane emissions} &= \text{Annual sludge production (tons per year)} \\ &\times \text{methane potential (g CH}_4 \text{ per ton)} \times \text{emission factor} \end{aligned} \quad (4)$$

The flow rate of wood solids in the wastewater stream is 3000 lb/hr, and around 10% of the solid forms sludge. Thus,

$$\begin{aligned} \text{Annual production of sludge} &= 3000 \text{ lb/hr} \div 2.205 \text{ lb/kg} \times 24 \text{ hr/day} \times 345 \text{ day/yr} \times \\ &10\% = 1.13 \times 10^6 \text{ kg/yr} \end{aligned} \quad (5)$$

The methane potential is assumed to be 200 kg CH<sub>4</sub> per ton solids,<sup>5</sup> that is

$$200\text{kg CH}_4/\text{ton} = 200 \text{ kg CH}_4/1000 \text{ kg} = 0.2 \text{ kg CH}_4/(\text{kg sludge}) \quad (6)$$

Emission factor is 0.18, therefore,

$$\begin{aligned} \text{Annual methane emissions} &= 1.13 \times 10^6 \text{ kg/yr} \times 0.2\text{kg CH}_4/(\text{kg sludge}) \times 0.18 = 4.07 \times \\ &10^6 \text{ kg CH}_4/\text{yr} \end{aligned} \quad (7)$$

#### 4.2. CO<sub>2</sub>

Another emission that needs to be considered due to the WWT is the carbon dioxide from the utilization of fertilizer (from fossil C in urea fertilizer). The input of fertilizer is  $9.07 \times 10^5$  kg/yr, with the ratio of nitrogen to phosphorus containing fertilizers as 5:1 (5/6 kg N / kg fertilizer).

Urea ammonium nitrate is used to provide the nitrogen, which has an N-content of 32%.

Thus,

$$\begin{aligned} & \text{The amount of N in the fertilizer} \\ & = 9.07 \times 10^5 \text{ kg/yr} \times \frac{5}{6} \times 32\% = 2.42 \times 10^5 \text{ kg N/yr} \end{aligned} \quad (8)$$

The ratio of CO<sub>2</sub> released during WWT to nitrogen in urea is 0.786, therefore,

$$\text{The emission of CO}_2 = 2.42 \times 10^5 \text{ kg N/yr} \times 0.786 = 1.90 \times 10^5 \text{ kg CO}_2/\text{yr} \quad (9)$$

#### 4. GHG emission from processing water

In order to assess the GHG emission from industrial water, an evaluation was conducted on the industrial water used in the biorefinery plant. “Water, completely softened, at plant/RER S” and “Water, decarbonised, at plant/RER S” from ecoprofile were selected to simulate industrial water used in the biorefinery plant as shown in Table S4. The burden of these two items were expressed as “kg CO<sub>2</sub> eq/ kg water” in the second row of Table S4. Take “Water, completely softened, at plant/RER S” for example, with the annual input of water in the biorefinery plant ( $3.5 \times 10^8$  kg), and annual ethanol production in the form of energy ( $6.04 \times 10^7$  MJ), the burden of industrial water per MJ ethanol were calculated as

$$\begin{aligned} & 2.43 \times 10^{-5} \text{ kg CO}_2 \text{ eq/kg water} \times 3.5 \times 10^8 \text{ kg water} \div 6.04 \times 10^7 \text{ MJ} \times \\ & 1000 \frac{\text{g CO}_2 \text{ eq/kg water}}{\text{kg CO}_2 \text{ eq/kg water}} = 0.14 \text{ g CO}_2 \text{ eq/kg ethanol} \end{aligned} \quad (10)$$

With the same method, “Water, decarbonised, at plant/RER S” from the ecoprofile simulates the burden of industrial water as 0.05 g CO<sub>2</sub> eq/kg ethanol. Therefore, we can conclude that the GHG impact from industrial water is little compared to other inputs.

#### 5. Allocation factor calculation

##### 5.1 Mass allocation

As shown in Table S5, the annual production of 50% solution of potassium acetate is  $3.84 \times 10^6$  kg, and that of ethanol is  $2.28 \times 10^6$  kg.

