Supplementary Information

Techno-economic and carbon-intensity assessment of lignin–methanol oil production for marine fuel applications

Stuart Scott, Neal Morgan, Aldo Caiazzo, Andrew Smallbone

This document supports the main manuscript submitted to *Fuel*. Aspen flowsheet diagrams, elemental mass balances, compositional data and sensitivity-analysis parameters are presented in the main article. Sections SI-1–SI-4 below provide yield-adjustment methods, energy balance tables, equipment sizing and full economic breakdowns referenced in the main text.

Contents

1 SI-1: Yield-adjustment method for ash and waste lignin

1.1 Yield Distributions

Ash was treated as an inert dilutant to be removed in the filtration phase. Following this reasoning and to simplify modelling, all ash was moved into the char parameter in the *RYield* block. It was assumed that no ash remained in the CLO product after filtration. Yield distributions were adjusted using the following formula to enable the model to respond dynamically to ash content in the feed:

$$Y = M_{\text{Dry}} \times (1 - Ash\%) \times \frac{Y_{\text{old}}}{0.98} \times \frac{1}{M_{\text{total}}}$$

Where Y is the ash-adjusted *RYield* fraction, $Ash\%$ is the decimal fraction of feedstock ash, M_{Dry} is the dry mass of lignin feed, Y_{old} is the original yield fraction and M_{total} is the total throughput mass. Using this formula, yields are replicated exactly at the original Protobind ash concentration of 2 wt%, and lowered proportionally with increasing ash content.

The formula normalises the yield by a factor of 0.98 to account for the 2% ash found in the Protobind lignin used in the Kouris et al. research. This ensures the yield replicates experimental results at 2 wt% ash, but increases or decreases proportionally when the feed composition changes. The char mass yield, M_{char}, was calculated as:

$$M_{char} = M_{feed} - M_{volatiles} + M_{ash}$$

Where M_{feed} represents the total elemental mass of the feedstock (dry basis), $M_{volatiles}$ is the cumulative elemental mass of the produced soluble, insoluble, and gaseous products, and M_{ash} is the mass of the inorganic fraction present in the feed.

1.2 Methanol Entrainment

It was assumed that any methanol reported missing in the experimental data not consumed in the 1.1 wt% was entrained in the char, due to its high porosity relative to lignin. Ash and char were assumed to entrain a similar quantity of methanol, and therefore entrainment is scaled proportionally to char mass. Entrained methanol was modelled by physically removing methanol after the flash with a theoretical separator block, which slightly overestimates steam consumption.

A entrainment factor, K, was defined to establish an estimate for how much methanol is removed per unit of char during filtration:

$$K = M_{\text{loss}}/M_c \approx 0.96$$

Where M_{loss} and M_c are the unaccounted methanol mass and the mass of char produced in the base case experimental data, respectively. The *Sep2* block was then encoded with a fractional separation, f, calculated as follows:

$$f = K \times \frac{M_{char}}{M_{\text{H2O}} + M_{\text{MeOH}}}$$

Where M_{H2O} and M_{MeOH} are the mass of methanol and water exiting the reactor. Due to perfect mixing assumptions, water and methanol were assumed entrained in the same fractional composition as the main stream, hence this factor was applied to both in the SEP2 block.

2 SI-2: Energy balance tables

Table 1: Mass and energy balance for all process streams.

