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Abstract

The pressing need to transition shipping operations toward net-zero emissions has catalyzed innovations in energy storage and propulsion technologies. Liquid organic hydrogen carriers (LOHC) have emerged as a promising medium to safely store and transport hydrogen at ambient temperatures and pressures. This enables usage of hydrogen fuel in proton exchange membrane fuel cells (PEMFC) for efficient onboard power generation.

This study examines the feasibility of using the LOHC-PEMFC technology combination tailored for marine applications. A case study design of LOHC storage, distribution, and PEMFC consumption onboard a 100m coastal general cargo vessel is presented. The analysis covers national infrastructure requirements, port interfaces, operational profile modeling and overall integration complexity.

Engineering analyses quantify the storage volumes, reactor productivity sizing, and PEMFC specifications to match propulsion duty cycles. Upgrades for port bunkering logistics and inland transport are elaborated. The maiden voyage consumption pattern verifies adequate capacity buffer between refueling cycles.

Applicability for marine usage is assessed based on fuel economy, safety, modular scaling and redundancy factors. Hybridization configurations using batteries and onboard generators are also explored to enhance flexibility. Initial cost projections find the life-cycle economics comparable or favorable against conventional options subject to incremental upstream investments.

Overall, LOHC-PEM systems display technical promise and infrastructure synergies to aid adoption as sustainable marine fuels. But rigorous testing and qualification milestones are vital prior to commercial deployment. Gradual industry transition can leverage the higher energy density and storage safety benefits over other hydrogen alternatives. Findings will inform holistic frameworks balancing environmental obligations and practical realities for ship owners.

Keywords:

Liquid organic hydrogen carrier (LOHC), proton exchange membrane fuel cell (PEMFC), green shipping, hydrogen storage, coastal vessel

Emission free costal cargo transport

CHAPTER-1: Introduction

1.1 Introduction, academic and industrial context, challenges.

Maintaining sustainability goals and cutting emissions are major challenges for the maritime transport sector. Targets to cut shipping emissions by at least 50% by 2050 have been established by the International Maritime Organisation (IMO), mostly from oceangoing commercial vessels (Kanberoğlu B. a., 2021). Widespread adoption of alternate energy sources, operating procedures, and propulsion technologies is necessary to achieve this. With the UK government aiming for net-zero domestic emissions by 2050, decarbonization is especially crucial in coastal and short-sea commercial transportation (Transport decarbonisation plan, 2021). The maritime sector must overcome obstacles to make the switch from fossil fuels to sustainable energy sources. The study investigates how autonomous coastal cargo ships with zero emissions might be made possible using liquid organic hydrogen carrier (LOHC) technology, offering a sustainable mode of transportation.

The freight transportation industry's carbon impact is mostly attributed to domestic coastal and short-sea cargo shipping. According to the (Transport decarbonisation plan, 2021), 11% of household goods carried in the UK was transported by water along inland and coastal waterways (Transport decarbonisation plan, 2021). However, most coastal vessels still run on outdated diesel-powered marine engines, which are quite inefficient and emit a lot of pollutants. Decarbonizing coastal shipping is essential to reaching the legally mandated net zero greenhouse gas emissions target set by the UK government for 2050.

Hydrogen is a zero-emission fuel that is becoming more and more popular in the marine industry. When it burns, it simply creates water vapour and has a better storage density than batteries. However, due to its high volatility and low ambient temperature liquefaction point, pure hydrogen presents difficulties for safe handling and storage on board ships. A novel approach is provided by Liquid Organic Hydrogen Carriers (LOHC), which attach hydrogen to a liquid organic substance via reversible chemical processes rather than high pressures or cryogenic temperatures (Rao, 2020). Compared to compressed gaseous or liquid hydrogen alternatives, LOHCs have benefits in terms of safety, supply chain compatibility, reusability, and infrastructure compatibility.

An innovative solution to overcome these barriers is using Liquid Organic Hydrogen Carriers (LOHC). LOHC systems rely on reversible chemical reactions to bind hydrogen to a liquid

organic compound without cryogenic temperatures or high pressures (Rao, 2020). The resulting carrier fluid allows hydrogen to be stored and transported via existing infrastructure at room temperature and modest pressures. LOHCs offer critical safety, infrastructure compatibility, reusability, and supply chain advantages over compressed gaseous or liquid hydrogen alternatives (Dagdougui, 2012).

