

## Supporting Information

### **Early-Stage Capital Cost Estimation of Biorefinery Processes: A Comparative Study of Heuristic Techniques**

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### Part A. Capital cost methods escalation

There are two ways to actualise a cost into a US cost: either convert at the reference year exchange rate and update with a US plant cost index or update with the reference country plant cost index and convert at 2011 exchange rate<sup>[1]</sup>.

The constant  $k_T$  in Taylor's method is expressed in (£, 1977) using the UK Engineering and Process Economics index (EPE = 280, 1977). This index was published monthly in the homonymous journal from 1970 (base= 100) until 1979<sup>[2]</sup>. Taylor, however, states that the constant can be updated using any other UK index. Bridgwater incorporates the UK PREDICT Plant Cost Index, which is published monthly in Process Engineering. This index, first appeared in 1973 and is rebased every five years. Values for this index were found from several sources and are carefully rebased in 2005, as shown in Fig. S1<sup>[3]</sup>. The 1970's was a period of extreme inflation in the UK and thus, a significant error in calculations is expected if UK indices of this period are used.

Therefore, in this study, the costs are converted to US\$ and plants are relocated in the US using appropriate factors for the reference year and then, an appropriate US plant cost index is used to escalate the costs. This necessity justifies the choice of such a location and currency for the needs of this comparative study. The Chemical Engineering Plant Cost Index (CEPCI) (base= 1958-59) is used to escalate the aforementioned correlations, as well as the constant  $k_k$  in Klumpar et al.'s method, while it is also used to update Petley's correlation<sup>[4]</sup>. Bridgwater's equation (5) employs the Engineering News Record (ENR) index which is being issued in the ENR magazine since 1908 (base= 1913)<sup>[5]</sup>. Furthermore, suitable relocation factors were used wherever required and were derived from publications by Bridgwater, Gerrard<sup>[3a, 6]</sup> and Compass International<sup>[7]</sup>. It should be noted that from 1972 until circa 1980 the UK plant costs were 90-97% of US plant costs<sup>[2b]</sup>.