Stream	**Location**	$\dot{m}$ **(kg/h)**	**T (°C)**	**P (bar)**	**H (MJ/h)**	**Q (MJ/h)**	**W (MJ/h)**	**|ΔE|**	**Energy balance**	**|ΔM|**	**Check**
Slurry	pump in	97118.0	25.0	10	-658986	–	–	–	–	–	–
Hpslurry	pump out	97118.0	26.4	55	-658357	0	629.20	0.16	OK	0.00	OK
S5	Ryield in	97118.0	200.0	55	-599705	58652	0.00	0.20	OK	0.00	OK
Intermediate	Ryield out	97118.0	200.8	55	-599705	0	0.00	0.00	OK	0.00	OK
Consumed	Me-loss out	852.6	–	–	–	–	–	–	–	–	–
R-Exit	60°C cooler in	96265.4	200.8	55	-593948	0	0.00	–	–	0.03	OK
Cooled	60°C cooler out	96265.4	60.0	55	-643552	-49604	0.00	0.30	OK	0.00	OK
Cond-E	20-bar valve out	96265.4	60.7	20	-643552	0	0.00	0.00	OK	0.00	OK
Solid1 M out	filter exit	11123.5	–	–	–	–	–	–	–	–	–
S3	1-bar valve in	85141.9	60.7	20	-579935	0	0.00	–	–	0.00	OK
CLO-M	Me-Flash in	85141.9	60.2	1	-579935	0	0.00	0.00	OK	0.00	OK
Recover1	MeFlash gases out	35061.8	64.2	1	-218464	39384	0.00	–	–	–	–
CLO-L	MeFlash liquid out	50080.1	64.2	1	-322088	0	0.00	0.70	OK	0.00	OK
Product	40°C cooler out	50080.1	40.0	1	-325519	-3432	0.00	0.59	OK	0.00	OK
Solid1	dry-heat in	11123.5	60.6	20	-63616	0	0.00	–	–	–	–
S4	dry-heat out / PD in	11123.5	90.0	20	-62871	746	0.00	0.05	OK	0.00	OK
Solid2	PD out / dryer in	11123.5	64.2	1	-62871	0	0.00	0.00	OK	0.00	OK
INTR	dryer liquids out	602.2	64.2	1	-3748	0	0.00	–	–	–	–
Drychar	dryer solids out	10521.3	64.2	1	-59123	0	0.00	0.02	OK	0.04	OK
MeSolids	entrained in char	3.4	–	–	–	–	–	–	–	–	–
Recover2	–	598.7	–	–	–	–	–	–	–	0.00	OK
H2OMEOH	RadFrac in	35660.5	64.2	1	-222187	0	0.00	–	–	0.01	OK
Meout	RadFrac tops	35627.5	44.4	1	-263144	-41466	–	–	–	–	–
Water	RadFrac bottoms	33.0	98.0	1	-509	–	–	0.19	OK	0.00	OK

3 SI-3: CAPEX equipment sizing and scaling

3.1 Reactor Volume Sizing

Assuming 100,000 tonnes of lignin solubilised per year and a plant uptime of 8000 hr/year, the required amount of feed lignin in the base case was calculated using the expected yield. Taking a 1:5 w/v ≈ 1:3.955 w/w ratio of lignin to methanol, it was also possible to calculate the input methanol requirements:

$$\frac{100000}{8000} = 12.5\,\text{tonnes/hr of solubilised lignin}$$

$$\frac{12.5}{0.6375} = 19.6\,\text{tonnes/hr of Protobind lignin}$$

$$19.6 \times 3.955 = 77.5\,\text{tonnes/hr methanol}$$

Assuming a lignin skeletal density of 1350 kg/m^3 and a methanol density of 791 kg/m^3, the volumes at mixing would be:

$$\frac{19.6 \times 10^3}{1350} = 14.518\,\text{m}^3/\text{hr}$$

$$\frac{77.518 \times 10^3}{791} = 98\,\text{m}^3/\text{hr}$$

$$\text{Total feed volume} = 112.518\,\text{m}^3/\text{hr}$$

Scaling the reactor to include a 30 min residence time, 25% headspace the required volume was calculated:

$$112.518\,\text{m}^3/\text{hr} \times 0.5\,\text{hr} = 56.25\,\text{m}^3$$

$$1.2 \times 56.26 = 70.3125\,\text{m}^3$$

Using a standard vessel size of 75m^3 will meet the required volumes.

