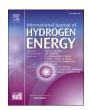
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A wind-to-wake approach for selecting future marine fuels and powertrains

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ABSTRACT

Global shipping contributes (2.8%) to greenhouse gas emissions and needs to find future fuels which will allow the International Maritime organisation's 2050 net zero targets to be met. There is much uncertainty as to which fuels should be used between hydrogen, ammonia or methanol as future costs are uncertain. We propose and evaluate a Wind-to-Wake ratio that provides an objective measure based on the amount of renewable energy required to propel a ship. Time domain voyage energy demand profiles are used to simulate the fuel used and emissions for a cruise ship, a research survey vessel, a container ship and a large multi-fuel Liquefied Natural Gas carrier. Alternative ship power systems are investigated using various carbon-based fuels, ammonia and hydrogen either using conventional engines or fuel cells. For all voyage and fuel scenarios the combination of hydrogen and fuel cells uses 30% less renewable energy than ammonia and 26% less than methanol. Hydrogen only emits steam whereas the other fuel scenarios still emit significant amounts of greenhouse gasses.

1. Introduction

The International Maritime Organisation (IMO) recently upgraded guidance on emissions regulations and reductions for all vessels across the globe with MEPC 80 [1] proposing new, more ambitious targets for shipping to meet both interim emission reductions (20% by 2030, 70% by 2040) and the long-term aim of 100% reductions by 2050. To achieve these goals, it will be imperative that new vessel builds are mostly zero carbon from 2030 to 2035 onwards [2]. The maritime industry is conservative in its adoption of new technologies because of the need for exceptional levels of reliability. The long lifetime of new built vessels, generally expected to be at least 25 years [3], requires confidence that decisions made in terms of net zero energy sources are future proof especially as whatever the new fuels that are selected a corresponding transition in the bunkering supply and energy infrastructure will be required.

The hydrocarbons that have powered the past century, and particularly oil, are remarkable fuels with only 15–20% of their embedded energy being consumed during production and refining, leaving the great majority of the energy available for useful work, although there are additional transportation losses [4]. It is noted that a steady and downward trend in the past decades of the Energy Return of Investment (EROI) as the energy required for oil and gas extraction has increased

[4–6] since more challenging reservoirs are brought into production. EROI does not include the significant proportion of energy required to carbon capture and store for such fuels to be net zero.

It is essential to understand and quantify the whole fuel supply budget in terms of greenhouse gas (GHG) emissivity and the amount of energy input required per GJ delivered to propel and power a ship. Currently established methods for measuring the carbon footprint of vessels only consider the assessments of funnel emissions, where NOx, SOx, CO2, CH4 are converted to a carbon dioxide equivalent (tCO2equiv) of greenhouse gas warming potential. Possible shipboard energy sources include those that are: carbon free at point-of-use such as hydrogen and nuclear; low carbon such as ammonia which requires a pilot fuel; net zero through carbon capture and utilisation (CCU) such as e-methanol. Each energy source and associated powertrain will influence ship design by altering its displacement (mass) and available cargo volume. Typically, as displacement increases, so does the propulsive power needed. Fuels with high specific energy density (kWh/kg) are attractive. A high volumetric energy density (kWh/L) is preferred but increased volume only has a small influence on propulsive power [7]. Fossil fuel tanks only occupy a small fraction of a ship's displacement and volume [8].

Fig. 1 compares the fuel supply chains from a renewable energy resource (wind) to the ship's rotating propeller shaft to drive the ship through the water (wake). Prior to July 2023 the International Maritime

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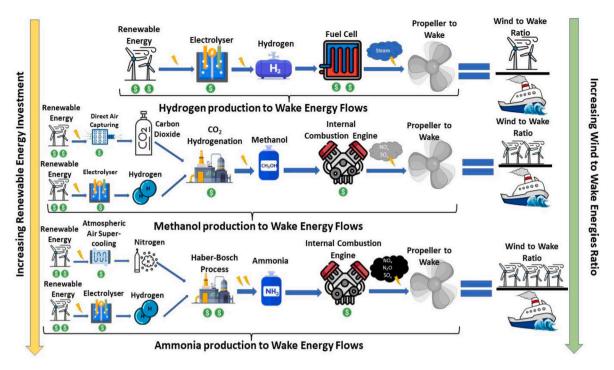


Fig. 1. Schematic of whole process to supply renewable energy onboard an identical ship ordered with increasing WtW ratio. Note that H2 production is a necessary step for both e-Ammonia and e-Methanol production.

Organisation (IMO) compared the Tank-to-Wake (TtW) assessment for comparison of GHG. A TtW approach ignores the energy and emissions required to produce and transport the fuels. IMO's MEPC 80 approach was revised to examine the whole fuel cycle, from extraction to use on board. Conventionally, comparison of alternative zero or low carbon fuels is done using an estimate of the likely fuel cost (e.g., \$/kg) in the utilisation phase [9,10]. While these are well understood for existing fuels, there is significant uncertainty looking at costs estimates for future fuels.

However, what is known to a reasonable degree of precision is how much energy is required to produce each low or zero carbon fuel. Kramel et al., constructed a Well-to-Wake assessment model for utilising current fossil fuels, looking at a global fleet level of impact [11]. Lindstad et al. looked into Well-to-Wake analysis which included e-fuels, using global energy demand data [12]. The aim of this work is to evaluate the use of a wind-to-wake ratio (WtWr) to assess the energy required to deliver the shaft energy needed for a ship to complete a voyage rather than the subjective approaches based on future fuel cost predictions [9,10, 13–15]. For those investing in new ships our proposed WtWr provides an objective measure that is related to the amount of renewable energy required with, as shown in in Fig. 1, liquid hydrogen, methanol and ammonia all requiring electrolysis of hydrogen.

