Supplementary information Role of biofuels, electro-fuels, and blue fuels for shipping: Environmental and economic life cycle considerations.

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This supplementary information covers details on the method, materials, case study vessels, technical descriptions of technologies, life cycle inventory data, and other detailed results from life cycle assessment.

A combined assessment of environmental and economic performance from a life cycle perspective is performed in the study. As explained in the main article an integrated life cycle framework adopted from study [1] is used. The pLCA used in this study is used to assess emerging technologies when the knowledge is sparse [2] and considers the environmental performance at a time in the future when the technology is likely to get developed. Similarly, LCC is a tool for assessing the economic dimension of sustainability and is capable of supporting decision-making at different stages of the life cycle, and also aligned with the LCA study with a life cycle thinking [1]. For the LCC and pLCA evaluation to be conducted without inconsistencies during the inventory assessment phase, it is crucial to consistently choose parameters for each technology/process, such as efficiency, energy use, and material consumption. The problem with using common inventories is that the flow parameters differ for cost and environmental impact assessments. To accomplish this, all parameters are calculated using Python codes written to perform cost calculation and integrate impact assessment calculation in openLCA.

Figure S 1: The midpoint indicators used in this study for impact assessment.

The midpoint level is used for the impact assessment and the sixth assessment report of the Intergovernmental Panel on Climate Change (IPCC) is used for calculating GWP100 [3] and other impact categories are assessed based on LCIA methods according to Environmental Footprint (EF) 3.0 recommended by the European Commission's Joint Research Centre [4] as shown in Figure 8.

S1 Method

S1.1 Size calculation

The propulsion system for each vessel is calculated based on the present installed capacity of the ships. Based on the present installed capacity the power required from the energy efficiency of components in the current installation. The components vary on the type of technical system considered in the study, termed configuration in the main article. Figure S2 shows the sizing of the component for different configurations.

Figure S 2: The calculations for the sizing of the component for different configurations.

S1.2 Fuel production cost.

The cost of e-fuels, biofuels, and blue fuels (CF_{LC}) is calculated by dividing it into capex cost, fixed OPEX cost, and variable OPEX. The capex cost (annualized capital cost) is calculated by converting the total investment to net present value using the capital recovery factor (crf) mentioned in the main article section 2.2.4. The investment costs for different processes in the fuel production pathways are taken from the literature review and the assumed costs are given in Table 4 of the main article. The higher and lower limits of the investment cost considered in the uncertainty analysis are given in Table S 6. The maximum fuel production capacity for all fuels assumed is 10000GJ/day and the investment cost is calculated towards these fuel production capacities using specific investment costs mentioned in Table 4 to get the total investment cost. The CAPEX is calculated for each of the production pathways separately. The same method is used for calculating the CAPEX for DAC and ASU, however the production capacity assumed is 50t/day. CAPEX varies usually with the economy of scale, however that is not considered. The fixed OPEX is calculated from the investment cost as these are yearly costs and are assumed to be directly related to the investment cost. These are also listed in Table 4. The variable operation cost is associated with the costs linked to the feedstock price e.g. energy, material, consumables, etc… which varies with the production output and also the process efficiencies.

S1.3 Replacements

The number of replacements is determined by comparing the life time of components and ships $(N_{\text{repl},i})$. The degradation of FCs is approximated at 0.4 percent per 1000 hours of operation, with the FC being deemed replaceable at the point of capacity loss of 20 percent. In uncertainty analysis, a higher degradation of 0.6 percent per 1000 hours of operation is considered. For battery replacement, a simplified assumption of ten years with a 60% depth of charge (DOC) as numerous factors influencing battery life (e.g., usage duration, charging cycles, and battery charging technology) are unknown and will only become apparent during the detailed design phase. SCR life is considered as 15 years as a simplified assumption for replacement.

S1.4 Normalization and weighting

The environmental impact results in the article are converted to a single score based on the normalization factors and weighing factors in Table S1. The global normalization factors (NFs) are taken from EF 3.0 [5]. Global NFs represent the relevance of the total environmental impact in a certain category in a global context [5]. The weighting factors are taken from the weighing approach suggested in EF 3.0 [6].