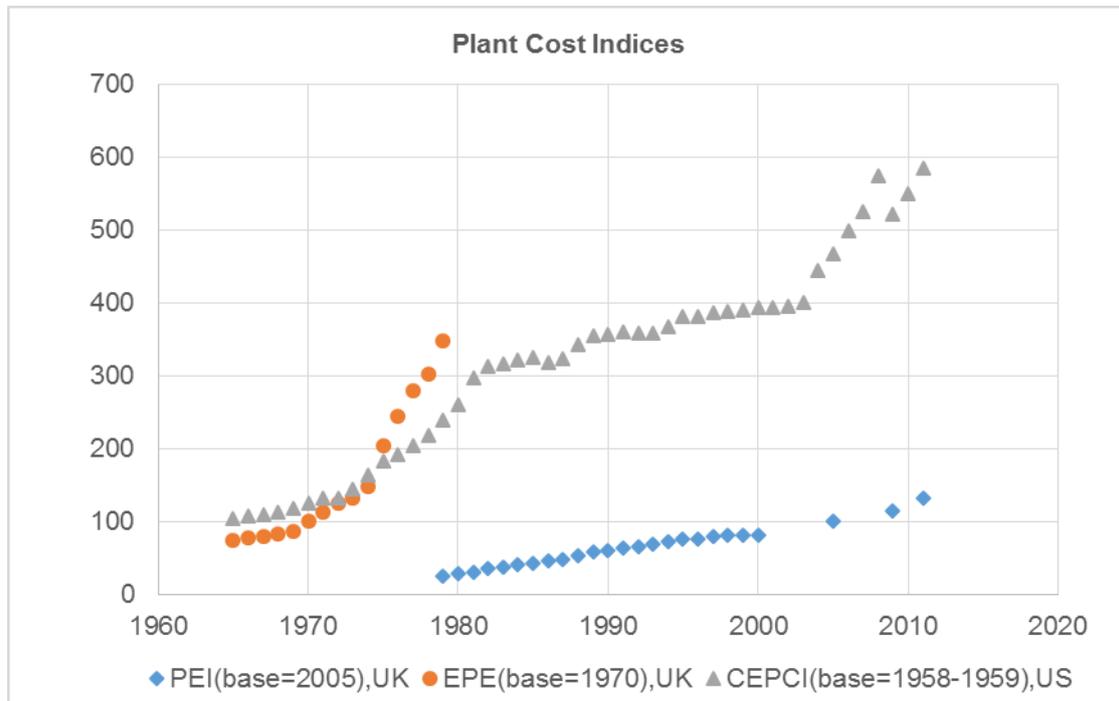


Figure. S1. Plant Cost Indices for the Chemical Industry

Taking into account the previous limitations and selecting the appropriate indices, the correlations under study were modified as follows:

#### Wilson

$$ISBL = f_I \cdot N \cdot (AUC) \cdot F_m \cdot F_p \cdot F_T, \text{ in } \text{£}, 1971, \text{ UK} \quad \text{Eq. (S.1)}$$

$$\text{CEPCI (1971)} = 132.3, \text{ CEPCI (2011)} = 585.7$$

$$1\text{£} = 2.43\text{\$ (1971)}$$

$$\text{Location factor (UK)} = 0.77 \text{ (base=US, 1971)}$$

$$ISBL = 13.97 \cdot 10^{-6} \cdot f_I \cdot N \cdot (AUC) \cdot F_m \cdot F_p \cdot F_T, \text{ in M}\$, 2011, \text{ US} \quad \text{Eq. (S.2)}$$

### **Taylor**

$$ISBL = 0.042 \cdot \sum_1^N (1.3)^S \cdot Q^{0.39}, \text{ in M}\pounds, 1977, \text{ UK} \quad \text{Eq. (S.3)}$$

$$CEPCI (1977) = 204.1, CEPCI (2011) = 585.7$$

$$1\pounds = 1.74\$ (1977)$$

$$\text{Location factor (UK)} = 0.9 \text{ (base=US, 1977)}$$

$$ISBL = 0.233 \cdot \sum_1^N (1.3)^S \cdot Q^{0.39}, \text{ in M}\$, 2011, \text{ US} \quad \text{Eq. (S.4)}$$

### **Bridgwater (A)**

$$GC = 50.26 \cdot N \cdot \left(\frac{Q}{0.5}\right)^{0.85} \cdot \left(\frac{T \cdot n}{N}\right)^{-0.17} \cdot \left(\frac{P \cdot n'}{N}\right)^{0.14} \frac{ENR}{1300}, \text{ Grassroots cost in } \pounds, \text{ UK,} \quad \text{Eq. (S.5)}$$

$$ENR = 9096.82 (2011), ISBL = 75\% \text{ of Grassroots Cost}$$

$$1\pounds = 1.8\$ (1976)$$

$$\text{Location factor (UK)} = 0.97 \text{ (base=US, 1976)}$$

$$ISBL = 489 \cdot 10^{-6} \cdot N \cdot \left(\frac{Q}{0.5}\right)^{0.85} \cdot \left(\frac{T \cdot n}{N}\right)^{-0.17} \cdot \left(\frac{P \cdot n'}{N}\right)^{0.14}, \text{ ISBL in M}\$, 2011, \text{ US,} \quad \text{Eq. (S.6)}$$

### **Bridgwater (B)**

$$ISBL = 158 \cdot N \cdot \left(\frac{Q}{S}\right)^{0.675} \cdot \frac{PEI(UK)}{100}, \frac{Q}{S} > 60000 \text{ tn/yr}, \text{ in } \pounds, \text{ UK} \quad \text{Eq. (S.7)}$$

$$ISBL = 13850 \cdot N \cdot \left(\frac{Q}{S}\right)^{0.3} \cdot \frac{PEI(UK)}{100}, \frac{Q}{S} < 60000 \text{ tn/yr}, \text{ in } \pounds, \text{ UK} \quad \text{Eq. (S.8)}$$