LOHC systems enable hydrogen fuel storage and transportation in a chemically bonded liquid carrier at ambient temperatures and modest pressures (Teichmann, 2012), offering safety and infrastructure advantages over compressed gaseous or liquid hydrogen. This technology avoids the boil-off and containment challenges of cryogenic liquid hydrogen while achieving higher volumetric density (Makaryan, 2020). This project aims to design LOHC-powered, potentially autonomous cargo vessels that can serve UK coastal routes with zero direct emissions. LOHC systems use chemical compounds to reversibly bind hydrogen through a hydrogenation process, allowing it to be shipped and handled like conventional liquid fuels without cryogenic temperatures or pressurization (Preuster, 2016). This report explores the feasibility of adopting LOHC technology for a new coastal cargo vessel design, potentially eliminating emissions and reducing the UK's reliance on carbon-intensive heavy goods vehicle (HGV) freight.

.However, practical implementation, fuelling infrastructure requirements, regulations, and economic viability remain questions. Transitioning coastal shipping to LOHC-hydrogen propulsion aligns with UK government goals to achieve net zero greenhouse gas emissions by 2050 and promote sustainable domestic freight ((DfT), 2022). LOHCs offer logistical advantages and reuse potential, but challenges include developing efficient release and recovery systems, assessing onboard storage needs, and designing compatible port interfaces and bunkering facilities.

The project aims to evaluate the technical and financial viability of low-emission coastal shipping (LOHC) in the UK, focusing on zero direct emissions cargo transport. It will evaluate the potential of LOHC in collaboration with a hydrogen and fuel cell technology specialist. The study will offer a unique design idea for a ship, focusing on cargo capacity, energy alternatives, autonomy features, and shore infrastructure needs. LOHCs could significantly increase efficiency and decarbonization of coastal shipping, fulfilling sustainability objectives and anticipated freight demand. The outcomes will guide industry investments, regulatory frameworks, infrastructure developments, and pilot projects.

CHAPTER-2: Literature review

Liquid organic hydrogen carriers (LOHCs) are a promising hydrogen storage and transportation solution. They allow hydrogen to be stored at ambient temperatures and moderate pressures by chemically binding with a liquid carrier oil, providing safety benefits, and utilizing existing fuel infrastructure. LOHCs can efficiently transport hydrogen from renewable energy sources to end-use mobility applications. (Preuster, 2016) conducted a technical and economic analysis of LOHCs for ship propulsion, finding favourable storage density and safety properties compared to compressed H₂ or ammonia. LOHCs also offer advantages such as standard fuel infrastructure, ambient storage conditions, and high cyclability (Preuster, 2016).

2.1 LOHC Fundamentals

Liquid hydrogen storage using organic chemical compounds relies on reversible binding with the fuel molecules through hydrogenation. (USA Patent No. 3883372, 1975) developed early LOHC concepts using catalytic reactions for low-pressure hydrogen loading into aromatic carriers like toluene. The loaded LOHC compound serves as a liquid vector for safe hydrogen transportation and storage without high volatility or the need for constant refrigeration compared to liquid H₂ itself (Teichmann, 2012).

LOHCs utilize either exothermic “absorption” reactions or slightly endothermic “adsorption” mechanisms for hydrogenation loading (Preuster, 2016). Thermal energy input enables controlled hydrogen release via dehydrogenation back to the original carrier compound, which can then be reused. Studies suggest excellent cycling stability over 100s of absorption-desorption loading cycles without efficiency declines, albeit using catalysts to accelerate kinetics. Various organic liquids have LOHC potential depending on hydrogenation conditions and kinetics, including aromatic hydrocarbons like toluene or dibenzyl toluene and heterocyclic saturated compounds such as N-ethyl carbazole (Rao, 2020).

2.1 Policy Landscape

The regulatory landscape is evolving to address alternative marine fuels, but gaps remain regarding LOHCs explicitly. Class rules traditionally focused on containing fossil diesel hazards may wrongly treat LOHC systems as conventional oil, missing unique risks (DNV, 2021). The (IMO, 2022) provides codes for very low flashpoint fuels, but ambiguities exist for hydrogen via carriers. Updates lag ongoing technology developments.

Greater clarity on safety zones, bunkering processes, tank storage limits, and redundancy levels will be necessary through iterative risk assessments with pioneering projects. Design standards explicitly addressing LOHC system integration could accelerate innovation. Staged requirements for crew training, system monitoring, and redundancy based on operational maturity can enable incremental automation (Rødseth, 2014). An enhanced regulatory framework can spur adoption.