While any renewable energy source could be used, we have chosen wind rather than, for instance, solar as its embedded ${\rm CO}_{\rm 2equiv}$ required to capture renewable energy from wind is typically an order less than solar [16].

Section 2 overviews the possible fuels and powertrains and assesses the energy required to bunker them on board. Section 3 details the WtW ratio approach by applying a time-domain, bottom-up method to match the required energy demand to power the vessel with a simulation of energy supply required. This is specific to every powertrain and fuel combination selected. Four representative ship types with differing

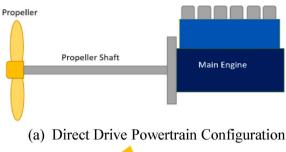
operational voyage energy demands are chosen to be benchmarked against a combination of conventional and future fuels for a variety of power trains. The results of these powertrain simulations are presented in Section 4. The effective WtWr for the various fuel/powertrain combinations are compared alongside their other environmental emissions in Section 5 as an objective framework for comparing alternative fuels for marine application concluded in Section 6.

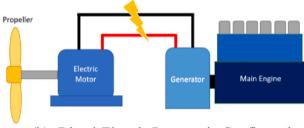
2. Future marine fuels & powertrains

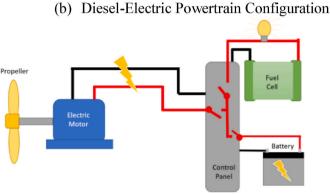
The effectiveness with which energy is transmitted from TtW is dependent on the fuel type and powertrain used. Conventional ship propulsion uses combustion of fossil fuels in reciprocating engines or gas turbines with their rotational power transmitted through a shaft attached to a propeller, with possibly a reduction gearbox in between (direct drive, Fig. 2a), or by converting to electricity through generators, with the propellers being connected to Direct Current motors (diesel-electric, Fig. 2b) [17]. This is a common approach in cruise ships or other vessels which have a high hotel (non-propulsive electrical) load or manoeuvring requirements.

Fuel cell technologies offer higher overall efficiencies (55–65 %) [18] compared to current internal combustion engines (40–50 %) [19] as well as only emitting water. Fuel cell electrical output is combined with load levelling batteries [20] to power electric motors (Fig. 2c). Only a few smaller vessels have adopted this approach [21] but are an attractive alternative due to their higher electrical efficiency yield [22–25].

Fuel cell options include Proton Exchange Membrane Fuel Cells (PEM FC) and Solid Oxide Fuel Cells (SOFC) that both display potential electrical efficiencies of over 50% [26]. Fuel cells are capable of providing this efficiency when utilising hydrogen [27], so are a zero-emission alternative for vessel propulsion. Internal reforming







(c) Fuel Cell Electric Powertrain Energy Management System

Fig. 2. Schematic of different propulsion powertrains indicating the main elements required.

technologies can be utilised to dissociate fossil fuels such as Liquefied Natural Gas (LNG) or other hydrogen carriers (e.g., methanol, ammonia) to hydrogen.

Heavy Fuel Oil (HFO), Marine Diesel Oil (MDO) or variants, power the vast majority of ships, with an increasing use of LNG and a limited number of nuclear vessels [28]. Hydrogen, e-Methanol, Ammonia, synthetic Methane & Bio-Diesel are some of the major contenders of zero and low carbon fuels [28]. Table 1 compares the key properties of some of the main fuels considered as future fuels [29,30]. It is assumed that these new fuels produced by utilising renewable electricity, the capture

of atmospheric CO₂ for methanol and nitrogen for ammonia. In this comparison we exclude the sole use of battery storage due to their low energy density (0.09 kWh/L) which is required to double before they are viable for long distance shipping [20].

Green hydrogen production is required for liquid hydrogen, (LH2), liquid ammonia (LNH3) and methanol (Fig. 1). Only the most space efficient storage method of storing hydrogen in its liquid state is considered. Alternative e-fuels such as e-Diesel require more energy to produce as it is more C-rich and so will perform less well than Methanol.

Ammonia (NH₃) is a major energy intensive industrial commodity (>175 Mt/a), essential to produce fertilizers, plastics, explosives and other industrial uses. It has been shipped and moved by pipelines for many decades [31], and considered as a potential future maritime fuel [32,33] as the ammonia molecule contains no carbon. Ammonia can be used as a fuel in internal combustion engines in combination with diesel as a pilot fuel. It is also potentially attractive as a hydrogen carrier as with 17.8 % hydrogen by mass [34,35]. Ammonia is liquid at -37 °C and contains 45% more hydrogen molecules per unit of volume compared to liquid H₂. However, energy is be required to dissociate, 'crack' the ammonia and to purify the hydrogen for use in fuel cells [36]. It is a highly toxic substance and its safe handling as a marine fuel, as opposed to a maritime commodity, remains unproven due to lack of commercial applications [37]. Although ammonia can be detected in very small concentrations (5 ppm) in the air, it is colourless and hydrophilic, with a strong pungent odour [35]. It is lethal when ingested. Due to its toxicity, an ammonia spillage in the environment could severely impact marine biodiversity [38]. The use of ammonia as a maritime fuel may be unacceptable to the general public [39] especially if large bunkers are stored in port cities. Finally, ammonia use in internal combustion engines can significantly impact emissions due to the formation of the N2O gases, which have a 265 times greater greenhouse gas warming potential than CO₂ [40].

