Supporting Information

Optimal production of Furfural and DMF from algae and switchgrass

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Cost analysis

Note: The equipment cost correlations are obtained directly from the source. Later, the final cost of the equipment is updated to 2014 prices. Due to the operating liquids across the plants, stainless steel is selected.

Equipment

1. Washing unit

The Washing operation was considered to be like a screw, so the cost can be estimated as:

$$C_{Wash} = 28,899 \cdot \left(\frac{Load_{(Solids+water)}(lb/h)}{277 \cdot d_{screw}(in) - 494} \right)$$

The typical d_{screw} is taken to be 24 in.¹ The water used inside this unit is half the load of solids.

2. Grinding unit

The grinding cost was estimated using a Rod mill to be \$1,741,545 using a diameter of

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12.5 ft.² The best efficiency is achieved for d = 12.5 ft. ³

3. Vessels

In order to calculate the sizes of the equipment in the plant either volume or weight of the vessel is required.

The sizes of the premix tank, flash units, the vessel that contain the adsorbent beds, are calculated based on their volume using with the following formula:

$$Volume = \left(\frac{m}{\rho} \right) \tau$$

ρ is taken to be 1000 Kg/ m³. τ is the residence time (in sec). For the pretreatment tanks 10 min residence time is assumed,⁴ for the acid pretreatment tank, 30 min is recommended based on experimental data. For the ammonia separation column and flash, a residence time of 20 min is assumed, for storage tanks, 1800 min is assumed, for liquid-liquid separators, 30 min is considered.

The diameter of the vessels is calculated considering spherical heads for the vessels as well as a length $L = 4D_c$ so

$$D_c = \sqrt[3]{\frac{6 \cdot Volume}{7 \cdot \pi}}$$

and the weight if needed is calculated as

$$W = \rho_{steel} \left(\pi \left[\left(\frac{D_c}{2} + e \right)^2 - \left(\frac{D_c}{2} \right)^2 \right] L + \frac{4}{3} \pi \left[\left(\frac{D_c}{2} + e \right)^3 - \left(\frac{D_c}{2} \right)^3 \right] \right)$$

where the thickness e (m) is taken to be:

$$e = 0.0023 + 0.003D_c$$

that has been derived from a table of minimum thickness within⁵

Columns, flash, and separation vessels are vertical vessels and its cost will be estimated as:²

$$C_{column}(\$) = 56.181 \cdot W^{0.878}$$

Weight is in Kg. Where the weight (W) es calculated as above. Columns made of stainless steel; medium size; no internals)

For the recovery of gases an gas separation including flash or the one for hydrogen recovery after DMF production or NH₃ recovery use:

$$C_{column}(\$) = 209W^{0.716}$$

Weight is in Kg. Where the weight (W) es calculated as above.

The cost of **Horizontal vessels** for liquid- liquid separation such as the biodiesel-glycerol mixture, the DMF-water mixture, is estimated using the following equation with 1h residence time, 30 min:

$$C_{Vessel} = 12080 \cdot \text{Volume}^{0.55}$$

The cost of the **storage tanks** will be calculated as a vertical **tank**² (cone roof, and flat bottom made of stainless steel)

$$C_{Str} = 5723.3 \cdot \text{Volume}^{0.65}$$

Volume is in m³

4. Reactors (Hydrolysis, Fermentation and dehydration units)

The cost correlation is taken to be:

$$C_{Fermentors} = 66532 \cdot \text{Volume}^{0.5}$$

The volume is computed using the mass flow rate (m (kg/s)) and the residence time (τ)

$$\text{Volume} = \left(\frac{m}{\rho} \right) \tau$$

Volume is in m³ and the residence time is 21600 s for dehydration. 3600 s for saccharification, 1800 s for liquefaction and 40 h for hydrolysis.

Cost correlation updated from,²

(A Fermenter Reactor made of Stainless steel 316 operating up to 25 psi)

The **transesterification reactor** is a jacketed reactor with agitation

$$C_{Biodiesel} = 15000 \text{Volume}^{0.55}$$

The neutralization reactor, pretreatment reactors for AFEX and Acid processing, and the biomass-oil separation are considered mixing tanks

$$C_{Reactors} = 12.325 \cdot W + 14639$$

Weight is in Kg. Where the weight (W) as calculated as above.