2.2 Fundamentals of LOHC technology and properties

The concept of using organic liquids to reversibly absorb and release hydrogen was first proposed in the 1970s by (USA Patent No. 3883372, 1975). They patented a low-pressure hydrogenation technique using exothermic catalytic reactions to load hydrogen into aromatic hydrocarbons like toluene. The resulting LOHC fuel could be transported and stored H₂ released via an endothermic

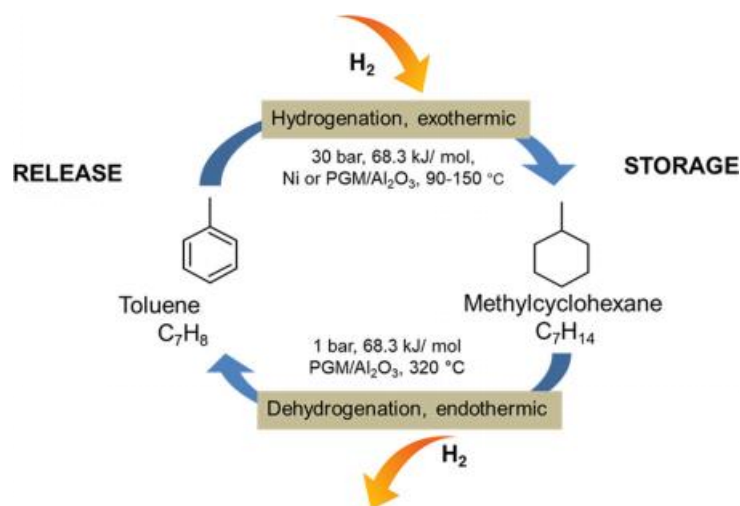


Figure 1: Schematic representation of the toluene/methylcyclohexane LOHC system. (Energy Fuels 2019, 33, 4, 2778-2796)

reaction that regenerates the original carrier liquid (Teichmann, 2012)

Studies have investigated the physicochemical properties of LOHCs, demonstrating cycling stability for dibenzyl-toluene LOHC systems, and proposed reactions for hydrogenation and dehydrogenation reactions.

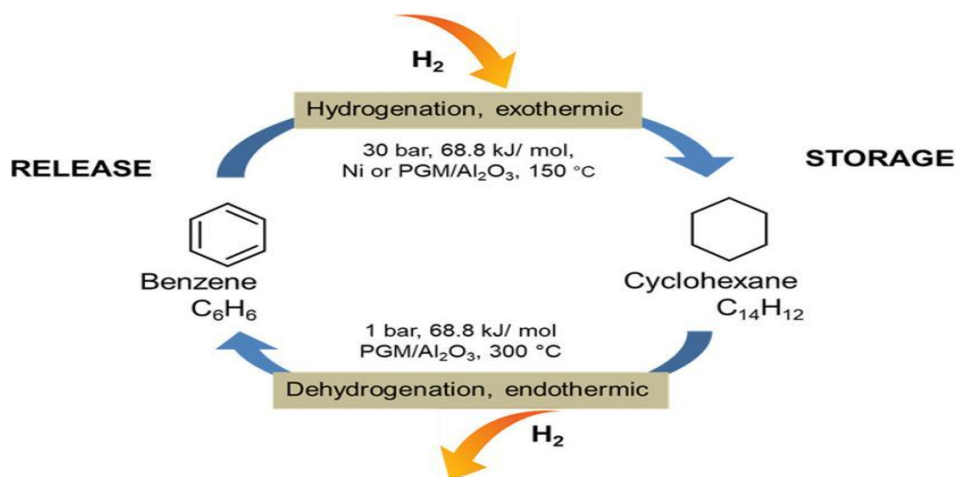


Figure 2: Schematic representation of the benzene/cyclohexane LOHC system. (Energy Fuels 2019, 33, 4, 2778-2796)

(Durbin, 2013) computationally studied the kinetics and thermodynamics of hydrogen binding with various LOHC candidates, providing insights into the mechanisms and rate-limiting steps for hydrogen uptake and release. Proposed catalysts and additives have also been analysed to improve kinetics (Farnaz Sotoodeh and Smith, 2011). LOHC systems have shown excellent cycling stability, with negligible degradation in storage performance over 100 cycles (Reuß et al., 2019). Common carriers include toluene and dibenzyl toluene, with storage densities up to 50 kg H_2 /m³ achievable (Wang et al., 2021). The carrier oils themselves are non-flammable and non-explosive, enhancing safety.