The use of synthetic methanol (CH₃OH) could be a potential decarbonisation option [41] despite still having CO₂ tailpipe emissions due to the presence of carbon in the molecule. Methanol is liquid at ambient conditions and relatively easy to handle. Overall safety precautions are likely to be similar to currently used fossil fuels, with only a few handling and storage modifications required such as the use of double walled tanks and special anti-corrosion coatings [42]. Its potential synthesis is most likely as a biofuel, requiring land that is essential for growing food or would instead be more efficient to use to deploy solar panels for energy production [43]. Methanol can also be produced by combining green hydrogen with CO₂ removed from the atmosphere by Direct Air Capture (DAC) systems, to produce e-methanol, that would be net zero with respect to emissions footprint after utilisation. DAC technologies are energy intensive and unproven at industrial scales [44,45].

The properties in Table 1 show that fuel transition for ships will require significant changes in practice for all possible solutions examined. Others have explored what these will be [7,25,30,46,47], along

Table 1Key properties of main fuels examined [34,49–59]. For the WtWr, the smaller the ratio of fuel generation energy to fuel exergy the better.

Fuel Type	Conventional		Zero/low carbon		
	MDO	LNG (Methane)	LH ₂	LNH ₃	Methanol
Density ρ (kg/m³)	890	440	71	653	780
Lower Calorific Value (LCV) (MJ/kg)	42.8	50	120	18.6	20
Volumetric Energy Density (MJ/L)	38	22	8.5	12.1	15.6
Boiling point (°C)	60	-163	-253	-33	64.7
Minimum Embedded Production Energy (per kg)	9 MJ	10 MJ	170 MJ [60,61]	43.2 MJ [62]	39.6 MJ [63,64]
Ratio of Energy for Fuel Generation to Fuel exergy (WtWr)	N/A	N/A	1.4:1	2.3:1	2:1
Flammability limits (Air conc. [% v/v])	1.3-6	5–15	4–74	14.8-33.5	6-36.5
Ignition temp. (°C)	350-380	537	520	650	433
Hazards	Flamm- able	Flammable, cryogenic	Highly Flamm-able; cryogenic	Highly Toxic, cryogenic	Flammable & Toxic corrosive

Table 2Case study vessels' key characteristics.

Vessel Type	Power (MW)	Service	Capacity	Time Duration (Days)
Container Vessel (A)	25	Port to port	3800 TEU	3
Survey Vessel (B)	2.5	Sea floor scanning	2 ROVs	30
Cruise Ship (C)	64	Tourist sightseeing	6000 Passengers	365
LNG Carrier (D)	41	Port to Port	138,000m ³ of LNG	28

Vessel A is a proposed 3800 TEU container vessel for short sea shipping route from Southampton to Liverpool. Vessel B is a research vessel carrying out a 30-day survey, utilising fuel cells. Vessel C is an operational 6000 passenger cruise ship with detailed data available for a year's annual operation and Vessel D is a tri-fuel LNG carrier, powered by Heavy Fuel Oil, LNG and MDO with detailed data for several years' operation.

with requirements for increases in onboard fuel storage and consequent range implications.

These will necessitate changes to current marine bunkering strategies that bunker with the most inexpensive fuel at any given journey point or distribution hub to ones where only the fuel required and a safe margin are bunkered for the next voyage.

All the alternative fuels discussed require the input of substantial energy in their manufacture (Table 1). The TtW approach does not take this into account, or the emissions associated with the production process. For example, a methane reformation process used to generate methanol to power a vessel, will result in a 17% increase of total $\rm CO_{2e}$ emissions, when compared to combusting LNG direct [48].

3. Application of wind-to-wake ratio approach

While the fuel energy required to supply onboard is known, we consider how the voyage energy requirement affects the eventual WtWr. Four case studies are chosen to compare alternative fuels and power-trains (Table 2). These are chosen to represent typical ship types that make up the global merchant fleet and their respective voyage energy demand [65].

To investigate different powertrain approaches, operational voyage power demand data at time increments between 30 and 90 s are used for the typical voyages considered. Different Python based models of all the components of power trains assessed allowed the fuel use and emissions per voyage to be compared. Vessels A and C used predicted voyage demand based on likely sea state and different voyage phases. Vessels B and D used measured data. For each time interval fuel consumption, battery state, and resultant emissions were determined.

3.1. Vessel A: container ship (3 fuels, 1 powertrain)

To compare potential retrofits, in this case methanol and ammonia, a diesel-powered 230 m long 'feeder' container ship servicing a 500-mile route between Southampton and Liverpool is selected. Based on a 3.8 m scale model tested in the University of Southampton's towing tank through a series of sea states, power demand was derived, from which a time series was developed using typical sea states for the route. Additional auxiliary equipment power was taken into consideration and a powering profile fluctuation during manoeuvring was acquired by comparison with the LNG tanker. Finally, the machinery specifications of a similar vessel design were used to match the powering requirements in terms of fuel consumption either when running on MDO, methanol or ammonia.