	Normalization	Weighing	
	Factors [5]	Factors [6]	
Acidification	$5.56E + 01$	6.2	
Ecotoxicity, freshwater	$4.27E + 04$	1.92	
Eutrophication, freshwater	$1.61E + 00$	2.8	
Eutrophication, marine	$1.95E + 01$	2.96	
Eutrophication, terrestrial	$1.77E + 02$	3.71	
Human toxicity, cancer	1.69E-05	2.13	
Human toxicity, non-cancer	2.30E-04	1.84	
Ionizing radiation	$4.22E + 03$	5.01	
Land use	$8.20E + 0.5$	7.94	
Ozone depletion	5.36E-02	6.31	
Particulate matter	5.95E-04	8.96	
Photochemical ozone formation	$4.06E + 01$	4.78	
Resource use, fossils	$6.50E + 04$	8.32	
Resource use, minerals & metals	6.37E-02	7.55	
Water use	$1.15E + 04$	8.51	
IPCC 2021 GWP 100	$8.10E + 03$	21.06	

Table S 1:Normalization factors and weighing factors used in the study.

S1.5 IAM prospective scenarios

SSP scenarios are developed by IAM community to structure the uncertainty around socio-economic developments such as national GDP, education and demographics. In this study SSP2 'Middle-of-the-Road' socio-economic pathway is considered, and this pathway describes development in line with historically observed. Table S2 summarize the IAM prospective scenarios considered in the study and is adopted from [7, 8]

SSP/RC	GMST	Society/economic trend		Climate policy	Model name
P	increase by				
scenario	2100				
$SSP2-$	\sim 2.5 °C	Extrapolation	from	Nationally Determined	REMIND
None		historical developments.		Contributions (NDCs).	SSP2-NDC
$SSP2-$	1.6-1.8 °C	Extrapolation	from	Paris Agreement objective.	REMIND
RCP2.6		historical developments.			$SSP2-$
					PkBudg1150
$SSP2-$	1.2-1.4 $^{\circ}$ C	Extrapolation	from	Paris Agreement objective.	REMIND
RCP1.9		historical developments.			$SSP2-$
					PkBudg500

Table S 2: IAM prospective scenarios considered in the study [7, 8].

S2 Technological system description

S2.1 Fuel production

All e-fuel production pathways except for e-methane are based on our previous studies [9, 10].

E-methane can be produced from electricity from renewable, e-hydrogen, and captured $CO₂[11]$. The study assumes that methane is produced by the Sabatier reaction process, which requires 2.939 kg of carbon dioxide, 0.506 kg of hydrogen, and 0.33 kWh of electricity and heat [11]. Hydrogen is assumed to come from electrolysis and CO2 is assumed from DAC as modeled in our previous studies [9, 10]. Liquefaction of methane is assumed to require 0.292 kWh of electricity per kg of methane [12]. The infrastructure for the e-methane synthesis is adopted from [13] and for liquefaction is from Ecoinvent 3.8.

Liquid blue-hydrogen is generated through the process of methane reforming of natural gas, along with CO2 capture and storage. Methane reforming of natural gas can be achieved through either steam methane reforming or auto-thermal reforming. Simulation results from the study [14] show that auto-thermal reforming can attain high $CO₂$ capture rates, hence auto thermal reforming is considered. Amine-based absorption is being considered for $CO₂$ capture technology with a 90% capture rate. The inventory data for blue hydrogen is sourced from the LCA study [14]. The data for natural gas is taken from Ecoinvent 3.8 (market group for natural gas, high pressure | natural gas, high pressure). 1.5% methane leakage is considered in the supply chain for natural gas till the production plant. The captured $CO₂$ is transported from the facilities to the port, then transferred by tanker to an injection site located 1000 km away from the port, where it is injected into geological storage. Inventory data for CO₂ transport and injection is extracted from the study [15]. The infrastructure for the blue hydrogen is considered from [14] and from Ecoinvent 3.8. The hydrogen liquefaction is modeled as in previous studies [9, 10].