$$PEI (1975) = 100. \text{ Therefore:}$$

$$CEPCI (1975) = 182.4, CEPCI (2011) = 585.7$$

$$1\pounds = 2.21\$ (1975)$$

$$\text{Location factor (UK)} = 0.95 \text{ (base=US, 1975)}$$

$$ISBL = 0.001 \cdot N \cdot \left(\frac{Q}{S}\right)^{0.675}, \frac{Q}{S} > 60000 \text{ tn/yr}, \text{ in M}\$, 2011, \text{ US} \quad \text{Eq. (S.9)}$$

$$ISBL = 0.103 \cdot N \cdot \left(\frac{Q}{S}\right)^{0.3}, \frac{Q}{S} < 60000 \text{ tn/yr}, \text{ in M}\$, 2011, \text{ US} \quad \text{Eq. (S.10)}$$

### **Bridgwater (C)**

$$ISBL = [401600 + 1.304 \cdot \left(\frac{Q}{S}\right)] \cdot N \cdot \left(\frac{PEI(UK)}{100}\right), \text{ in } \pounds, \text{ UK} \quad \text{Eq. (S.11)}$$

$$PEI (1975) = 100. \text{ Therefore:}$$

$$CEPCI (1975) = 182.4, CEPCI (2011) = 585.7$$

$$1\pounds = 2.21\$ (1975)$$

$$\text{Location factor (UK)} = 0.95 \text{ (base=US, 1975)}$$

$$ISBL = \left[3 + 9.7 \cdot 10^{-6} \cdot \left(\frac{Q}{S}\right)\right] \cdot N, \text{ in M}\$, 2011, \text{ US} \quad \text{Eq. (S.12)}$$

### **Bridgwater (D)**

$$ISBL = 193 \cdot N \cdot \left[\left(\frac{Q}{S}\right)^{0.665}\right] \cdot [e^{(2.58 \cdot 10^{-7} Q)}] \cdot [T^{-0.022}] \cdot [P^{-0.064}] \cdot \left[\frac{PEI(UK)}{100}\right], \text{ in } \pounds, \text{ UK} \quad \text{Eq. (S.13)}$$

$$PEI (1975) = 100. \text{ Therefore:}$$

$$CEPCI (1975) = 182.4, CEPCI (2011) = 585.7$$

$$1\pounds = 2.21\$ (1975)$$

$$\text{Location factor (UK)} = 0.95 \text{ (base=US, 1975)}$$

$$ISBL = 1.44 \cdot 10^{-3} \cdot N \cdot \left[\left(\frac{Q}{S}\right)^{0.665}\right] \cdot [e^{(2.58 \cdot 10^{-7} Q)}] \cdot [T^{-0.022}] \cdot [P^{-0.064}], \text{ in M}\$, 2011, \text{ US} \quad \text{Eq. (S.14)}$$

### **Klumpar, Brown, Fromme (A) & (B)**

$$ISBL = 180 \cdot F \cdot N \cdot G^e, e=0.57 \text{ or } e=v, \text{ in } \$, 1981 \text{ (US)} \quad \text{Eq. (S.15)}$$

$$CEPCI (1981) = 297, CEPCI (2011) = 585.7$$

$$ISBL = 3.55 \cdot 10^{-4} \cdot F \cdot N \cdot G^e, \text{ in M}\$, 2011, \text{ US} \quad \text{Eq. (S.16)}$$

### **Petley**

$$ISBL = 55882 \cdot Q^{0.44} \cdot N^{0.486} \cdot T_{max}^{0.038} \cdot P_{max}^{-0.02} \cdot F_m^{0.341}, \text{ in } \$, 1988, \text{ West Germany} \quad \text{Eq. (S.17)}$$

$$CEPCI (1988) = 342.5, CEPCI (2011) = 585.7$$

Location factor (Germany) = 1.03 (base=US, 2011)

$$ISBL = 0.093 \cdot Q^{0.44} \cdot N^{0.486} \cdot T_{max}^{0.038} \cdot P_{max}^{-0.02} \cdot F_m^{0.341} \text{ in M\$, 2011, US} \quad \text{Eq. (S.18)}$$