3.2. Vessel B: survey vessel (2 fuels, 1 powertrain)

A 78-m-long survey vessel, conducting a 30-day seafloor scanning mission, is proposed to employ PEM FC, fed by an ammonia cracker which is electrically powered by an internal combustion engine genset. The ammonia cracker utilisation examined in this case, is used as a comparison with direct use of LH2. A model was developed to generate power demand profiles specific to this survey vessel, accounting for factors such as speed and load variation associated with the many activities carried out by the vessel, such as remotely operated vessel deployment or cranes and monitoring equipment mobilisation using winches.

3.3. Vessel C: cruise ship (3 fuels, 2 powertrains)

The cruise ship is a 6000-passenger carrying vessel with four Ottocycled generator-sets (gen-sets) fuelled by Liquified Natural Gas (LNG), providing a combined maximum power output of 62 MW. This vessel mostly operates short overnight voyages, with passengers able to disembark daily. Due to the large number of passengers and consequent large crew carried, the vessel has a significant accommodation demand for heating, ventilation, and air-conditioning (HVAC), steam production, and other electrical demands required to sustain passenger needs. All energy demands were evaluated, based on data recordings worth of one year's operation [66]. For this case, a Solid Oxide Fuel Cell (SOFC) system was implemented to support the baseload energy demand, firstly with an internal reformer unit to convert LNG into Hydrogen. In a second scenario the running of the SOFC on pure hydrogen was investigated. A final comparison was made with a methanol combustion retrofit.

3.4. Vessel D: LNG carrier (4 fuels, 2 powertrains)

The large LNG carrier used in this case study, has 41 MW of rated power. The propulsion system used is tri-fuel diesel electric (TFDE), as the machinery employed on board can run on Heavy Fuel Oil (HFO), Marine Diesel Oil (MDO) and LNG, all converted into a MDO_{eq} equivalent consumption. An example case study voyage was from Singapore to Trinidad and Tobago, which takes 28 days and represents the longest duration voyage this vessel underwent during its recorded period of service. For this case study, ammonia and methanol retrofits as well as a fuel cell running on a hydrogen conversion scenario were investigated. More detailed investigations on this vessel and associated fleet are given in McKinlay et al. [48].

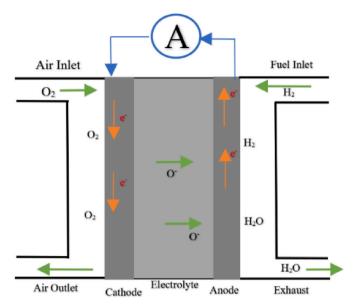


Fig. 3. Illustration of SOFC operating principles, where fuel (hydrogen) is fed to the anode, oxygen is supplied to the cathode, and electrochemical reactions occur to produce electricity. Note for LNG or NH_3 feedstock, this needs to be reformed into H_2 and purified.

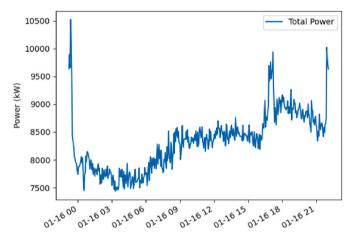


Fig. 4. Typical example of demand fluctuation whilst in port (Cruise ship scenario) (month-day/hour).

3.5. Powertrain simulation

Ship engines or fuel cells must respond to various loads (demands) throughout a specific voyage, with power demand on board constantly fluctuating, depending on speed, sea-state and the operational condition of the vessel at any given time. For all vessel case studies presented above, a time accurate powertrain simulation of operation was developed using Python. This simulation matched the power demanded to propel the ship and power its onboard systems (the 'hotel' load). The time step used was $\sim\!60$ s which is sufficiently refined to capture power fluctuations in waves and follows a bottom-up approach (from electric demand, up to the larger system's energy needs) [67]. The required power demand is related to the fuel consumption required and

associated CO2e emissions. Two types of power generation devices are considered: internal combustion engines and fuel cells with batteries.

3.5.1. Internal combustion engine simulation

A few commercial companies supply the world's market for large ship engines. In general, engine emissions and performance data are not made available. A first principles internal combustion engine simulation was developed to generate consumption and emission profiles over various engine loads. The same theoretical internal combustion model was employed on an engine that is offered in the market, for evaluating basic thermodynamic parameters such as cylinder mean effective pressure, thermal and mechanical efficiency, allowing a comparison of these results to the limited performance test data available (Table 3). The same model was then adopted for potential methanol and ammonia retrofits (Table 4).

For a fair comparison amongst the different vessels, as most of the dual fuel genset powertrains presented in this case run on the theoretical Otto-4 stroke cycle, it is assumed that this will remain the case for both methanol and ammonia scenarios, as it constitutes a realistic representation of a marine engine retrofit [41,43,48,68,69]. An exception is made when running on MDO, where the theoretical engine cycle is that of a 4-Stroke Diesel engine.

When considering the combustion of methanol, a means of initiating combustion is required due to significantly higher auto-ignition temperature of methanol compared to diesel because of the lower cetane number. One method considers increasing the compression ratio to 27:1 which requires extensive modification of the engine's internal architecture. Another method for methanol autoignition is through the introduction of a chemical ignition improver or through the utilisation of pilot diesel fuel. The amount of diesel pilot fuel required was estimated based on published results [70,71]. The same is also applied for the ammonia combustion scenarios, where the amount of pilot fuel required is based on published experimental studies [72–75], with respect to the total consumption, assuming that thermal efficiency remains the same across all fuelling scenarios.