5. Mechanical Separation/ solid-liquid separations or Filters

The mechanical separation is considered as a centrifuge (Centrifugal Separator Bottom Driven)²:

$$C_{MechSep} = 892 \cdot d \cdot \left(\frac{\text{Load}(\text{gal} / \text{min})}{200(\text{gal} / \text{min})} \right)$$

d is typically 24 in and the maximum capacity of 200 gal/min for a single centrifuge is taken from Walas.⁴

6.-Compressor costs

Centrifugal compressors have been considered and two correlations will be used depending on the final pressure of the stream:²

For Low pressures till 125 psi $C_{Compressor} = 302 \cdot P(kW) + 32650$

For pressure till 1000psi $C_{Compressor} = 2283.6 \cdot P(kW)^{0.8302}$

7. Molecular sieves and PSA systems.

The **molecular sieves** are cost estimated using the price of the adsorbent and vertical vessels. Two beds are needed to ensure continuous operation. We use an over-design factor of 10% for safety reasons.

Molecular sieves with a bulk density of 45 lb/ft^{3.6}

$$\text{Volume of bed} = \frac{\text{Bed size}}{\text{Bulk density}} = \frac{1.1 \cdot \text{Mass(Kg)}}{41.5 \frac{\text{lb}}{\text{ft}^3} \cdot 0.454 \frac{\text{Kg}}{\text{lb}} \cdot \left(\frac{1 \text{ ft}}{0.3048 \text{ m}}\right)^3}$$

Molecular sieves data:

The price is around 1000\$ per ton either for zeolite 13x^{7,8}, 5A⁹ or silica gel.¹⁰

The molecular sieves are assumed to be a combination of two vertical vessels and the cost will be estimated as:

$$C_{MS} = 2 \cdot (\text{cost of bed} + 56.181 W^{0.878})$$

Weight is in Kg.

8. Heat exchangers

We compute the area of the heat exchanger as

$$A = \frac{Q}{U \Delta T}$$

Where

$$U \approx \left(\frac{1}{h_{in}} + \frac{1}{h_{out}} \right)^{-1}$$

The film coefficients for the streams are taken from Brannan¹¹

Next, we separate the reboilers:²

$$C_{Reboiler} = 734.58A - 5961.5$$

From the other shell and tube exchangers:²

$$C = 293.59A^{1.4915}$$

$$A < 25\text{m}^2$$

$$C = 1436.4A + 2275.3$$

$$25 < A < 140\text{m}^2$$

$$C = 20044A^{0.4669}$$

$$A > 140\text{m}^2$$

C in \$, A is the area in m².

Heat Exchanger, Stainless steel 316 working up to 150 psig. The type of the heat exchanger is either reboiler or Shell / Tube Fixed U, small, medium and big.

The hydrogenation reactor cost is estimated as a heat exchanger.

9. Columns

The **distillation columns** are cost estimated as vertical vessels including the cost of the sieve trays^{5,12}

The diameter of the columns is calculated as:

$$D_c = 2 \cdot \sqrt{\frac{1}{\pi} \cdot \frac{\text{Vapor rate (kg/s)}}{\rho_v \cdot (\text{vapor velocity (m/s)})}}$$

$$\text{Vapor rate (kg/s)} = (1 + R) \cdot D$$

R is the reflux ratio, assumed 2, and D is distillate withdrawn from top.

In case the diameter of the column is bigger than 3m the feed should be split into as many columns as those which allow a D_c of around 3m,⁵

$$\text{vapor velocity (m.s)} = 0.8 \cdot \text{max vapor velocity} = 0.8 \cdot 0.3048 \cdot 0.3 \cdot \sqrt{\frac{\rho_L - \rho_v}{\rho_v}}$$

- 0.8 is the fraction of the flooding velocity⁵

- $0.3 \cdot \sqrt{\frac{\rho_L - \rho_v}{\rho_v}}$ ft/s is the maximum vapor velocity¹¹ corresponding to a plate separation of

2 ft.

(0.3048 if because 0.3 is given for a velocity in ft/s instead of m/s.