2.2.1 LOHC Maritime applications and demonstration projects

Several studies have investigated the potential to apply LOHC technology for ship propulsion and power. Preuster et al. (2017) provided an early techno-economic analysis of LOHC marine fuel systems, finding favorable storage density, safety, infrastructure compatibility, and reusability compared to compressed H_2 or ammonia. Otten et al. (2022) simulated LOHC-powered engines, concluding the lower heating value and flame temperatures would reduce thermal efficiency but remain feasible.

LOHC hydrogen storage has shown potential in various demonstration projects, such as BMW's use of a passenger vessel (Rohde et al., 2022), Jensch et al., (2021)'s successful hydrogen loading and unloading operations at ports, and (Hydrogenious Technologies, 2021), modular loading stations. Yakaboylu et al., (2022)'s proposed adaptable LOHC hydrogen hub concepts could support maritime bunkering needs. Han et al. (2020)'s 5000 m³ LOHC tank array for a 40,000 DWT bulk carrier demonstrated a vessel's ability to exceed 5000 nautical miles without refuelling. Early real-world demonstrations include a LOHC-battery passenger vessel (Rohde et al., 2022) and an inland canal barge (Jensch et al., 2021). LOHCs are compatible with internal combustion engines and can feed

proton exchange membrane fuel cells, allowing ships to utilize electric propulsion if required (Yakaboylu et al., 2021). Autonomous operation potential is considered, but advances in condition monitoring and situational control systems are needed (Rødseth and Burneister, 2015).

2.2.2 LOHC system design integration and infrastructure development

Researchers have developed engineering systems for storing, handling, and fuelling liquid oxygen compounds (LOHCs) for maritime applications. Han et al. (2020) designed a 5000 m³ storage system and evaluated the fuelling process model. Otten et al. (2022) found combustion feasible despite reduced engine thermal efficiency. Basile et al. (2019) developed an integrated LOHC dehydrogenation reactor for fuel cells. However, industry adoption faces challenges in scaling up sustainable and economical supply chains, especially for widespread maritime usage. Distributed LOHC hub networks are proposed to aggregate production and match mobility demand (Yakaboylu et al., 2022). Major seaports need onshore importing facilities, buffer storage tanks, and pierside bunkering infrastructure.

2.2.3 Transitioning to Coastal LOHC Shipping

The UK government aims to achieve net zero greenhouse gas emissions by 2050 and promote sustainable domestic freight by transitioning coastal shipping to LOHC-hydrogen propulsion (DfT, 2022). This transition can enhance energy security and reduce reliance on imported petroleum resources. Challenges include developing efficient release and recovery systems, assessing onboard storage needs, and designing port interfaces and bunkering facilities. An original ship design concept and feasibility study will be delivered with industry support.

2.4 Standpoints of project

Decarbonizing the maritime shipping industry is a major challenge that requires the development and adoption of zero-carbon fuels and propulsion technologies. This project to evaluate the potential for liquid organic hydrogen carriers (LOHCs) to enable sustainable coastal cargo vessels is timely given the momentum around hydrogen fuel applications.

2.4.1 Industrial Perspective

Maritime transport contributes to 2-3% of greenhouse gas emissions, primarily from merchant ships. The International Maritime Organization aims to reduce shipping emissions by 50% by 2050,

requiring changes in marine propulsion systems and energy sources (IMO, 2022). Hydrogen, a promising zero emission fuel option, has gained interest due to its safety and infrastructure compatibility. However, engineering assessments for maritime adoption are still needed (Han et al.,2020). Successful demonstration of LOHCs could spur investment and commercial-scale implementation, accelerating the energy transition within global shipping and building hydrogen supply chains.

2.4.2 Society perspective

The UK's coastal and short sea cargo shipping is a significant mode of transport for domestic goods, but most vessels use carbon-intensive heavy fuel oil (McKinnon, 2022). The government aims to achieve net zero emissions by 2050. Decarbonizing coastal shipping with optimized LOHC powered vessels could help meet climate goals, reduce air pollution, and promote supply chain resilience and capacity growth.