3.5.2. Fuel cell simulation

A fuel cell (Fig. 3) operates by using a fuel, hydrogen in the cases discussed, which reacts with oxygen ions to form water molecules through an ion-conducting electrolyte between the anode and cathode where the electrolyte is a non-porous solid metal oxide, in the case of SOFC. In PEMFCs, the hydrogen itself is converted to ions that travel through the electrolytic membrane. In both cases, due to ion formation, an electrical potential difference is induced within the system, as ions are attracted to their ionic counterparts, with the end byproduct being water vapour, once these ions bond [26,27].

A first principles fuel cell operational simulation was developed, based on the main working principles of a fuel cell system, described above and compared to data supplied by fuel cell manufacturers. This gave comparable performance with regards to efficiency, power output and fuel consumption of both SOFC (Table 5) and PEMFC (Table 6).

Parameters include internal cell resistance, fuel utilisation factor, fuel cell plate thickness and cross-sectional area, the required voltage and amperage output to be compatible with current machinery, the total power required, and the heat developed from the resulting reactions. With some parameters for both fuel cell types being confidential, the simulations were based on the main theoretical equations (eqs. (1)–(6)) to estimate performance indexes [27,76]. These equations are:

$$W_{out} = \Delta G = RT_{ref} \ln(Ko) - RT\ln(Kp)$$
 (1)

where, W_{out} is the work extracted by the cell for a given product of partial pressures (Kp), based on the Gibb's energy principle, R ($J/mol\cdot K$) is the gas constant, T_{ref} is the reference temperature (K) of the cell and the equilibrium constant Ko:

$$Voc = \frac{W_{out}}{n_{el}F} \tag{2}$$

where, *Voc* is the open cell voltage, n_{el} is the number of electron exchange within the reaction 2H- + O₂- \rightarrow H₂O and F is the Faraday Constant;

$$P_{stack} = V_{cell} \bullet I_s \tag{3}$$

where P_{stack} is the power output of each cell that depends on the fixed voltage of the cell (V_{cell}) and the cell's current supply Is which are found through the following equations;

$$I_s = n_{el} \bullet F \bullet \dot{m}_{H2} \tag{4}$$

where Is is the combined amperage output, directly related to the fuel consumption;

$$V_{cell} = V_{oc} - R_{ohm} *i - V_{Act} - V_{Con}$$

$$\tag{5}$$

where i is the cell's current, $R_{\rm ohm}$ is the ohmic resistance, V_{Con} is the concentration loss and V_{Act} is the activation loss; where;

$$V_{Act} = bln(i), V_{Con} = me^{ni}$$
 (6)

As part of the fuelling system for one of the case studies examined here for the powering of a PEM-FC stack, the energy demand for an ammonia cracker is modelled using equations used to calculate fuel reformation and storage methods:

$$Heat input = M_{NH3} \bullet Cp(T_{in} - T_{out})$$
 (7)

where.

a) Simulated Value

- $M_{NH3} = \text{Mass flow of ammonia fuel input}$
- Cp = Specific heat capacity of ammonia (2.175 kJ/kg.K)

Table 3 Wärtsilä 12W32/40 Engine Power output against load.

Load (%)	Power (kW)		fic Fuel Imption [S.F.C.] Vh)	Brake Mean Effective Pressure [B.M.E.P.] (bar)	Efficiency (%)
100	7095	189		28.2	44.4
75	5282	181		22.1	46.4
50	3557	185		14.2	45.4
(b) Manufacturer Values [80]					
Load (%)	Power	r (kW)	S.F.C. (g/kWh)	B.M.E.P. (bar)	Efficiency (%
100	6960		186	28.8	45.2
75	5220		182	N/A	46.2
50	3480		189	N/A	44.9

Table 4a
Methanol simulation results.

Load (%)	Power (kW)	S.F.C. [g/kWh]	Pilot Fuel (% m/m)
100 75	7098 5282	376 364.7	5 10
50	3458	373	15

Table 4b
Ammonia simulation results.

S.F.C. [g/kWh]	Pilot Fuel (% m/m)
417.7	10
391.1	14
370.5	23

Table 5Simulated efficiency and consumption for Solid Oxide Fuel Cells.

Power (kW)	Efficiency %	SFC LNG (g/kWh)
7875	65.5	115.2
8925	64	114.3
10,500	62.5	118.2

Table 6
Simulated efficiency and consumption for Proton Exchange Membrane Fuel cells.

Power (kW)	Efficiency %	SFC H ₂ (g/kWh)
1000	54.8	54.7
1500	56	53
2000	52.6	57
2500	49	68

- T_{in} = Inlet temperature of ammonia after heat exchanger
- T_{out} = Outlet temperature of ammonia at cracking temp

Energy input =
$$M_{H_2}(h_{in} - h_{out})$$
 (8)

where.

- M_{H_2} = Mass flow of hydrogen input, subsequent of ammonia consumption requirement
- h_{in} = Specific enthalpy of hydrogen prior to compression and cooling at specific temperature and pressure
- h_{out} = Specific enthalpy of hydrogen after compression and cooling at specific temperature and pressure.

3.5.3. Batteries

Fig. 4 shows the power demand recordings of a specific vessel case study with examples of rapid fluctuations that require power smoothing using a battery.

Engines are intrinsically faster in changing their power output to service fluctuating demands, due to their ability to change the air-fuel mixture entering the combustion chamber within milliseconds [77, 78]. In contrast, fuel cells, require slower alteration of flow to avoid damage of the electrolytic structure, either by water droplet development or thermal damage [79]. Consequently, batteries are required to respond to sudden peaks in power demand, providing enough time for the fuel cell to ramp up its electrical output. Likewise, excessive power will be used for charging during sudden drops in demand, maintaining an acceptable level of charge. An optimal level of charge of 80% is set as a target, to enhance battery longevity and performance.