Thus,

$$\text{Mass allocation factor of ethanol} = \frac{2.28 \times 10^6}{3.84 \times 10^6 \times 50\% + 2.28 \times 10^6} = 0.54 \quad (11)$$

## 5.2 Market value allocation

The price of potassium acetate used in this analysis was obtained from alibaba website.<sup>16</sup> The price range offered by five sellers were listed in Table S6, the average price was calculated as 1.35 \$/kg, with the standard deviation 23%. The price of ethanol ranges from 1.94\$/gal to 2.72\$/gal during 2011-2013,<sup>17</sup> and the average price was calculated as 2.33\$/gal, with the standard deviation 24%. Therefore, it is reasonable to assume the wholesale price of potassium acetate as 1.5\$/kg, that of ethanol is 2.5\$/gal, and the price fluctuation of the two products are  $\pm 25\%$ .

As shown in Table S7, the wholesale price of potassium acetate is assumed to be 1.5\$/kg, and that of ethanol is assumed to be 2.5 \$/gal.<sup>17,18</sup>

$$\begin{aligned} \text{The annual value of potassium acetate produced in integrated biorefinery} &= 1.5 \text{ \$/kg} \times \\ &1.92 \times 10^6 \text{ kg/yr} = 2.88 \times 10^6 \text{ \$/yr} \end{aligned} \quad (12)$$

$$\begin{aligned} \text{The annual value of ethanol produced} &= 2.5 \text{ \$/gal} \times \frac{1}{0.789 \text{ kg/l}} \times \frac{1}{3.785 \text{ l/gal}} \times 2.28 \times \\ &10^6 \text{ kg/yr} = 1.91 \times 10^6 \text{ \$/yr} \end{aligned} \quad (13)$$

Consequently,

$$\text{Market value allocation factor of ethanol} = \frac{1.91 \times 10^6}{2.88 \times 10^6 + 1.91 \times 10^6} = 0.4 \quad (14)$$

## 5.3 Scenario 5-Yield of KAC

In scenario 5, the environmental impacts of the two products were evaluated when the yield of potassium acetate had 10 % fluctuation. As allocation factor is related to the yield of both ethanol and potassium acetate, the calculation procedure of both situations are shown in equations (15) to (18).

When yield of potassium acetate is 10% more,  $2.11 \times 10^6$  kg/yr,

$$\begin{aligned} \text{The annual value of potassium acetate produced in integrated biorefinery} &= 1.5 \text{ \$/kg} \times \\ 2.11 \times 10^6 \text{ kg/yr} &= 3.17 \times 10^6 \text{ \$/yr} \end{aligned} \quad (15)$$

Thus,

$$\text{Market value allocation factor of ethanol} = \frac{1.91 \times 10^6}{1.91 \times 10^6 + 3.17 \times 10^6} = 0.38 \quad (16)$$

While when the yield of potassium acetate is 10% less,  $1.73 \times 10^6$  kg/yr,

$$\begin{aligned} \text{The annual value of potassium acetate in the integrated biorefinery} &= 1.5 \text{ \$/kg} \times 1.73 \times \\ 10^6 \text{ kg/yr} &= 2.60 \times 10^6 \text{ \$/yr} \end{aligned} \quad (17)$$

Thus,

$$\text{The Market Value Allocation Factor of Ethanol} = \frac{1.91 \times 10^6}{1.91 \times 10^6 + 2.60 \times 10^6} = 0.42 \quad (18)$$

#### 5.4 Scenario 7-Price fluctuation

The price of the two products has an influence on the analysis by effecting the allocation factor, when market value allocation method is applied. 25% price fluctuation was evaluated to get the range of market value allocation factors of ethanol, that is, a 25% increase in price for ethanol plus a 25% decrease in price for potassium acetate and vice versa.