Blue-ammonia is produced from the reforming of methane from natural gas and combined with $CO₂$ capture and storage similar to blue hydrogen. However, additional energy is required for the Haber Bosch process, and operation of ASU is assumed from renewable electricity. Parameters for auto-thermal reforming, CO₂ capture technology, $CO₂$ transport, and storage are assumed similar to the blue hydrogen production mentioned above. The infrastructure for the blue ammonia production plant is adopted from the study [16].

Bio-methanol is assumed to be produced from biomass using biomass gasification technology where biomass is converted to syngas and is taken from the study[17] and summary is shown in Figure 3. Residual biomass from the sustainably managed forest is assumed as feedstock for gasification where the inventory data is taken from Ecoinvent. Dried biomass is subjected to gasification with steam in a high-pressure

gasifier. Heat pipes transfer the heat from the combustor to the gasifier to facilitate the endothermic steam gasification reactions. Char, a byproduct of the gasification process, is burned along with extra wood in the combustion chamber using air. The syngas produced is nearly nitrogen-free due to the separation of the two chambers. It is assumed that for processing 1 kg dry biomass 0.5 kg water, 0.33kg Olivine (bed material), 0.002 kg ammonia, and 0.0008 kg sulphur are required [18, 19]. The raw syngas is treated using acid gas removal and waste gas shift and are sent to the methanol synthesis plant for production of the methanol. It is assumed that except for the carbon that flows into the methanol, all remaining carbon in the biomass is emitted as $CO₂$. The overall efficiency of the process is assumed 60% and total biomass needed is 1.79 kg per tonne of biomethanol.

Liquid bio-methane is also produced similarly to bio-methanol except that the treated syngas is sent to methanation for the production of methane gas. Similar to bio-methanol it is assumed that the remaining carbon in the biomass other than that flows into methane is emitted as $CO₂$. The overall efficiency of the process is assumed 60% and total biomass needed is 4.50 kg per tonne of biomethane. bio-methane is then upgraded and liquefied (same process as mentioned in e-methane) to produce liquid biomethane.

Liquid bio-hydrogen is also produced using similar process as shown in Figure S3. However, syngas is treated differently at acid gas removal and waste gas shift where the H_2 concentration in treated syngas is maximised during syngas treatment. Afterwards, the treated syngas containing raw H_2 is purified and separated in pressure swing adsorption to obtain hydrogen with a purity of >99.97% [17]. The tail gas from pressure swing adsorption is combusted with air in the gasification combustion chamber to recover energy. The carbon in the biomass is assumed to be emitted as $CO₂$ into atmosphere. The overall efficiency of the process is assumed 55% and total biomass needed is 11.79 kg per tonne of biohydrogen. The hydrogen is then liquified similar to the liquid e-hydrogen which is mentioned in previous studies [9, 10].

Bio-ammonia is assumed to be produced from bio-hydrogen and nitrogen using Haber Bosch process as shown in Figure x. The electricity required for Haber Bosch process and ASU is assumed similar to the eammonia pathway with only difference that hydrogen comes from biomass gasification route. The infrastructure for Haber Bosch and the ASU is also same from previous study[9, 10].

Figure S 3: Biofuel production pathway considered in the study.

S2.3 Power train system

Engine and SCR: Engine configuration depends on the type of ship and also on the fuel type. Vessel operating long distance are often 2 stroke engine with slow speed, 4S engines with medium speed engines,

and diesel electric which is usually 4S engines with generator and electric motors. The material data for the engine, selective catalytic reduction, batteries, electric motor, PEMFC, SOFC are assumed same as in our previous study [9, 10]. MeOHICE is a propulsion option fueled by methanol in a dual-fuel engine and the pilot fuel is MGO. To meet the Tier III requirement, 2 stroke engine requires SCR as NOx abatement technology. 4S engine have lesser NOx emissions than 4S engine but still requires SCR for NOx abatement system however need lesser urea. The NH3ICE and H2 ICE are also dual fuel engine which also includes gas injection system, and the pilot fuel is MGO. The emissions are assumed based on stoichiometric efficiencies, percentage of pilot fuel, and also comparing to gas engine parameters. The exhaust of NH3 ICEs contains unburned NH3 and NOx emissions because of fuel-bound nitrogen [32, 33]. The SCR system can convert NOx emissions by utilizing NH3 in the exhaust. Experts recommend that fine-tuning the engine to optimize NH3 combustion can effectively reduce NOx in SCR and meet tier III standards. It is assumed that the NH3 and NOx emissions post-SCR would be comparable to emissions from existing SCR systems. An uncertainty analysis is conducted in this study to assess the impact of nitrous oxide emissions on GWP. For methane and LNG, low pressure dual fuel (LPDF) engine is considered technology for 4S engine, SCR is not required for this type of engine. However, for 2S LNG/methane engine SCR is considered for meeting tier III requirement. Methane slip is main concern for methane/LNG engine and uncertainty analysis is conducted in this study to assess the impact of methane slip on GWP.