4. Simulation results

4.1. Powertrain simulations

4.1.1. Internal combustion engine simulation

Using the typical thermodynamic equations for both Diesel and Otto cycle 4 Stroke engines, the mechanical and thermal efficiencies were approximated and compared to an engine whose values were already known (Table 3) and is advertised as dual fuel ready.

Table 3a shows the results gathered from the theoretical approximation which indicate less than 2% deviation from manufacturer's

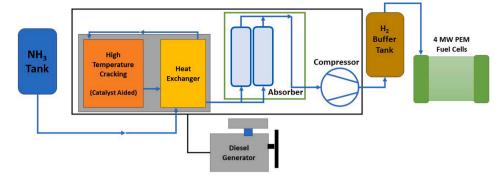


Fig. 5. Ammonia cracker on board the Survey vessel showing the multiple stages between tank and fuel cell to ensure sufficiently pure H₂.

values in Table 3b. Following this approach, the simulation was adjusted to provide a realistic engine operation under methanol and ammonia utilisation, by altering the fuel properties, and the air to fuel ratio accordingly (Table 4).

4.1.2. Fuel cell simulation

As in the case of internal combustion engines, a simulation of operation was developed to cross reference values from manufacturers, using Eqs. (1)–(6) for the proposed fuel cell-battery hybrid powertrain to provide performance output parameters. (Tables 5 and 6).

4.2. 3800 TEU container vessel

Three scenarios were considered for the container ship, with methanol or ammonia combustion compared to the current and traditional MDO fossil fuel utilisation, having the power output supplied by two ICE-gensets, totalling 25 MW. For a single trip from the Port of Southampton to the Port of Liverpool (500 nm), the total consumption of MDO was 168 tonnes, resulting in a total of 539 tonnes of $\rm CO_{2equiv}$.

Considering the proposed methanol retrofit solutions, 334 tonnes of methanol and 3.6 tonnes of diesel are consumed, resulting in 574 tonnes of CO_2 . As such, fuel consumption increased 2.2 times and CO_2 funnel emissions by 6.4%. Consequently, methanol consumption increases funnel emissions when compared to fossil fuels, although the same emissions are offset during production, by utilising previously captured CO_2 , but this requires large amounts of valuable renewable electricity to power DAC (Fig. 7). Instead, onboard carbon capturing can be used, but this increases fuel consumption by 10–20% while still not capturing all of the funnel emissions [81]. The use of bio-methanol would avoid much of these emissions, albeit at the expense of utilising an amount of useful cropland. With the ammonia retrofit, total consumption amounted to 318 tonnes of liquid ammonia and 41 tonnes of diesel as pilot fuel, releasing 127 tonnes of $\mathrm{CO}_{2\mathrm{equiv}}$, emissions.

4.3. LNG carrier

For this vessel, the original powertrain consists of three diesel generators that can be run on HFO, MDO or LNG boil off from the cargo carried. The later fuelling option, although abundant on board, does not necessarily mean that it will be utilised on every trip, as it depends on charter and management agreements. For example, in some cases, it is of economic benefit for the managers to run on the cheaper HFO option and reliquefy the boil off gas, than to utilize it directly by combusting it. Moreover, an LNG carrier does not always carry cargo at full capacity, as it can sometimes be empty and run in ballast, meaning that there is not

Table 7Fuel cell hydrogen consumption according to power output and subsequent power supply required for the ammonia cracker to meet the fuel demand.

FC power (kW)	H ₂ Consumption (kg/s)	NH ₃ required (kg/s)	Cracker (kW)
1000	0.017	0.10	245
1500	0.025	0.15	360
2000	0.036	0.21	514
2500	0.047	0.28	681

enough boil-off to fuel the main propulsion engines and diesel equivalent fuel is used instead of a reserve LNG tank.

This voyage considered from Singapore to South America, uses HFO as the main propulsion fuel. The total consumption was converted to an MDO equivalent, a total of 2878 mt. GHG emissions are consequently 7373 mt $\rm CO_2e$, using factors set by the IMO [82]. Methanol and ammonia retrofits, both anticipated to greatly reduce GHG emissions, were also considered for this voyage. Total methanol and ammonia consumption were estimated to be 5063 and 4993.5 tonnes, with pilot fuel consumption being 446.1 and 644.5 tonnes for each case, respectively. NOx, SOx and Particulate Matter emissions will not be compared between the scenarios, since they do not translate directly in terms of $\rm CO_2$ equivalence.

As a zero-tail pipe emission alternative, a completely new powertrain and fuelling scenario is considered, in terms of 40 MW fuel cells with 10 MWh batteries and pure hydrogen as the main fuel. For the same voyage, 913 tonnes of hydrogen are required.

4.4. Cruise ship

As a baseline, the annual LNG utilisation through internal combustion engines was compared to that through SOFCs. Significant reduction in terms of fuel consumption and $\rm CO_{2equiv}$, emissions was found, when only subsidising part of the powertrain to cover the baseload demand, with SOFC. The original LNG Genset powertrain amounted to a total annual consumption of 26,746 tonnes of LNG, emitting 92,099 tonnes of $\rm CO_{2equiv}$. By substituting a pair of the original gensets with two smaller ones and a complete SOFC powertrain of 10.5 MW, a drop of 35% and 27% in $\rm CO_{2equiv}$, emissions and LNG consumption respectively, was gained, partially due to the reduction of methane slip [66].