3.2 Reactor & Filter CAPEX

The pressure vessel was assumed to have a length:diameter ratio of 3:1. Solving for a 75 m^3 volume gives a diameter D ≈ 3.2 m and a length L of 9.6 m. A maximum allowable stress (S) of 135 MPa was selected as a typical ASME design value for carbon steel pressure vessels. Using an internal radius of 1.6 m and a working pressure (P) of 5.5 MPa, the minimum thickness (t_{min}) was calculated using a thick wall pressure vessel formula:

$$\begin{aligned} t_{\text{min}} = R \times (e^{\frac{P}{S}} - 1) &= 66.53\,\text{mm} \\ +6\,\text{mm corrosion resistance} &= 72.5\,\text{mm} \\ +12.5\%\,\text{tolerance} &= 81.6\,\text{mm} \end{aligned}$$

The volumes of the stainless steel (SS) cladding and outer carbon steel (CS) were calculated as below using standard densities. Hemispherical reactor caps were assumed.

$$\text{Volume} = \pi(R_1^2 - R_2^2)L$$

$$\text{Heads Volume} = \frac{4}{3}\pi(R_1^2 - R_2^2)L$$

$$\text{SS Total Volume} = 0.77\,\text{m}^3$$

$$\text{SS Mass} = 0.77\,\text{m}^3 \times 8000\,\text{kg/m}^3 = 6200\,\text{kg}$$

$$\text{CS Total Volume} = 10\,\text{m}^3$$

$$\text{CS Mass} = 10\,\text{m}^3 \times 7850\,\text{kg/m}^3 = 78500\,\text{kg}$$

$$\text{Total Mass} = 84700\,\text{kg}$$

An averaged cost per kilogram of pressure vessel material was calculated using MEPS world steel prices, incorporating estimated fabrication, inspection and waste material costs:

$$(79000\,\text{kg} \times 1.1\,\$/\text{kg}) + (6200\,\text{kg} \times 6.50\,\$/\text{kg}) = \$127,200$$

$$\frac{\$127,000}{84700\,\text{kg}} \approx 1.5\,\$/\text{kg}$$

$$+20\%\,\text{waste material} = +1.80\,\$/\text{kg}$$

$$+\,\text{fabrication costs} = +10\,\$/kg$$

$$+\,\text{inspection and testing costs} = +4\,\$/kg$$

$$= 15.80\,\$/\text{kg}\,\text{in total}$$

This leads to a cost of \$1.33 million for the pressure vessel materials. However, the pressure vessel requires agitation. Based on Matches agitator cost estimates for a 70 hp, 316 stainless steel agitator (adjusted from 2014 to 2026 USD), alongside seals, gearbox and shaft estimates, \$300,000 was added to the cost. Applying a Lang Factor of 4 gives an estimated final cost of \$6.52 million, or £4.89 million.

To scale the plant to full capacity, five 150 m^3 reactors were assumed. Using standard cost scaling factors. the scaled reactor costs were calculated as follows:

$$C_{\text{scale}} = 5 \times C_{\text{pilot}} \left(\frac{150}{75} \right)^{0.6} = \pounds\,37.164\,\text{million}$$

A conservative estimate of the filter cost was selected using intelmarketresearch.com data on large-scale industrial rotary drum vacuum filter units. This gave an estimated cost of $500,000 (£375,000) before Lang factor application.

4 SI-4: OPEX assumptions and full expenditure breakdowns

4.1 Base Case Breakdowns

Table 2: Base case economic breakdown at pilot scale (100,000 tonnes of soluble lignin per operating year).