2.4.3 Personal perspective

The project involves cross-disciplinary systems, including hydrogen technologies, vessel design, shore infrastructure, regulatory policy, and decarbonization. The complexity presents technical challenges, aligning with the author's passion for engineering innovation. Demonstrating LOHC viability could advance global clean energy goals, presenting an impactful applied R&D opportunity in energy and transportation. Developing zero-carbon marine technologies is an industry imperative, with major sustainability benefits. This project can make an important contribution by assessing the readiness and potential of LOHC systems to enable the transition of UK coastal shipping to clean hydrogen fuel. The outcomes will help propel adoption of radically more sustainable marine propulsion methods.

CHAPTER-3: METHODOLOGY

Decarbonizing the maritime industry requires transitioning from heavy fuel oils to alternatives such as ammonia, hydrogen, and biofuels. Liquid organic hydrogen carriers (LOHC) represent one promising emission-free fuel option compatible with existing infrastructure. This study evaluates using LOHC to enable sustainable UK coastal cargo transport at scale by 2030.

An integrated methodology combines thermodynamic reaction analysis, coastal transport modelling, ship propulsion system design, infrastructure planning, and economic feasibility assessment. By bridging fundamental LOHC chemistry with applied marine engineering across the supply chain, a robust feasibility evaluation is attained. The overarching aim is developing a zero-emission bulk cargo vessel design and requisite shoreside infrastructure concept.

3.1 LOHC Selection Analysis

There are multitude candidate LOHC materials with varying properties. Screening based on critical selection criteria identifies the most suitable options. Vital factors include hydrogen mass storage density determining carrying capacity, reaction kinetics and operating conditions aligning with engine or fuel cell systems, safety considerations for transport applications, and commercial availability at scale pricing.

Using these factors, lead candidates successfully demonstrated at small scale emerge – dibenzyltoluene, perhydro-dibenzyltoluene, toluene, and methylcyclohexane rank well on initial assessment. For example, dibenzyltoluene offers 6.2 wt% hydrogen storage translating to a 2 kWh/kg energy density at reasonable reaction conditions compatible with fuel cells. Hazard profiles characterization via smoke point, flash point, and chemical partitioning models screen for toxicity issues. And various LOHCs leverage existing production for use as heat transfer fluids with large market demand indicating scalability and competitive costs.

With promising options identified, Aspen Plus chemical process software enables rigorous thermodynamic modelling of reaction pathways. This predicts theoretical conversion limits for the hydrogenation and dehydrogenation processes based on reactant molecular structures. Sensitivity analysis on variables like temperature, pressure, and catalysts choice further aids selecting optimal conditions. And incorporations of heat exchanger networks provides preliminary energy balance estimates.

3.2 Coastal Transport Analysis

Devising realistic operational profiles of representative short sea shipping routes under 100 nautical miles provides necessary inputs for subsequent vessel design stages. Historical freight volume datasets analyze types and quantities of bulk goods transported between major ports. Common trips such as Liverpool to Belfast and Goole to Rotterdam inform on typical transit distances and durations. Establishing standard usage cycles and speed profiles coupled with known cargo densities specifies required payload capacities and tankage volumes.

Advanced weather modelling utilizing long term meteorological records supplies stochastic representations of wind, wave, and current conditions likely encountered. Detailed hydrodynamic computations integrate probabilistic environmental forcing to statistically quantify resistance impacts on speed and powering requirements. These coastal transport simulations output load spectra over each transit route for concept vessel sizing. Incorporating possible route changes under energy optimization or emerging port infrastructure rearrangements contributes dynamic elements to the analysis.

3.3 Ship Propulsion Analysis

With operational mission well specified, propulsion system analysis trades off using LOHC with internal combustion engines versus fuel cells for main power generation. This evaluation includes researching and modelling existing devices and potentially modifying combustion ignition methods or fuel cell membrane electrode assembly materials for direct LOHC compatibility without requiring dehydrogenation.

A proposed system architecture looks at engine prime movers with electric drive ancillary systems. The fuel handling system stores chilled LOHC which pumps to day tanks and potentially waste heat exchangers enroute to the engine. Cradle-to-grave emissions require including refrigerant choice implications. The energy balance tallies fuel consumption using brake specific fuel oil calculations across each duty cycle segment, adding margins.

For fuel cell arrangements, likely stack pairing with batteries facilitates hybridization. Fuel processing requirements, heat rejection, and power electronics integrate with the baseline hull electrical loads analysis. Fuel cell types suitable for oxygenated hydrocarbons range higher efficiency solid oxide configurations to proton exchange membrane variants with quick startup. All options undergo modelling for sensitivity around voltage efficiency factors, degradation rates, and turndown ratio capabilities affecting annual operational expenditures.