The new powertrain system design required a methane reformer, powered by the SOFCs' exhaust heat and a Waste Heat Recovery System (WHRS) to satisfy the demand of steam production on board. Due to the heat demanding reforming process requiring, steam output was insufficient [66]. Consequently, the utilisation of auxiliary gas boilers was accounted for in the final analysis.

If hydrogen is used with the same fuel cell powertrain, to cover the base demand on board, the emissions could be reduced by 65%.

When the original genset configuration was retrofitted for utilising methanol, the total consumption of MDO and methanol was 6771 and 49,558 tonnes, respectively, meaning 2.1 times higher in total fuel mass capacity for the entire year. Moreover, although the $\rm CO_{2equiv}$ funnel emissions dropped by 2.6% compared to the original LNG genset scenario, this is mostly attributed to the lack of methane slip.

As a result, it is still unclear whether there is any improvement from converting this particular vessel to run on methanol, especially when comparing the utilisation of a higher efficiency SOFC powertrain whilst using LNG.

4.5. Survey vessel

For the survey vessel, in addition to the PEM fuel cells and batteries, an ammonia cracker and purifier must also be added to the system (Fig. 5).

A catalyst-aided cracking process is considered in this case and the process steps are: Vaporisation and preheat of ammonia; heating of ammonia at 450 °C, hydrogen formation; precooling of Hydrogen to 150 °C; compression of Hydrogen to 6 bar; cooling to -50 °C; and storage for use.

To estimate the total amount of energy required to completely dissociate ammonia into hydrogen, the energy demands of each process step is calculated separately (Equations (7) and (8)). The final energy demand is the sum of these results (Table 7).

The largest energy loads in this process are the ammonia heater, the hydrogen coolers and the compressors. The mass of the fluid is calculated based on the hydrogen demand of the Proton Exchange Membrane (PEM) fuel cells, assuming a 25% hydrogen loss during the purification process [83].

The average power requirement of the ammonia cracker just to feed the PEM fuel cells that power it, is >20% of their total power output (Table 7). This energy input requirement is significant and should be accounted for when selecting the appropriate fuel cell installation sizing, to accommodate the cracker's extra demand. For this study this extra energy was neglected as it was assumed, a bio-diesel generator was used.

An alternative zero-emission fuelling system, which uses liquid hydrogen stored in the vessel also considered. 27.9 tonnes of liquid hydrogen are required to carry out the same mission with total system weight of 172 tonnes, \sim 17% less weight compared to the ammonia cracker scenario, that requires 198.4 tonnes of ammonia as fuel, with total fuelling equipment space requirements showing a 7% increase to 994 m³. This highlights the feasibility of liquid hydrogen storage with appropriate allocation within the vessel's general arrangement, considering a small sacrifice for attaining a higher efficiency powertrain.

5. Effectiveness of WtW ratio

Although both ammonia and methanol can be net-zero in terms of ${\rm CO_2}$ equivalence, a distinction is made between these two and the pilot fuel used to ignite them. In most cases, MDO is essential to initiate combustion which results in significant contribution towards funnel emissions (Fig. 6). Therefore, neither fuels can be considered as truly net zero, unless other means of utilisation are employed, such as reforming and fuel cells.

Fig. 7 shows the amount of fuel that is consumed onboard each vessel case study, for the specific fuel and powertrain that is selected, along with the resulting net emissions footprint. These are accompanied by the

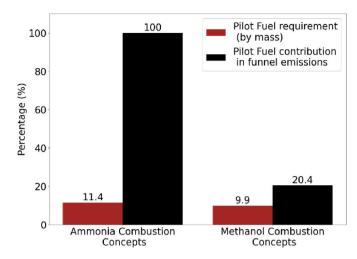


Fig. 6. Average contribution of Pilot fuel for ammonia and methanol combustion, in terms of fuel mass consumption and resulting CO₂ funnel emissions (TtW), for case studies examined.

total renewable energy investment, to indicate the shortcomings of the Tank-to-Wake concept compared to the Wind-to-Wake approach. These concepts challenge the efficacy of some net-zero fuels. Both ammonia and methanol combustion require a significantly higher energy invested during manufacturing compared to the energy required to carry out the services of each vessel, while still using pilot fossil fuels for their combustion (Fig. 6).

Considering Fig. 7, it appears that only hydrogen can provide the solution of zero emission shipping. Although ammonia can be used with PEM fuel cells, this requires the employment of an ammonia cracker, which contributes to a major parasitic loss onboard, therefore making its utilisation very inefficient (Fig. 8). When SOFCs are employed, the efficiency loss could be less, yet to the expense of internal material degradation [84]. Fig. 8 shows, on average, the amount of renewable energy investment required towards manufacturing of each fuel, with associated powertrain selected, compared to the energy that is required to carry out each service.

Through the WtWr approach an additional energy sacrifice of capturing that $\rm CO_2$ emission from atmospheric air to develop sustainable methanol is highlighted. This number is at least an additional 30% compared to a zero-emission fuel, such as hydrogen, implying a nonending and intensive cycle just for partially recycling carbon. The WtWr also indicates how important it is to utilize both higher efficiency powertrains for propulsion and fuels that require less energy for their production.

