Supplementary material to:

Environmental and economic assessment of a novel solvolysis-based biorefinery producing lignin-derived marine biofuel and cellulosic ethanol

Transportation of cargo - model

S-1. Methodology

For the tank-to-wake stage a panamax vessel, i.e. a medium-sized container ship that can go through the old Panama Canal locks, is considered. The vessel is assumed to be equipped with a slow speed two-stroke dual-fuel engine which can operate on both diesel oil and low-flashpoint liquid fuels. The auxiliary engine, in turn, is a medium speed engine. Specifications for the vessel and engines are shown in Table S-1.1 and Table S-1.2 respectively.

Table S-1.1. Specifications for the panamax ship

Parameter	Panamax ship
Average payload (TEUs)	4818
Average payload (t)	44533
Capacity of the fuel tank (m^3)	5678-7571

Table S-1.2. Specifications for the main and auxiliary engines

Parameter	Main engine	Auxiliary engine
Engine maximum continuous rating, MCR (kW)	37 457.04	8278.23
Engine load factor, LF	0.83	0.19
Brake-specific fuel consumption, BSFC (MJ/kWh)	7.91	9.28
Using methanol		
(g/kWh)	397.74	466.54
(L/kWh)	0.50	0.59
Using the CLO-methanol blend		
(g/kWh)	391.83	459.61
(L/kWh)	0.41	0.48

Trip distances were retrieved from the GREET-marine® model [1]. The trip is divided into three segments which all have distinctive fuel consumptions and emission factors owing to different speeds, load factors (i.e. portion of the rated engine power that is utilized during the work process), and the use of either the main or auxiliary engines. The container ship is assumed to travel at normal cruising conditions at the design speed of 21.17 knots (nautical miles/hour) which is equivalent to 39.21 km/h. This speed is lowered to 18.01 knots (= 33.35 km/h) during the transit through the reduced speed zones (RSZs). These RSZs are often established near ports and allow to limit fuel consumption and emissions within the designated region. Lastly, the time, the container ship spends at dockside in the port of departure and arrival (dwell time, hoteling) is assumed to be 22 hours.

The model described above can be used considering both methanol and the CLO-methanol blend as a marine fuel as can be seen in Figure S-1. Although these two low-flashpoint liquid fuels have similar LHVs (20.2 MJ/kg versus 19.9 MJ/kg), their volumetric energy densities vary significantly (19.4 MJ/L versus 15.7 MJ/L). This difference plays a crucial role in fuel storage on the container ships and on the distance these ships can travel without refueling. To calculate the difference in cruising distances between the two fuels, the RSZs and dockside activities will be kept the same for the two pathways.

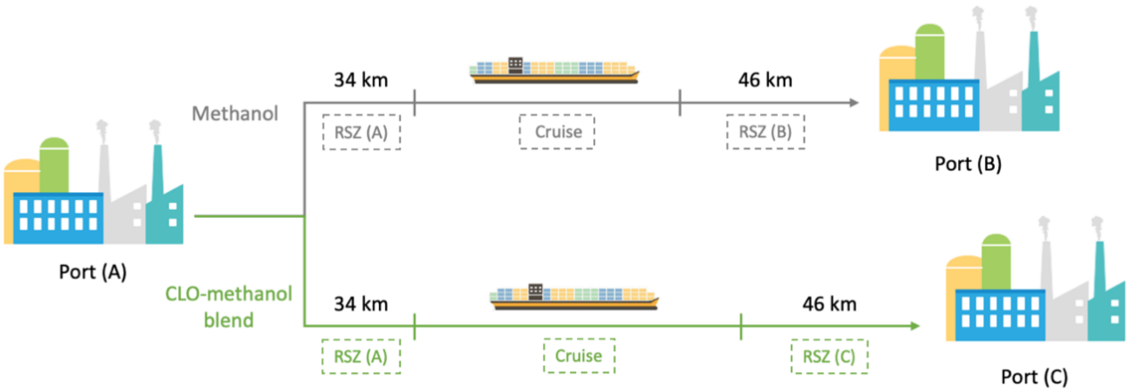

Figure S-1. Trip segments (RSZ – reduced speed zone)