Section	Item	£/tonne	£/year	Equipment cost (£)	Installed cost (£)
CAPEX (pilot)					
Equipment	DISTIL-cond	-	-	85,800	343,200
Equipment	DISTIL-cond acc	-	-	30,750	123,000
Equipment	DISTIL-reb	-	-	368,775	1,475,100
Equipment	DISTIL-reflux pump	-	-	9,150	36,600
Equipment	DISTIL-tower	-	-	500,625	2,002,500
Equipment	DRYHEAT	-	-	11,550	46,200
Equipment	200-DEG	-	-	109,050	436,200
Equipment	DRYER-flash vessel	-	-	18,825	75,300
Equipment	40-DEG	-	-	11,250	45,000
Equipment	FILTER	-	-	375,000	1,500,000
Equipment	SOLVOL	-	-	1,222,500	4,890,000
Equipment	ME-FLASH-flash vessel	-	-	26,850	107,400
Equipment	55-BAR	-	-	106,275	425,100
Equipment	HEATEX	-	-	142,875	571,500
Fixed Capital Investment (FCI)		-	-	3,019,275	12,077,100
Working Capital		-	-	-	1,811,565
Contingency (10%)		-	-	-	1,207,710
Total CAPEX		-	-	-	**15,096,375**
Annualised CAPEX		-	1,772,314	-	-
OPEX (Pilot)					
OPEX	Lignin cost	562.50	88,200,000	-	-
OPEX	Methanol makeup	225.00	73,500,004	-	-
OPEX	Steam	-	12,910,001	-	-
OPEX	Cooling water	-	2,109,096	-	-
OPEX	Electricity	-	211,424	-	-
OPEX	Labour	-	2,200,000	-	-
OPEX	Engineering/Supervision	-	330,000	-	-
OPEX	Maintenance	-	362,313	-	-
OPEX	Operating supplies	-	54,347	-	-
OPEX	Insurance	-	120,771	-	-
Total OPEX		-	**179,997,956**	-	-
CAPEX + OPEX		-	**181,770,270**	-	-
MSP (£/tonne output)		**454.51**	–	–	–
MSP (£/GJ)		**20.66**	–	–	–

Table 3: Base case economic breakdown at full scale (1,000,000 tonnes of soluble lignin per operating year).

Section	Item	£/tonne	£/year	Equipment cost (£)	Installed cost (£)
CAPEX (full scale)					
Equipment	DISTIL-cond	-	-	341,570	1,366,279
Equipment	DISTIL-cond acc	-	-	122,416	489,663
Equipment	DISTIL-reb	-	-	1,468,093	5,872,373
Equipment	DISTIL-reflux pump	-	-	36,426	145,705
Equipment	DISTIL-tower	-	-	1,992,988	7,971,953
Equipment	DRYHEAT	-	-	45,981	183,922
Equipment	200-DEG	-	-	434,128	1,736,512
Equipment	DRYER-flash vessel	-	-	74,942	299,769
Equipment	40-DEG	-	-	44,786	179,145
Equipment	FILTER	-	-	1,492,875	5,971,500
Equipment	SOLVOL	-	-	9,291,000	37,164,000
Equipment	ME-FLASH-flash vessel	-	-	106,890	427,559
Equipment	55-BAR	-	-	423,081	1,692,323
Equipment	HEATEX	-	-	568,785	2,275,142
Fixed Capital Investment (FCI)		-	-	15,875,176	65,775,845
Working Capital		-	-	-	9,866,377
Contingency (10%)		-	-	-	6,577,585
Total CAPEX		-	-	-	**82,219,806**
Annualised CAPEX		-	9,652,605	-	-
OPEX (Full Scale)					
OPEX	Lignin cost	562.50	882,000,000	-	-
OPEX	Methanol makeup	225.00	735,000,040	-	-
OPEX	Steam	-	129,100,013	-	-
OPEX	Cooling water	-	21,090,957	-	-
OPEX	Electricity	-	2,114,116	-	-
OPEX	Labour	-	2,600,000	-	-
OPEX	Engineering/Supervision	-	390,000	-	-
OPEX	Maintenance	-	1,973,275	-	-
OPEX	Operating supplies	-	295,991	-	-
OPEX	Insurance	-	657,758	-	-
Total OPEX		-	**1,775,222,151**	-	-
CAPEX + OPEX		-	**1,784,874,757**	-	-
MSP (£/tonne output)		**446.30**	–	–	–
MSP (£/GJ)		**20.29**	–	–	–

4.2 Waste case breakdowns

Table 4: Waste-base case economic breakdown at pilot scale (100,000 tonnes of soluble lignin per operating year).