The Wind to Wake approach emphasizes the importance of dissociating future marine fuels from current fossil fuel, to eliminate emissions. This extends on saving energy during each fuel's life cycle, something that is otherwise masked when using an energy source, whose extraction is treated as granted, even in the final stage of utilisation.

Finally, the high WtWr in Fig. 8 with regards to ammonia utilisation, results from the energy intensive process of nitrogen capturing and its bonding with hydrogen that could make it a hydrogen carrier, which is then "cracked" on board or, as is proposed, to create ammonia and then transporting it, before cracking either before bunkering or once on board. This comes with a significantly higher energy expense when compared to the solution of carrying liquid hydrogen. Both manufacturing processes can be traced back to Fig. 1.

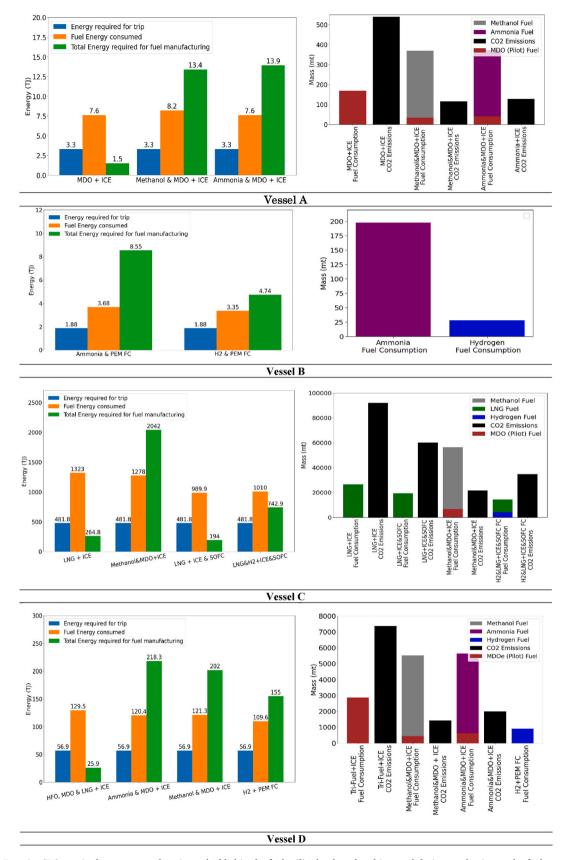


Fig. 7. (Left): Energies (TJ) required to carry out the trip, embedded in the fuel utilised onboard and invested during production to the fuels consumed. (Right): Amount of fuel consumed in each scenario with resulting carbon footprint emissions, by mass (mt).

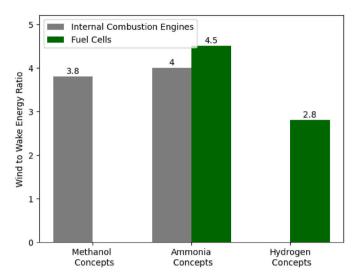


Fig. 8. Wind to Wake energy Ratio of e-fuels examined using an average of the various comparable scenarios.

6. Conclusion

New, low and zero-carbon fuel options are imperative for the maritime industry to reach net-zero emissions by 2050. Here, a range of alternative fuels are investigated alongside new powertrain solutions to test the lowest emission solutions, requiring the least amount of renewable energy investment towards their implementation. Although some alternative fuels may theoretically appear as zero emission, our full life-cycle energy feasibility studies challenge this.

Through taking a Wind to Wake approach, the cases of both ammonia and methanol indicate higher energy contribution towards their production compared to liquid hydrogen, while crucial steps such as carbon recycling and fossil fuel dependence are brought to light. A case is also made for utilising higher efficiency powertrains, as this allows for large savings on costly renewable energy sources, since lower

amounts of e-fuels are consumed. This is of high importance when planning to reform a global industry with the end goal being environmental sustainability, as set out by the IMO.

The results obtained show that for the fuels considered, liquid hydrogen requires the least amount of renewable energy investment from all fuels discussed, 30% less than ammonia and 26% less than methanol when used in combination with a fuel cell and battery hybrid powertrain. These results are consistent across the wide range of ship types. It is to be expected that this significant energy saving will drive the industry to adopt hydrogen as its fuel of the future with the additional benefits of zero greenhouse gas and other air pollutant emissions.

CRediT authorship contribution statement

Panagiotis Manias: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation. Charles McKinlay: Writing – review & editing, Software, Resources. Damon A.H. Teagle: Writing – review & editing, Writing – original draft, Project administration, Conceptualization. Dominic Hudson: Writing – review & editing, Writing – original draft, Methodology. Stephen Turnock: Writing – review & editing, Writing – original draft, Supervision, Project administration, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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NOMENCLATURE

NH_3	Ammonia
BMEP	Brake Mean Effective Pressure
CCU	Carbon Capture and Utilisation
CO_2	Carbon Dioxide
FC	Fuel Cell
GHG	Greenhouse Gas
HFO	Heavy Fuel Oil
H_2	Hydrogen
ICE	Internal Combustion Engine
IMO	International Maritime Organisation
LNG	Liquefied Natural Gas
LCV	Lower Calorific Value
MDO	Marine Diesel Oil
CH ₃ OH	Methanol
NO_x	Nitrogen Oxides
PEM	Proton Exchange Membrane (fuel cell)
SFC	Specific Fuel Consumption
SOFC	Solid Oxide Fuel Cell
SO_x	Sulphur Oxides

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