**Lange**

$$Direct Cost = 3.0 \times (energy losses [MW])^{0.84}, \text{ in M\$, 1993, US} \quad \text{Eq. (S.19)}$$

$$CEPCI (1993) = 359.2, CEPCI (2011) = 585.7$$

$$Direct Cost = 4.9 \times (energy losses [MW])^{0.84}, \text{ in M\$, 2011, US} \quad \text{Eq. (S.20)}$$

$$ISBL = 2.9 \times (energy transfer [MW])^{0.55}, \text{ in M\$, 1993, US} \quad \text{Eq. (S.21)}$$

$$CEPCI (1993) = 359.2, CEPCI (2011) = 585.7$$

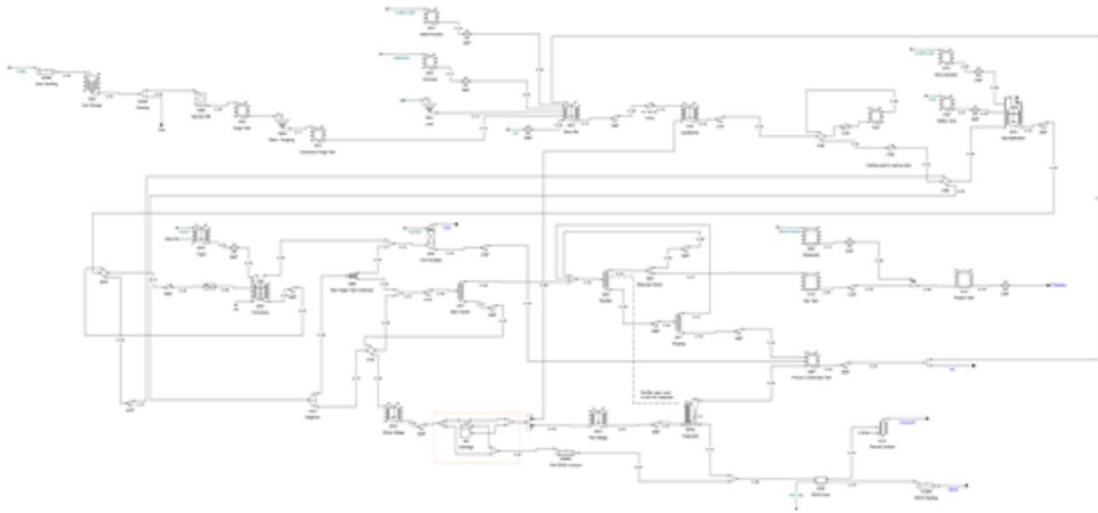
$$ISBL = 4.7 \times (energy transfer [MW])^{0.55}, \text{ in M\$, 2011, US} \quad \text{Eq. (S.22)}$$

Table S1. Updated cost estimation methods		
Author	Correlation	Accuracy (as reported)
Wilson	$ISBL = 13.97 \cdot 10^{-6} \cdot f_l \cdot N \cdot (AUC) \cdot F_m \cdot F_p \cdot F_T$	-30/+50%
Taylor	$ISBL = 0.233 \cdot \sum_1^N (1.3)^S \cdot Q^{0.39}$	±30%
Bridgwater (A)	$ISBL = 489 \cdot 10^{-6} \cdot N \cdot \left(\frac{Q}{S \cdot 0.5}\right)^{0.85} \cdot \left(\frac{T \cdot n}{N}\right)^{-0.17} \cdot \left(\frac{P \cdot n'}{N}\right)^{0.14}$	±25%
Bridgwater (B)	$ISBL = 0.001 \cdot N \cdot \left(\frac{Q}{S}\right)^{0.675}, \frac{Q}{S} > 60000 \text{ tn/yr}$ $ISBL = 0.103 \cdot N \cdot \left(\frac{Q}{S}\right)^{0.3}, \frac{Q}{S} < 60000 \text{ tn/yr}$	±20%
Bridgwater (C)	$ISBL = \left[3 + 9.7 \cdot 10^{-6} \cdot \left(\frac{Q}{S}\right)\right] \cdot N$	±20%
Bridgwater (D)	$ISBL = 1.44 \cdot 10^{-3} \cdot N \cdot \left[\left(\frac{Q}{S}\right)^{0.665}\right] \cdot [e^{(2.58 \cdot 10^{-7} Q)}] \cdot [T^{-0.022}] \cdot [P^{-0.064}]$	±20%
Klumpar, Brown, Fromme (A)	$ISBL = 3.55 \cdot 10^{-4} \cdot F \cdot N \cdot Q^{0.57}$	±30%
Klumpar, Brown, Fromme (B)	$ISBL = 3.55 \cdot 10^{-4} \cdot F \cdot N \cdot Q^v$	±30%
Petley	$ISBL = 0.093 \cdot Q^{0.44} \cdot N^{0.486} \cdot T_{max}^{0.038} \cdot P_{max}^{-0.02} \cdot F_m^{0.341}$	N.A.
Lange	$ISBL = 4.7 \times (energy transfer [MW])^{0.55}$	N.A.
Lange	$DCC = 4.9 \times (energy losses [MW])^{0.84}$	N.A.