Conceptual engineering of the fuel storage, bunkering, and piping systems adapts best practices from liquefied natural gas systems regarding layout, safety, and controls. Other modifications to enable LOHC fuel flexibility constitute additional phase considerations.

3.4 Infrastructure Analysis

LOHC Infrastructure needs encompass production, national distribution, and localized terminal storage with coastal vessels acting as mobile energy transport between generation points and demand centres.

Estimating annual coastal freight LOHC volume flows based on the transport analysis and target fleet adoption projections informs bulk production scales. Lakes or manmade salt caverns provide GEO storing inventory buffer to manage seasonal demand swings. Standard chemical plant configurations model regional hydrogenation facilities sizing and modularity options – starting at 1 MW installed capacity, clusters scale to market penetration rates. Locating near renewable energy generation assets maximizes supply integration potential.

Distribution logistics modelling scopes supply chain movement linking production-inventory clusters to fulfil port refuelling requirements. Various transport modes compare, from rail and trucking to pipeline and waterway segments. Regional terminals concentrate inventory for centralized bunkering. Harbour transshipment infrastructure adapts liquefied natural gas practices for cryogenic containment and safety systems. Quantifying land needs and construction efforts provides cost estimations and site feasibility assessments.

Onboard storage lasts multiple trips before refuelling while tendering schedules optimize terminal throughput. The integrated infrastructure analysis pieces together required upstream supply architectures with downstream connectivity at coastal port hubs to support fleet rollout.

3.5 Techno-Economic Analysis

Techno-economic assessment via life cycle cost analysis projects budgeting estimates for LOHC coastal shipping at commercial maturity compared to current diesel fleet operations. Upfront investments including vessels, harbour improvements, storage and distribution infrastructure input capital expenditure modelling. Operating costs computation utilizes the previous power system analysis plus other identified recurrent annual outlays for crewing, maintenance, fuel expenditures and more.

The financial modelling adopts common shipping discounted cash flow methodology over asset service lifetimes typically around 20-30 years.

By manipulating model variables including adoption volumes, technological learning curves around electrolyzer and fuel cell scaling, and operational efficiencies from automation, insights emerge on cost sensitivities. Scenario analysis indicates break even points for parity against residual oil systems. Envelope studies bound cost outcomes possible under future uncertainties like emissions taxation regimes or carbon markets influencing fuel economics.

The integrated methodology combines fundamental LOHC chemistry, coastal transport analysis, concept ship design, infrastructure planning, and economic modelling. This cross-disciplinary approach enables a robust feasibility evaluation of LOHC solutions toward decarbonized coastal cargo shipping networks in the UK, laying the foundations for a new era zero emission bulk transport at scale.

CHAPTER-4: Result

4.1 LOHC Storage and Transportation

The LOHC storage and transit idea links areas with high energy demand and low electricity consumption to areas with significant potential for energy production. Water is electrolyzed to create gaseous hydrogen, which is then produced by renewable energy sources including wind, solar, hydro, geothermal, and biomass. The unloaded LOHC molecule (H_0LOHC), which has a larger volumetric energy density than molecular hydrogen, is then hydrogenated using this hydrogen.