When the decreased price of ethanol and increased price of potassium acetate are applied,

$$\text{Market value factor of ethanol} = \frac{1.91 \times 10^6 \times (1-25\%)}{2.88 \times 10^6 \times (1+25\%) + 1.91 \times 10^6 \times (1-25\%)} = 0.28 \quad (19)$$

When the increased price of ethanol and decreased price of potassium acetate are applied,

$$\text{Market value factor of ethanol} = \frac{1.91 \times 10^6 \times (1+25\%)}{2.88 \times 10^6 \times (1-25\%) + 1.91 \times 10^6 \times (1+25\%)} = 0.52 \quad (20)$$

## 6. Scenario analyses: Results and discussion

Table S9, S10 and S11, the direct effect on net GHG emission due to a change of one parameter is shown.

In scenario 1, the energy resource alteration in the biorefinery process reduces GHG emission resulting from the energy used to produce steam. For ethanol, the utilization of natural gas and biomass reduces the GHG emission in this sector from 150 g CO<sub>2</sub> eq/MJ to 102 and 6.5 g CO<sub>2</sub> eq/MJ, respectively, in the system expansion method. In the market value allocation method, GHG emission from the same input is reduced from 60 g CO<sub>2</sub> eq/MJ to 41 and 2.6 g CO<sub>2</sub> eq/MJ respectively. For potassium acetate, net GHG emission is also reduced with the savings of energy for steam in the biorefinery process, in the market value allocation method, natural gas and biomass avoid GHG emission of 900 and 2707 g CO<sub>2</sub> eq/kg, respectively. As the use of natural gas and biomass could save around one third and more than 95% GHG emission from the energy for steam respectively, these changes can result in considerable life cycle GHG emissions.

In scenario 2, the net GHG emissions show leading negative impact to the environment. Compared to the basecase, both situations considered in WWTP cause more net GHG emissions due to a combined effect of lower credits from WWT savings and lower burden in the remaining WWTP. As the input in WWT savings is 100% of the original WWT plant, and the remaining input in biorefinery WWTP is only 40% of that, the WWT savings is the dominant factor. When the biorefinery plant is integrated in a forest product facility, whose power and steam in WWTP is generated by more sustainable energy, such as natural gas in scenario 2a, and biomass in scenario 2b, the life cycle GHG emission of the biorefinery products are considerably increased compared to those using hard coal. In system expansion method, 356 and 249 g CO<sub>2</sub> eq/ MJ of GHG emission was saved from the replacement of WWTP when natural gas and biomass are applied, instead of 500 g CO<sub>2</sub> eq/MJ. Thus the life cycle GHG emission are also brought from - 27.2 g CO<sub>2</sub> eq/ MJ to 102.8 and 258.1 g CO<sub>2</sub> eq/ MJ. In market value allocation method, similarly, net GHG emission are three and seven times more than that in basecase for ethanol; one and four times more for potassium acetate when the biorefinery plant partially replaces a natural gas or biomass driven WWTP that a hard coal fired one.

In scenario 3, the GHG emissions from each individual input is effected in ratio when there's a change in the yield of ethanol or potassium acetate. In scenarios 4 and 6, the fluctuation in the yield of KAc and price cause changes in allocation factors as calculated in section 1, thus the GHG emission from each individual input is allocated with the new allocation factors. In scenario 5, net GHG emissions are changed only due to the differences from the remaining biorefinery WWT plant.

**Table S1.** Michigan Grid Distribution<sup>19</sup>

<b>Category of Primary Energy</b>	<b>Michigan Net Electricity Generation (GWh)</b>	<b>Percentage</b>	<b>Inventory Data Sources (ecoinvent)</b>
<b>Petroleum-Fired</b>	11	0%	-
<b>Natural Gas -Fired</b>	1820	18%	Electricity, natural gas, at power plant/US S
<b>Coal - Fired</b>	5531	56%	Electricity, hard coal, at power plant/US S
<b>Nuclear</b>	2293	23%	Electricity, nuclear, at power plant/US S
<b>Other Renewables</b>	272	3%	Electricity, Renewable Energy MI (Table S2)
<b>Sum</b>	9927	100%	Electricity, Renewable Energy MI (Table S2)