**Part B. Biorefinery processes description & flowsheets**

**Ethanol production by dry corn milling**

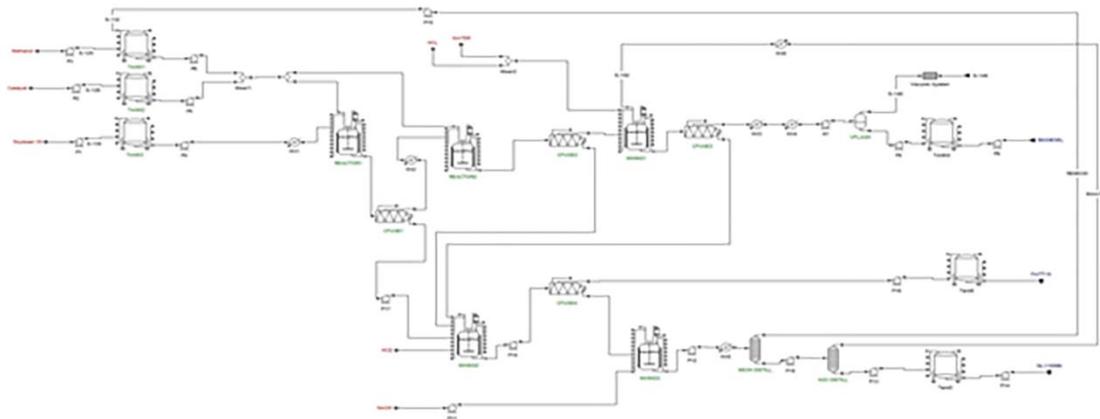
Corn is received, cleaned from foreign materials, ground in hammer mills and sent onto the hoppers. The ground corn is first, mixed with α-amylase, ammonia and lime and then, hydrolysed into polysaccharides via steam injection for 1 hr at 88 °C. The output from the liquefaction is combined with a recycle stream from DDGS production and cooked for 15 min at 110 °C, before being fed to the saccharification reactors for the final conversion of the dextrans into glucose (5 hrs, 61 °C). The glucose is fed to six fermenters, which operate at batch mode (68 hrs) and at 32 °C. CO2 emitted from the fermenters is sent to a scrubber for recovery. Beer from the fermentation is first heated to flash off the vapor and then is fed to the beer column (along with the condensed vapors), where water is removed from the bottom. 99 % of the ethanol is recovered as a distillate from the rectifier, while the stripping column removes the remaining water and the rest of the mixed ethanol is recycled back to the rectifier. The recovered ethanol is driven into the molecular sieves for final purification. The non-fermented material from the beer column's bottom is fed to the whole stillage tank and then water is removed by centrifugation to produce wet distillers grains and a thin stillage. The thin stillage is further dried in a four-effect evaporator, before being mixed with a part of the wet distillers grains and sent to a rotary drum dryer to produce the Dried Distillers Grains<sup>[8]</sup>.