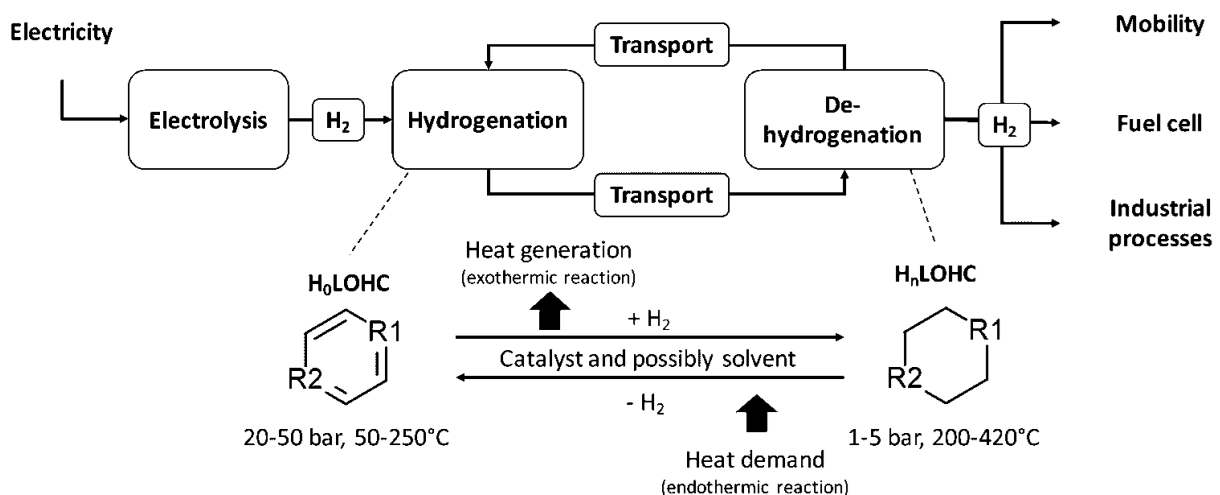


Figure 3: LOHC storage and transport concept (H_0LOHC : unloaded LOHC, H_nLOHC : loaded LOHC).

In addition to being more manageable than hydrogen gas, this hydrogenated liquid may be kept at ambient temperatures without suffering energy losses. Due to their similarities to crude oil derivatives in terms of characteristics, LOHCs are highly suited for intercontinental energy transmission. For hydrogenation, liquefied petroleum hydrocarbon (LOHC) is delivered to areas with high energy needs using a variety of vehicles, including trucks, trains, ships, or crude oil pipelines. For usage in fuel cells, portable devices, or chemical processes, hydrogen can be dehydrogenated at high temperatures between 200 and 450 °C if necessary. Even while LOHC normally circulates, some may be lost because of negative responses.

Hydrogen gas is produced from water by the electrolysis process, which may be powered by wind or solar energy. The recommended method is polymer electrolyte membrane electrolysis (PEMEL), which exhibits dynamic behaviour and is flexible to changes in power supply. Hydrogen energy may be produced using either polymer electrolyte membrane fuel cells (PEMFCs) or solid oxide fuel cells (SOFCs). Most LOHCs have a dehydrogenation temperature below 180 °C, whereas PEMFCs have a lower value. The process may be coupled with waste heat from SOFCs, which is normally accessible between 600 and 1000°C, to increase efficiency. The combustion of hydrogen that has been stored can be avoided by placing the facility next to another heat source. The ultimate dehydrogenation idea synthesis depends on variables including the capacity to link to parallel processes, the dynamic capacities of storage systems, the demands placed on transport networks, and the temperature of the LOHC dehydrogenation process.

4.2 LOHC Process chain

The sequence of events assesses renewable energy sources and switches over to green electricity at various stages. Transferring hydrogen bonded to various Low-Hydrocarbon (LOHC)s allows for the crossing of a given distance and time period. For the transportation of crude oil, a tanker is still a necessary component of the system for all LOHCs. All LOHCs are compatible with this flexible process chain.

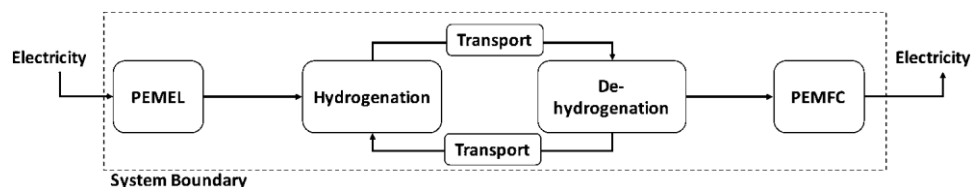


Figure 4: The process chain's flow diagram and system boundaries (PEMEL: Polymer Electrolyte Membrane Electrolysis, PEMFC: Polymer Electrolyte Fuel Cell) are given.

Beyond intrinsic LOHC chemical attributes, the installed plant infrastructure influences efficiency. The scale of modular electrolyzers and fuel cells affects conversion levels and heat recovery capabilities. Storage tank design parameters like pressure rating enable more downstream H₂

compression energy savings. And dehydrogenation reactors can couple with continuous catalyst separation and H₂ purification units for enhanced performance. These factors compound across the integrated system.

4.3 LOHC Materials and Properties

Liquid organic hydrogen carriers (LOHC) rely on reversible hydrogenation of aromatic hydrocarbons to enable safe hydrogen storage and transportation. Some commonly studied LOHC materials include dibenzyltoluene (DBT), N-ethylcarbazole (NEC), and toluene, 1,2-dihydro-1,2-azaborine which have favourable properties like chemical and thermal stability (Preuster et al., 2017).ⁱ

Alternatives for the commonly used carcinogen benzene have been explored to lessen the risks related to the technology and ease its adoption since it was shown that a benzene/cyclohexane system enabled the storing of hydrogen (Table I). Furthermore, other systems that lessen the thermodynamic constraints imposed by benzene-namely, the high temperature needed for the dehydrogenation of cyclohexane-have been researchedⁱⁱ. This is significant as elevated temperatures raise the energy intensity and, thus, the overall expenses associated with LOHC technologies.