**Table S2.** Distribution of Renewable Power in Michigan Grid<sup>19</sup>

<b>Generation</b>	<b>Value (thousand megawatthours)</b>	<b>Percent of State Total</b>	<b>Percentage of Renewable Net Generation</b>	<b>Inventory Data Sources (ecoinvent)</b>
<b>Total Renewable Net Generation</b>	<b>4,084</b>	<b>3.7%</b>		<b>Electricity, Renewable Energy MI</b>
Geothermal	-	-	-	-
Hydro Conventional	1,251	1.1%	31%	Electricity, hydropower, at power plant/DE S
Solar	-	-	-	-
Wind	360	0.3%	9%	Electricity, at wind power plant/RER S
Wood/Wood Waste	1,670	1.5%	41%	Electricity, biomass, at power plant/US
MSW/Landfill Gas	795	0.7%	19%	Electricity from waste, at municipal waste incineration plant/CH S
Other Biomass	8	0%	0%	-

**Table S3.** Inputs and Outputs: Inventory Data with Sources

<b>Input and Output Category</b>	<b>Inventory Data Sources (ecoinvent)</b>
<b>Inputs</b>	
Electricity	
Electricity (from MI Grid) (MJ)	The distribution is shown in Tables S1 and S2
Electricity (from WWTP Mix) (MJ)	Electricity in DPI
Energy Savings (MJ)	Hard coal, burned in industrial furnace 1-10MW/RER S
Steam	
Steam for Process Heat from Coal (MJ)	Hard coal, burned in industrial furnace 1-10MW/RER S
Steam from WWTP Mix (MJ)	Electricity, Michigan Grid Mix (See Tables S1 and A2 for detail)
Chemical Inputs	
KOH, 50% wt. (kg)	Potassium hydroxide, at regional storage/RER S
Lime (kg)	Lime, hydrated, packed, at plant/CH S
H <sub>2</sub> SO <sub>4</sub> (kg)	Sulphuric acid, liquid, at plant/RER S
Fertilizer 5:1 N:P ratio (kg) as N	Urea ammonium nitrate, as N, at regional storehouse/RER S
Fertilizer 5:1 N:P ratio (kg) as P	Thomas meal, as P <sub>2</sub> O <sub>5</sub> , at regional storehouse/RER S
Yeast (kg)	Yeast paste, from whey, at fermentation/CH S
Yeast Extract (kg)	Yeast paste, from whey, at fermentation/CH S
Polymer Flocculants (kg)	Acrylonitrile-butadiene-styrene copolymer, ABS, at plant/RER S
Al <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> (kg)	Aluminium sulphate, powder, at plant/RER S
Ca(NO <sub>3</sub> ) <sub>2</sub> (kg)	Calcium nitrate, as N, at regional storehouse/RER S
<b>Outputs</b>	
KAc (50% soln)	Potassium hydroxide, at regional storage/RER S; Acetic acid, 98% in H <sub>2</sub> O, at plant/RER S
Ethanol	-

**Table S4.** GHG Emission from Industrial water

<b>Catogory</b>	<b>Unit</b>	<b>Water, completely softened, at plant/RER S</b>	<b>Water, decarbonised, at plant/RER S</b>
<b>GHG Emission from the IPCC GWP 100a Method</b>	kg CO <sub>2</sub> eq/kg water	$2.43 \times 10^{-5}$	$7.74 \times 10^{-6}$
<b>Annual GHG Emission from Water in Biorefinery Plant</b>	kg CO <sub>2</sub> eq	$8.58 \times 10^3$	$2.73 \times 10^3$
<b>GHG Emissions on Basis of Per MJ of Ethanol Produced</b>	g CO <sub>2</sub> eq/MJ ethanol	0.14	0.05

**Table S5.** Mass Allocation Factor Calculation

	Basecase	Scenario 5	
	Value	KAC Yield 10%+	KAC Yield 10%-
<b>K Acetate Production (kg/yr)</b>	$1.92 \times 10^6$	$2.11 \times 10^6$	$1.73 \times 10^6$
<b>KAC Wholesale Price (\$/kg K-Acetate)</b>	1.50	1.50	1.50
<b>K Acetate Value Production (\$/yr)</b>	$2.88 \times 10^6$	3.17E+06	$2.59 \times 10^6$
<b>Ethanol Production (kg/yr)</b>	$2.28 \times 10^6$	2.28E+06	$2.28 \times 10^6$
<b>EtOH Wholesale Price (\$/gal ethanol)</b>	2.50	2.50	2.50
<b>Ethanol Value Production (\$/yr)</b>	$1.91 \times 10^6$	1.91E+06	$1.91 \times 10^6$
<b>Total Value Production (\$/yr)</b>	$4.79 \times 10^6$	5.08E+06	$4.50 \times 10^6$
<b>Market Value Allocation Factor Ethanol</b>	0.40	0.38	0.42