**Figure. S2.** Ethanol production by corn dry milling SuperPro® flowsheet (with permission from Intelligen, Inc)

**Biodiesel production by soyoil transesterification**

Methanol is combined with soyoil triglycerides and sodium methoxide into the first steam jacketed agitated reactors, where transesterification takes place for 1 hr at 60 °C, followed by a centrifugation step to remove the produced glycerol. The upper-rich fatty acid methyl esters phase is fed to a second transesterification reactor to complete the reaction, while a second centrifuge separates the esters from the glycerol. The methyl esters are then washed with water to remove soaps and then centrifuged to remove the aqueous phase and finally, they are sent to a dryer for the final water removal. The glycerol-rich phases are sent to the glycerol purification stage, where they are washed with HCl to transform soaps into fatty acids. The fatty acids are centrifuged and sent to waste. The remaining glycerol phase is neutralised with sodium hydroxide and sent to the methanol recovery column. The remaining water is removed by distillation to produce 80 % w/w glycerol product<sup>[9]</sup>.



**Figure. S3.** Biodiesel production by soyoil transesterification SuperPro® flowsheet (with permission from Intelligen, Inc.)

## Ethanol production by indirectly-heated biomass gasification

The process was modelled using Aspen Plus, the only commercially available software capable of handling sorbent solid components, to handle the rigorous material and energy balances. The NREL's design for the Batelle Columbus Indirectly Heated Gasifier is taken as a base case. Pine chips of appropriate size (<75 mm) and moisture content 15 % enter the Gasifier (RYield, 870 °C, 1.6 bara) which is of a dual fluidized bed design. Heat for the endothermic gasification reactions is supplied by circulating hot olivine sand between the Gasifier vessel and the char combustor (RStoic). The gasification medium is steam and the temperature of the boiler is 982 °C. The majority of the olivine and char (99.9 % of both) is separated in the primary Gasifier cyclone and sent to the char combustor. A secondary cyclone removes 90 % of any residual fines. The char that is formed in the Gasifier is burned in the combustor to reheat the olivine. The primary combustor cyclone separates the olivine (99.9 %) from the combustion gases and the olivine is sent back to the Gasifier. Ash and any sand particles that are carried over are removed in the secondary combustor cyclone (99.9 % separation) followed by an electrostatic precipitator which removes the remaining residual amount of solid particles. The sand and ash mixture is diluted with water and discarded as waste. After immediate cooling of the produced gas at a temperature of 148 °C and at a point where the gas remains above its dew point, a filter is used to remove ash from the gas stream. Any condensate is removed, and the gas is then scrubbed (RadFrac) with water to remove HCl, along with most of the residual ammonia content and any residual particulate material. The product gas still contains H<sub>2</sub>S.

After the syngas is properly conditioned, it passes into the fermenter. The fermenter (RStoic) operates at 3 bar and 37 °C, and contains bacteria (*C. ljundahlii*) which convert part of the CO and H<sub>2</sub> into ethanol, producing CO<sub>2</sub> and consuming water. Unconverted gas which passes out of the fermenter is cooled and chilled to maximize recovery of ethanol. The gas is then scrubbed by a counter-current flow of water, recycled from the distillation area. Liquor from the fermenter, which contains 3 % w/w ethanol and 10 g/l of biomass, is pumped through the membrane unit. The membrane permeate passes to the distillation area, and the thickened retentate returns to the fermenter, first passing through a cooler to remove the heat generated by the ethanol formation and thereby control the fermenter operating temperature. The fermentation liquor from the membrane separator is heated to 100 °C and passes into the first distillation column which operates at 1.9 bar (Stripping column-RadFrac). The column removes CO<sub>2</sub> and removes about 92 % of the water as a bottoms product. The gases are vented to the atmosphere from the top of the column. The ethanol is withdrawn from the column as a vapour side stream. The column bottoms water contains ethanol and is recycled to the fermenter. The vapour stream passes to the rectifier (RadFrac) to produce 92.5 % w/w ethanol which is withdrawn from the column top as vapour at 116 °C. The rectifier bottoms stream still contains ethanol and is cooled and passes to the gas scrubber, before returning to the fermenter. There is a small make-up of water to the top of the scrubber. The ethanol vapour stream from the rectifier passes to the ethanol dehydration unit. Molecular sieve dryers are used to remove the remaining water to produce anhydrous ethanol. The dried ethanol vapour is condensed and pumped off to storage. The water/ethanol vapour stream is condensed in a vacuum set.