S3 Ship details

Bulk carriers Container ships Cruise ships Row Labels 25000 - 49999 GT 50000 - 99999 GT $> = 100000$ GT **Average statistics No of IMO's** 6,434 1,049 103 **Avg ME kw Installed** 8,990 52,650 67,300 **Avg design speed (Knop)** 14.2 24.1 21.1 21.1 **Avg DWT** 65,500 85,670 **Avg gross tonnes** 36,740 75,790 143,550 **Average time in each mode Maneuvering** 5.8 % 8.4 % 6.3 % **Harbour** 44.5 % 30.5 % 35.2 % **At sea** 49.7 % 61.1 % 58.5 % Total Operations **Sum of Distance (NM)** 562,833,937,000 158,802,147,000 15,210,943,000
 SALE ANGLES AN Sum of AIS Hours 52,236,000 8,779,000 877,000 FUEL totals per consumer (tonne) **Sum of (Total Fuel Consumption (MetricTon)** 28,107,100 20,158,000 3,737,300 **Sum of (ME Fuel Consumption (MetricTon)** 23,994,900 16,182,800 2,940,900 **Sum of (AE Fuel Consumption (MetricTon)** 3,339,100 3,562,300 702,300 **Sum of (Boiler Fuel Consumption (MetricTon)** 773,100 412,900 94,200 Fuel totals per mode (tonne) **At sea (ME+AE)** 24,845,100 17,417,000 3,281,200 **Harbour (AE+B)** 2,598,800 1,800,000 348,900 **Maneuvering (ME+AE+B)** 663,200 941,000 107,200

Table S 3: Statistics of the ship used in the study

S4 Summary of Technological Readiness Level

Summary of technology readiness level (TRL) of different technologies are given in Figure S4. It is crucial to acknowledge that technologies are currently at different stages of readiness, and the advancement in technological development is influenced by investment choices. In the assessment, it is assumed that all technologies will have reached maturity by 2035. This assumption is crucial in conducting a prospective life cycle assessment, as it allows for a comprehensive understanding of the impact of each technology when fully developed. This understanding is essential in making informed decisions regarding investment.

Figure S 4: Technological readiness level of different pathways

S5 Uncertainty analysis

As the evaluated technologies are immature, performance parameters may undergo different changes as they mature. We ran a Monte Carlo simulation uncertainty analysis to see how results would change if the parameters were changed compared to the base assumptions could have affected the outcomes. A developing scenario method is used (Figure S2) where ranges of parameters in different development pathways are considered. In the article, the lower range is named the pessimistic scenario, and the high range is the optimistic scenario. For base value, the parameter in between is considered is considered. The values for these parameters are considered from the literature review. Tables S3 to S6 show ranges of the values for different key parameters considered in the study. Apart from the parameters listed in the Tables, emissions from the ammonia and LNG/LMG engine operation are also varied as given below.

- Ammonia engines: Nitrous oxide emission range min 0.03 max 0.2g/kWh
- LNG/LMG 2S engines cruising: Methane emission range min 0.1; max 0.5g/kWh
- LNG/LMG 2S engines maneuvering: Methane emission range min 1; max 10g/kWh
- LNG/LMG 4S engines cruising: Methane emission range min 2; max 6g/kWh
- LNG/LMG 4S engines maneuvering: Methane emission range min 10; max 25g/kWh

Figure S 5:Different development pathways possible for emerging technologies [1]

Table S 4: Ship parameters considered in uncertainity analysis.