**Table S6.** Price of Potassium Acetate and Price Fluctuation Estimate<sup>12</sup>

<b>Seller</b>	<b>Price Range</b>	
<b>#1</b>	1.40-1.55	
<b>#2</b>	0.99-1.35	
<b>#3</b>	1.00-2.00	
<b>#4</b>	1.30-1.50	
<b>#5</b>	1.00-1.35	
	Average	Standard Diviation
	1.34	23%

**Table S7.** Market Value (Price) Allocation Factor Calculation

	Basecase	Scenario 7	
	Value	Ethanol Price 25%-/ KAC Price 25%+	Ethanol Price 25%+/ KAC Price 25%-
<b>K Acetate Production (kg/yr)</b>	$1.92 \times 10^6$	$1.92 \times 10^6$	$1.92 \times 10^6$
<b>KAC Wholesale Price (\$/kg K-Acetate)</b>	1.50	1.875	1.125
<b>K Acetate Value Production (\$/yr)</b>	$2.88 \times 10^6$	$3.60 \times 10^6$	$2.16 \times 10^6$
<b>Ethanol Production (kg/yr)</b>	$2.28 \times 10^6$	$2.28 \times 10^6$	$2.28 \times 10^6$
<b>EtOH Wholesale Price (\$/gal ethanol)</b>	2.50	1.875	3.125
<b>Ethanol Value Production (\$/yr)</b>	$1.91 \times 10^6$	$1.43 \times 10^6$	$2.39 \times 10^6$
<b>Total Value Production (\$/yr)</b>	$4.79 \times 10^6$	$5.04 \times 10^6$	$4.55 \times 10^6$
<b>Market Value Allocation Factor Ethanol</b>	0.40	0.28	0.52

**Table S8.** Ecoprofiles of Alternative Energy Resources in Scenarios 1&2

Scenario		Inventory Data Sources (ecoinvent)	
	Alternative Energy Resources	Natural Gas	Biomass
#1	Used in biorefinery plant for heat	Heat, natural gas, at industrial furnace >100kW/RER S	Heat, mixed chips from forest, at furnace 1000kW/CH S
#2	Used in the WWTP for heat and power	Heat, natural gas, at industrial furnace >100kW/RER S	Heat, mixed chips from industry, at furnace 1000kW/CH S

**Table S9.** Scenario Analysis-GHG impact of ethanol from different stages in system expansion method

GHG Emission of Ethanol(D)-Scenario Analysis (g CO <sub>2</sub> eq/MJ)	Biorefinery Inputs			Emission Credits			Biorefinery WWTP	Total
	Electricity	Energy for Steam	Chemicals	Credits from KAC	Energy Saved from Hot Water	WWTP P Savings	Remaining Biorefinery WWTP	
<b>Basecase</b>	261.0	150.0	66.0	-65.1	-139.0	-500.0	200.0	-27.1
<b>Scenario 1a</b>	261.0	102.0	66.0	-65.1	-139.0	-500.0	200.0	-75.1
<b>Scenario 1b</b>	261.0	6.5	66.0	-65.1	-139.0	-500.0	200.0	-170.6
<b>Scenario 2a</b>	261.0	150.0	66.0	-65.3	-94.9	-356.0	142.0	102.8
<b>Scenario 2b</b>	261.0	150.0	66.1	-65.1	-4.4	-249.0	99.5	258.1
<b>Scenario 3a</b>	290.0	167.0	73.4	-72.3	-154.0	-555.0	222.0	-29.0
<b>Scenario 3b</b>	237.0	136.0	59.8	-58.9	-126.0	-453.0	181.0	-24.1
<b>Scenario 4a</b>	261.0	150.0	66.0	-58.5	-139.0	-500.0	200.0	-20.5
<b>Scenario 4b</b>	261.0	150.0	66.0	-71.6	-139.0	-500.0	200.0	-33.6
<b>Scenario 5a</b>	261.0	150.0	66.0	-65.1	-139.0	-500.0	250.0	22.9
<b>Scenario 5b</b>	261.0	150.0	66.0	-65.1	-139.0	-500.0	150.0	-77.1