For the gasification part, the system thermodynamics are modelled using the RKS-BM (Redlich Kwong Soave with Boston Matthias alpha function) –which is widely used in coal treatment processes, while for the syngas fermentation, NRTL provided for accurate results<sup>[10]</sup>.

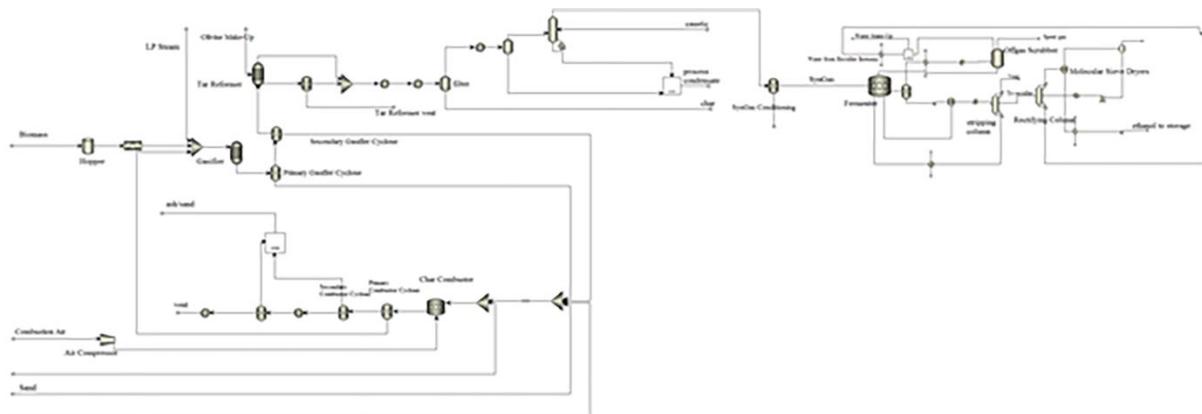
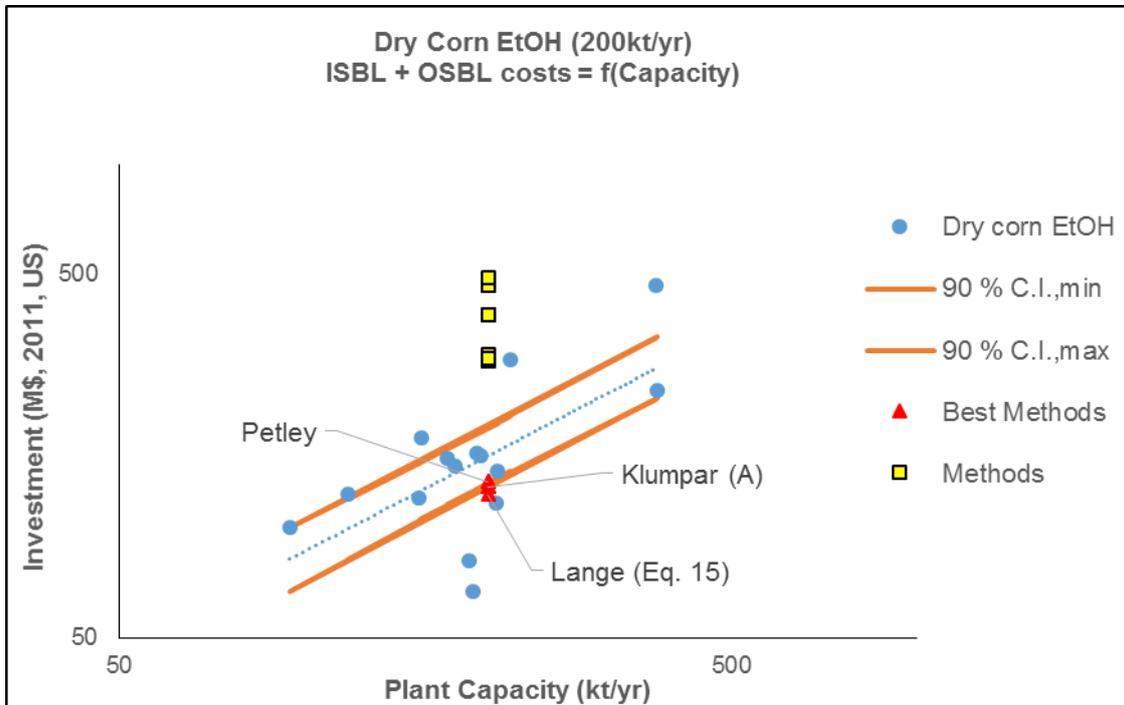