Section	Item	£/tonne	£/year	Equipment cost (£)	Installed cost (£)
CAPEX (pilot)					
Equipment	DISTIL-cond	-	-	85,800	343,200
Equipment	DISTIL-cond acc	-	-	30,750	123,000
Equipment	DISTIL-reb	-	-	368,775	1,475,100
Equipment	DISTIL-reflux pump	-	-	9,150	36,600
Equipment	DISTIL-tower	-	-	500,625	2,002,500
Equipment	DRYHEAT	-	-	11,550	46,200
Equipment	200-DEG	-	-	109,050	436,200
Equipment	DRYER-flash vessel	-	-	18,825	75,300
Equipment	40-DEG	-	-	11,250	45,000
Equipment	FILTER	-	-	375,000	1,500,000
Equipment	SOLVOL	-	-	1,222,500	4,890,000
Equipment	ME-FLASH-flash vessel	-	-	26,850	107,400
Equipment	55-BAR	-	-	106,275	425,100
Equipment	HEATEX	-	-	142,875	571,500
Fixed Capital Investment (FCI)		-	-	3,019,275	12,077,100
Working Capital		-	-	-	1,811,565
Contingency (10%)		-	-	-	1,207,710
Total CAPEX		-	-	-	**15,096,375**
Annualised CAPEX		-	1,772,314	-	-
OPEX (Waste Base Case)					
OPEX	Lignin cost	45.00	7,056,000	-	-
OPEX	Methanol makeup	225.00	47,174,267	-	-
OPEX	Steam	-	21,013,442	-	-
OPEX	Cooling water	-	2,828,058	-	-
OPEX	Electricity	-	211,424	-	-
OPEX	Labour	-	2,200,000	-	-
OPEX	Engineering/Supervision	-	330,000	-	-
OPEX	Maintenance	-	362,313	-	-
OPEX	Operating supplies	-	54,347	-	-
OPEX	Insurance	-	120,771	-	-
Total OPEX		-	**81,350,622**	-	-
CAPEX + OPEX		-	**83,122,936**	-	-
MSP (£/tonne output)		**360.94**	–	–	–
MSP (£/GJ)		**16.41**	–	–	–

Table 5: Waste-base case economic breakdown at full scale (1,000,000 tonnes of soluble lignin per operating year).

Section	Item	£/tonne	£/year	Equipment cost (£)	Installed cost (£)
CAPEX (full scale)					
Equipment	DISTIL-cond	-	-	341,570	1,366,279
Equipment	DISTIL-cond acc	-	-	122,416	489,663
Equipment	DISTIL-reb	-	-	1,468,093	5,872,373
Equipment	DISTIL-reflux pump	-	-	36,426	145,705
Equipment	DISTIL-tower	-	-	1,992,988	7,971,953
Equipment	DRYHEAT	-	-	45,981	183,922
Equipment	200-DEG	-	-	434,128	1,736,512
Equipment	DRYER-flash vessel	-	-	74,942	299,769
Equipment	40-DEG	-	-	44,786	179,145
Equipment	FILTER	-	-	1,492,875	5,971,500
Equipment	SOLVOL	-	-	9,291,000	37,164,000
Equipment	ME-FLASH-flash vessel	-	-	106,890	427,559
Equipment	55-BAR	-	-	423,081	1,692,323
Equipment	HEATEX	-	-	568,785	2,275,142
Fixed Capital Investment (FCI)		-	-	15,875,176	65,775,845
Working Capital		-	-	-	9,866,377
Contingency (10%)		-	-	-	6,577,585
Total CAPEX		-	-	-	**82,219,806**
Annualised CAPEX		-	9,652,605	-	-
OPEX (Waste Base Case)					
OPEX	Lignin cost	45.00	70,560,000	-	-
OPEX	Methanol makeup	225.00	471,742,667	-	-
OPEX	Steam	-	210,134,423	-	-
OPEX	Cooling water	-	28,280,578	-	-
OPEX	Electricity	-	2,114,238	-	-
OPEX	Labour	-	2,600,000	-	-
OPEX	Engineering/Supervision	-	390,000	-	-
OPEX	Maintenance	-	1,973,275	-	-
OPEX	Operating supplies	-	295,991	-	-
OPEX	Insurance	-	657,758	-	-
Total OPEX		-	**788,748,932**	-	-
CAPEX + OPEX		-	**798,401,537**	-	-
MSP (£/tonne output)		**346.69**	–	–	–
MSP (£/GJ)		**15.76**	–	–	–