**Table S10.** Scenario Analysis-GHG impact of ethanol from different stages in market value allocation method

GHG Emission of Ethanol (P)-Scenario Analysis (g CO <sub>2</sub> eq/MJ)	Biorefinery Inputs			Emission Credits		Biorefinery WWTP	Total
	Electricity	Energy for Steam	Chemicals	Energy Saved from Hot Water	WWTP Savings	Remaining Biorefinery WWTP	
<b>Basecase</b>	105.0	60.0	26.4	-55.4	-200.0	80.0	16.0
<b>Scenario 1a</b>	105.0	41.0	26.4	-55.4	-200.0	80.0	-3.0
<b>Scenario 1b</b>	105.0	2.6	26.4	-55.4	-200.0	80.0	-41.4
<b>Scenario 2a</b>	105.0	60.1	26.4	-37.9	-142.0	56.9	68.5
<b>Scenario 2b</b>	105.0	60.1	26.4	-2.4	-99.5	39.8	129.4
<b>Scenario 3a</b>	107.0	61.6	27.2	-57.0	-205.0	82.2	16.0
<b>Scenario 3b</b>	99.4	57.0	25.1	-52.7	-190.0	76.1	14.9
<b>Scenario 4a</b>	110.0	63.0	27.7	-58.2	-210.0	84.0	16.5
<b>Scenario 4b</b>	99.3	57.0	25.1	-52.7	-190.0	76.0	14.7
<b>Scenario 5a</b>	105.0	60.0	26.4	-55.4	-200.0	100.0	36.0
<b>Scenario 5b</b>	105.0	60.0	26.4	-55.4	-200.0	60.0	-4.0
<b>Scenario 6a</b>	73.2	42.0	18.5	-38.8	-140.0	56.0	10.9
<b>Scenario 6b</b>	136.0	78.0	34.3	-72.1	-260.0	104.0	20.2

**Table S11.** Scenario Analysis-GHG impact of KAC from different stages in market value allocation method

GHG Emission of Ethanol (P)-Scenario Analysis (g CO <sub>2</sub> eq/kg)	Biorefinery Inputs			Emission Credits		Biorefinery WWTP	Total
	Electricity	Energy for Steam	Chemicals	Energy Saved from Hot Water	WWTP Savings	Remaining Biorefinery WWTP	
<b>Basecase</b>	4930.0	2830.0	1246.0	-2620.0	-9440.0	3770	716
<b>Scenario 1a</b>	4930.0	1930.0	1246.0	-2620.0	-9440.0	3770	-184
<b>Scenario 1b</b>	4930.0	123.0	1246.0	-2620.0	-9440.0	3770	-1991
<b>Scenario 2a</b>	4930.0	2830.0	1246.0	-1790.0	-6700.0	3780	1546
<b>Scenario 2b</b>	4930	2830	1246	-114	-4680	3360	3862
<b>Scenario 3a</b>	5180.0	2970.0	1308.0	-2750.0	-9910.0	3960	758
<b>Scenario 3b</b>	4770.0	2740.0	1204.0	-2530.0	-9120.0	3650	714
<b>Scenario 4a</b>	5290.0	3030.0	1337.0	-2810.0	-10100.0	4050	797
<b>Scenario 4b</b>	4630.0	2650.0	1169.0	-2450.0	-8850.0	3540	689
<b>Scenario 5a</b>	4930.0	2830.0	1246.0	-2620.0	-9440.0	4720	1666
<b>Scenario 5b</b>	4930.0	2830.0	1246.0	-2620.0	-9440.0	2830	-224
<b>Scenario 6a</b>	3950.0	2260.0	996.3	-2090.0	-7550.0	3020	586
<b>Scenario 6b</b>	5920.0	3400.0	1494.0	-3140.0	-11300.0	4530	904

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