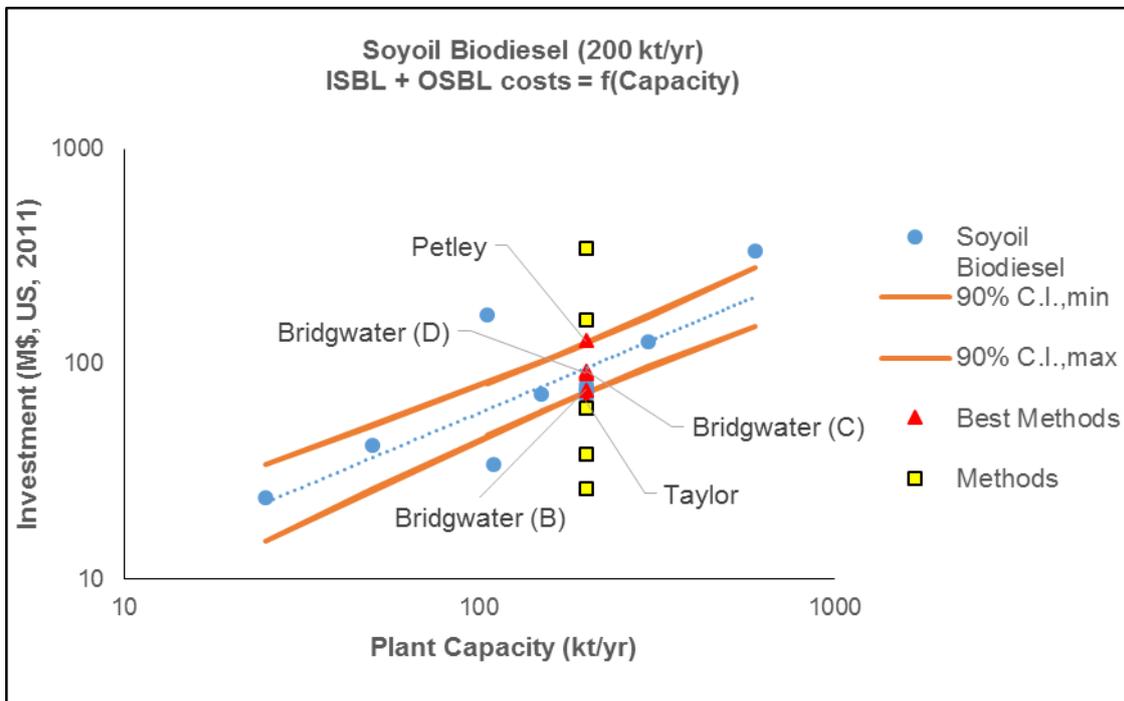
Figure. S4. Ethanol production by indirectly-heated biomass gasification AspenPlus® flowsheet<sup>[10a]</sup>

**Part C. Probabilistic comparison with commercial capital costs: Corn-to-Ethanol and Soyoil Biodiesel at 200 kt/yr**

The biochemical ethanol and soyoil biodiesel processes are upscaled to 200 kt/yr, which is close to the median commercial operating capacity. The upscaled SuperPro flowsheets were prepared and provided by Intelligen, Inc. Careful application of the cost methods on the validation processes provided the following figures:



**Figure. S5.** Corn to Ethanol Biorefineries: Inside + Outside Battery limits cost (M\$, 2011, US) vs plant capacity (kt/yr)



**Figure. S6.** Soyoil Biodiesel Biorefineries: Inside + Outside Battery limits cost (M\$, 2011, US) vs plant capacity (kt/yr)

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