Parameter	unit	Base value	Pessimistic value	Optimistic value	<u>Ref</u>
2SICE eff cru		0.48	0.46	0.5	$[9, 20]$ ¤
2SICE_NH3_eff_cru		0.46	0.44	0.48	$[9, 20]$ ¤
4SICE eff cru		0.46	0.44	0.48	$[9, 20]$ ¤
4SICE_NH3_eff_cru		0.44	0.42	0.46	$[9, 20]$ ¤
2SICE eff man		0.42	0.4	0.44	$[9, 20]$ ¤
2SICE NH3 eff man		0.4	0.38	0.42	$[9, 20]$ ¤
4SICE eff man		0.4	0.38	0.42	$[9, 20]$ ¤
4SICE NH3 eff man		0.38	0.36	0.4	$[9, 20]$ ¤
OCC el MGO 2S	kWh/kWhoutengine	0.059	0.06	0.058	$[21-24]$ ¤
OCC el LNG 2S	kWh/kWhoutengine	0.03	0.031	0.029	$[21-24]$ ¤
OCC el MGO 4S	kWh/kWhoutengine	0.062	0.064	0.06	$[21-24]$
OCC el LNG 4S	kWh/kWhoutengine	0.029	0.03	0.028	$[21-24]$ ¤
OCC th MGO 2S	kWh/kWhoutengine	0.19	0.18	0.2	$[21-24]$ ¤
OCC th LNG 2S	kWh/kWhoutengine	0.11	0.1	0.12	$[21-24]$ ¤
OCC th MGO 4S	kWh/kWhoutengine	0.15	0.14	0.16	$[21-24]$ ¤
OCC th LNG 4S	kWh/kWhoutengine	0.06	0.06	0.07	$[21-24]$ ¤
PEMFC eff		0.55	0.53	0.57	[9, 10]
SOFC NH3 eff		0.58	0.56	0.6	[9, 10]
SOFC CH4 eff		0.6	0.58	0.62	$[25]$ ¤
SOFC MeOH eff		0.58	0.56	0.6	[9, 10]
2SMGO CCS capacity	kgCO2/h/kW	0.57	0.59	0.55	\ast
2SLNG CCS capacity	kgCO2/h/kW	0.44	0.46	0.42	\ast
4SMGO CCS capacity	kgCO2/h/kW	0.59	0.61	0.57	\ast
4SLNG CCS capacity	kgCO2/h/kW	0.44	0.46	0.42	\ast
*Own calculations, ¤adapted					

Table S 5: Costs associated with component and fuel distribution considered in uncertainty analysis

Table S 6: Parameters of fuel production pathways used in uncertainty analysis.

Table S 7: Cost parameters of the fuel production considered in the uncertainty analysis

Weight of the components used to calculate the capacity loss is shown in Table S8.

Table S 8: The specific weight and volume of components used for the calculation of the weight and volume of power train components including fuel storage.

S5 Results

S5.1 Environmental impacts

The LCA results for impact categories other than GWP are shown in figures S5 to S19 for bulk carrier. All results including life cycle cost, life cycle impacts for all categories for all assessed ship types are attached in supplementary excel files.

Figure S 7:LCA result on impact category resource use, fossils

Figure S 8:LCA result on impact category Particulate matter

Figure S 9: LCA result on impact category- Photochemical ozone formation

Figure S 10: LCA result on impact category-Ozone depletion

Figure S 11: LCA result on impact category-Land use

Figure S 12: LCA result on impact category-ionising radiation

Figure S 13: LCA result on impact category-Human toxicity, non cancer

Figure S 14:LCA result on impact category-Human toxicity cancer

Figure S 15: LCA result on impact category- Eutrophication, terrestrial

Figure S 16:LCA result on impact category-marine eutrophication

Figure S 17: LCA result on impact category-Freshwater eutrophication

Figure S 19: LCA result on impact category- Acidification potential

Figure S 20-LCA result on impact category- water use

S5.2 Monte-carlo simulation box plot for CAC

Figure S 21: CAC box plot for bulk carrier.

Figure S 23: Box plot for cruise ship.

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