The vessel, engine, and trip characteristics described above together with Equations S-1.1, S-1.2, and S-1.3 are used to calculate the fuel consumption per trip (F). Importantly, the load factor of the main engine is reduced to 0.60 when the ship transits through an RSZ.

$$F_{Port} = BSFC_{Aux} \cdot MCR_{Aux} \cdot LF_{aux} \cdot t_{dwell} \quad \text{(Eq. S-1.1)}$$

$$F_{RSZ} = BSFC_{Main} \cdot MCR_{Main} \cdot LF_{Main} \cdot D_{RSZ} \cdot \frac{1}{v_{RSZ}} \quad \text{(Eq. S-1.2)}$$

$$F_{cruise} = BSFC_{Main} \cdot MCR_{Main} \cdot LF_{Main} \cdot D_{cruise} \cdot \frac{1}{v_{cruise}} \quad \text{(Eq. S-1.3)}$$

These fuel consumptions for the individual trip segments were then used to calculate the fuel consumption of the entire trip using Equation S-1.4.

$$F_{total} = F_{Port(A)} + F_{RSZ(A)} + F_{cruise} + F_{RSZ(B)} + F_{Port(B)} \quad \text{(Eq. S-1.4)}$$

Finally, the fuel consumption in the cruise mode (F_{cruise}) and the maximum cruising distance (D_{cruise}) can be found using the next equations:

$F_{cruise} = \text{capacity of the fuel tank} - (F_{Port(A)} + F_{RSZ(A)} + F_{RSZ(B)/(C)} + F_{Port(B)/(C)})$ (Eq. S-1.5)

$$D_{cruise} = \frac{F_{cruise}}{BSFC_{Main} \cdot MCR_{Main} \cdot LF_{Main} \cdot \frac{1}{v_{cruise}}} \quad \text{(Eq. S-1.6)}$$

S-2. Results

S-2.1. Maximum cruising distances for methanol and the CLO-methanol blend using the full tank

Table S-2.1 summarizes the fuel consumption, in m^3, per trip using the full tank of methanol and the full tank of the CLO-methanol blend.

Table S-2.1. Volume-based fuel consumption per trip using the full tank

	F (m^3)	
	Methanol	**CLO-methanol blend**
Port (A)	$2.05 \cdot 10^1$	$1.66 \cdot 10^1$
RSZ (A)	$1.16 \cdot 10^1$	$9.35 \cdot 10^0$
Cruise	$\mathbf{5.61 \cdot 10^3 - 7.50 \cdot 10^3}$	$\mathbf{5.62 \cdot 10^3 - 7.52 \cdot 10^3}$
RSZ (B)/(C)	$1.56 \cdot 10^1$	$1.26 \cdot 10^1$
Port (B)/(C)	$2.05 \cdot 10^1$	$1.66 \cdot 10^1$
Total	$5.68 \cdot 10^3 - 7.57 \cdot 10^3$	$5.68 \cdot 10^3 - 7.57 \cdot 10^3$

Therefore, the maximum cruising distances are found to be $1.40 \cdot 10^4 - 1.88 \cdot 10^4$ km for methanol and $1.74 \cdot 10^4 - 2.32 \cdot 10^4$ km for the CLO-methanol blend.

The higher volumetric energy density of the blend enables a CLO-methanol-propelled vessel to travel 3347-4463 km (23.9%) further than if it was fueled with methanol. In other words, when a 4818 TEU panamax ship fueled with the CLO-methanol blend leaves the port of Rotterdam it can reach the port of Shanghai in China which is 19535 km away without refueling. The same container ship propelled with methanol, however, will have to hotel in the port of Bangkok in Thailand to refuel on its way to China.

The travelling time of a panamax ship from the port of Rotterdam to the port of Shanghai amounts to 542.70 hours (=22.6 days). Specifications per trip segments can be found in Table S-2.2.