The number of plates for each column is calculated as:¹³

$$n_{\text{plates}} = \text{Round} \left(\frac{\ln \left(\frac{\xi_{\text{etho}} (1 - \xi_{\text{wa}})}{\xi_{\text{wa}} (1 - \xi_{\text{etho}})} \right) - 1}{\frac{\ln(\alpha_{\text{etho/wa}})}{\text{Efficiency}}} + 1 \right)$$

$$\text{Efficiency} = 0.5 / (0.3 \cdot \alpha_{\text{etho/wa}})^{0.25}$$

The height of the column will be

$$H = n_{\text{plates}} \cdot \text{Esp} + 4 \cdot 1.5$$

Esp is the separation between plates and is commonly taken as 0.6m.¹³ The factor 4

times 1.5m is a consideration¹⁴ for space above the top plate and below the bottommost plate.

Since the column thickness is small compared to its diameter, we can calculate its weight using:

$$W = \rho_{steel} \left[\pi \cdot D_c \cdot e \cdot H + \frac{4}{3} \cdot \pi \cdot \left[\left(\frac{D_c}{2} + e \right)^3 - \left(\frac{D_c}{2} \right)^3 \right] \right]$$

$$\rho_L = 950 \text{ kg} / \text{m}^3 \quad (\text{Liquid phase density})$$

$$\rho_v = \frac{P \cdot M_{Water-EtOH}}{R \cdot T} (\text{kg} / \text{m}^3) \quad (\text{Gas phase density})$$

The bottoms pressure and temperature is used for calculating the vapor density.

Thickness calculation:⁵

$$P > atm \quad t = 0.0032 + \frac{P \cdot D_c}{2 \cdot S \cdot E - 0.2P}$$

$$P < atm \quad t = 0.0032 + 4 \cdot \frac{D_c}{2} \cdot \sqrt{\frac{P_{out}}{S}}$$

Corrosion allowance, 0.0032m⁵ (from 2 to 4 mm; typically 1/8 in = 3.2 mm is used)

t (m): thickness

E: joint efficiency, equal to 1

P (psi): Design pressure – We have selected 1.5 times the working pressure since bottoms pressures is higher than atmospheric pressure

P_{out} (psi): Pressure outside the column (= atmospheric pressure). units consistent with those of S

S (psi): Design stress (S = 13300 psi for stainless steel working at 100°C. From Walas,⁴

D_c (m): column diameter

Another correlation for thickness:

$$t \text{ (m)} = 0.0023 + 0.003D_c$$

where D_c is in m , as presented above.

The **cost of the trays** is given by⁵

$$\text{Cost Trays}(\$) = n_{\text{Trays}} \cdot 315 \cdot e^{0.72 \cdot D_c}$$

where D_c is in m

$$C_{column}(\$) = 56.181 \cdot W^{0.878} + \text{cost of Trays}$$

Summary of units and costs

AFEX		ACID		ALGAE	
Unit	Cost k\$(2009)	Unit	Cost k\$ (2009)	Unit	Cost k\$ (2009)
Washing	1010	Washing	1010	Ponds	16000
Grinding	1741	Grinding	1741	Belt	2350
Pretreat Reactor	135	Tank	57	Tank	81
Column	175	Pretreat Reactor	150	Mec Sep	86
Flash	25	Mec Sep	86	Distillation	450
Storage tank	1473	Neutralization	52	Transeste- rification	426
Hydrolysis reactor	5620	Tank	60	Separator	96
Storage tank	5636	Filter	65	Distillation (ethanol)	1260
Separator	100	Flash	20	Distillation (FAEE)	735
Reactor	360	Storage tank	1630	Liquefaction	363
Separator	97	Hydrolysis reactor	6100	Saccharification	513
Filter	645	Storage tank	1630	Storage tank	812
Distillation 1 (x 6 col)	58000	Separator	108	Reactor	3200
Distillation 2	30	Reactor	3200	Storage tank	4350
Distillation 3	121	Storage tank	5310	Separator	44
Distillation 4	135	Reactor	330	Storage tank	90
Separator	22	Separator	96	Reactor	2540
Compressors	7867	Filter	581	Separator	513
HXs	33400	Distillation 1 (x4 col)	92000	Filter	431
		Distillation 2	34	Distillation 1 (x 4 col)	70000
		Distillation 3	125	Distillation 2	24
		Distillation 4	116	Distillation 3	164
		Separator	20	Separator	26
		Compressors	1710	Compressors	2332
		HXs	44610	HXs	39000
Fixed Investment (2014)	130000	Fixed Investment (2014)	168000	Fixed Investment (2014)	158000

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