Table S-2.2. Time required to travel from the port of Rotterdam to the port of Shanghai with a 4818 TEU panamax ship

	Distance (km)	**Speed (km/h)**	**Time (h)**
Port (A)	0	0	22.00
RSZ (A)	34	33.35	1.02
Cruise	19455	39.20	496.30
RSZ (B)/(C)	46	33.35	1.38
Port (B)/(C)	0	0	22.00
Total	19535		542.70

S-2.2. Fuel consumption and CO_2 emissions

Table S-2.3 summarizes the fuel consumption per trip segment and for the entire trip assuming the vessel uses methanol. For F_{cruise} the lower bound of the distance range, $1.40 \cdot 10^4$ km (section S-2.1), was used.

Table S-2.3. Energy- and mass-based fuel consumption per trip using methanol

	F (MJ)	F (t)
Port (A)	$3.21 \cdot 10^5$	$1.61 \cdot 10^1$
RSZ (A)	$1.81 \cdot 10^5$	$9.11 \cdot 10^0$
Cruise	$8.81 \cdot 10^7$	$4.43 \cdot 10^3$
RSZ (B)	$2.45 \cdot 10^5$	$1.23 \cdot 10^1$
Port (B)	$3.21 \cdot 10^5$	$1.61 \cdot 10^1$
Total	$8.91 \cdot 10^7$	$4.48 \cdot 10^3$

Table S-2.4, in turn, summarizes the results for the use of the CLO-methanol blend. Similarly to methanol, the lower bound of the distance range given in section S-2.1. ($1.74 \cdot 10^4$ km) was used for the calculation of F_{cruise}.

Table S-2.4. Energy- and mass- based fuel consumption per trip using the CLO-methanol blend

	F (MJ)	F (t)
Port (A)	$3.21 \cdot 10^5$	$1.59 \cdot 10^1$
RSZ (A)	$1.81 \cdot 10^5$	$8.98 \cdot 10^1$
Cruise	$1.09 \cdot 10^8$	$5.40 \cdot 10^3$
RSZ (C)	$2.45 \cdot 10^5$	$1.21 \cdot 10^1$
Port (C)	$3.21 \cdot 10^5$	$1.59 \cdot 10^1$
Total	$1.10 \cdot 10^8$	$5.45 \cdot 10^3$

S-2.3. Emissions of CO_2 per tkm (considering hoteling, RSZs and cruising)

Table S-2.5. Emission factors for methanol and the CLO-methanol blend

Emission factors (gCO_2/MJ)	
Methanol	67.91
CLO-methanol blend	33.45

Table S-2.6. Emission of CO_2 per tkm for methanol and the CLO-methanol blend

	MJ/trip	gCO_2/trip	gCO_2/tkm
Methanol	$8.91 \cdot 10^7$	$6.05 \cdot 10^9$	9.634
CLO-methanol blend	$1.10 \cdot 10^8$	$3.68 \cdot 10^9$	4.740

S-2.4. Biorefinery capacity and shipping

Table S-2.7. Energy- and mass- based fuel consumption per trip from the port of Rotterdam to the port of Shanghai using the CLO-methanol blend

	F (MJ)	F (t of CLO-methanol blend)	F (t of CLO)
Port (A)	$3.21 \cdot 10^5$	$1.59 \cdot 10^1$	$7.95 \cdot 10^0$
RSZ (A)	$1.81 \cdot 10^5$	$8.98 \cdot 10^1$	$4.49 \cdot 10^0$
Cruise	$1.22 \cdot 10^8$	$6.05 \cdot 10^3$	$3.02 \cdot 10^3$
RSZ (C)	$2.45 \cdot 10^5$	$1.21 \cdot 10^1$	$6.07 \cdot 10^0$
Port (C)	$3.21 \cdot 10^5$	$1.59 \cdot 10^1$	$7.95 \cdot 10^0$
Total	$1.23 \cdot 10^8$	$6.10 \cdot 10^3$	$3.05 \cdot 10^3$

Given that the biorefinery capacity is 26610 t of CLO/year, 8.7 one-way trips from Rotterdam to Shanghai can be completed per year.

References

[1] ANL, GREET® Model. The Greenhouse gases, Regulated Emissions, and Energy use in Technologies Model.