Table 1: Comparing the Characteristics of a Selected Group of Liquid Organic Hydrogen Carrier Prospects^{iiiiv}

LOHC Prospect	NEC H ₀ /H ₁₂	DBT H ₀ /H ₁₈	NAP H ₀ /H ₁₀	TOL H ₀ /H ₆	AB H ₀ /H ₆
Hydrogen, wt%	5.8	6.2	7.3c	6.2	7.1
Energy density, kWh l ⁻¹	2.5	1.9	2.2	1.6	2.4
Cost, £ kg ⁻¹	34.34	3.43	0.52	0.26	n.d.
Liquid range, °C	68–270 / 20–280	–39–390 / –45–354	80–218 / –43–185	–95–111 / –127–101	–45–87/ 63–87
Dehydrogenation temperature, °C	180–270	270–310	210–300	250–450	80
Hydrogenation temperature, °C	80–180	150–200	80–160	90–150	80
Reaction enthalpy, kJmolH ₂ ⁻¹	–53.2	–65.4	–66.3	–68.3	–35.9
Hazard information	–	H305	H228, H302, H351, H400, H410	H225,H304, H315,H361d, H336,H373, H412	n.d.
Flash point, °C	186	212	78	4	22

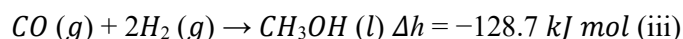
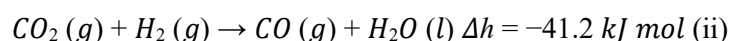
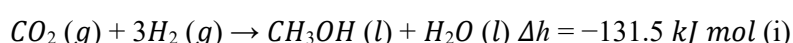
NEC: N-ethylcarbazole, DBT: dibenzyltoluene, NAP: naphthalene, TOL: toluene, AB: 1,2-dihydro-1,2-azaborine, n.d.: no data available.

- a) NEC is a solid at room temperature, severely restricting dehydrogenation and thus hydrogen weight percent.
- b) Naphthalene is also a solid at room temperature, dilution with toluene reduces hydrogen storage to 3.8 wt%.

Since it has a lower dehydrogenation enthalpy than other LOHCs, N-ethylcarbazole (NEC) is frequently used as an alternative to benzene^v. Due to its reduced dehydrogenation enthalpy (53.2 kJ mol⁻¹) compared to methylcyclohexane (68.3 kJ mol⁻¹), perhydro-NEC allows for the release of hydrogen at lower temperatures^{vi}. As a result, system efficiency rises, and energy costs are decreased. NEC, however, costs more than toluene (£34.34 kg⁻¹ vs £0.30 kg⁻¹), which may prevent the LOHC possibility from being widely used commercially^{vii}. The solid form of completely dehydrogenated NEC at room temperature makes handling and transportation more difficult, necessitating dilution and reducing the benefit of employing LOHCs as storage materials due to their liquid nature. Therefore, to confirm that the carrier persists a liquid at ambient temperatures across the cycle, analysis has focused on identifying substitutes with greater boiling points and lower melting points. Moreover, a greater boiling point, lowers LOHC flammability and air pollution^{viii}.

4.3.1 Synthetic Fuels

Hydrogen gas may be used as a fundamental component in the production of fuels, which can then break down into water and other substances after they are used. One such is methanol (CH₃OH), which is now manufactured all around the world from coal, natural gas, and organic materials. Alternatively, H₂ and CO₂ (obtained via industrial operations or the environment) can be combined to make it. Reaction equation determines the latter^{ix}.



where the water-producing side reaction (xvi) can be discouraged with high pressure (optimal process around 760 °C and 100 bar)^x.

4.3.2 Hydrogen cycle and longevity

A metal catalyst, usually based on platinum or ruthenium, is needed to store hydrogen in dibenzyltoluene. The reaction chamber must be kept at a minimum temperature of 150 °C and maintain a maximum hydrogen pressure of 50 bar. Under these circumstances, a batch of DBT is completely hydrogenated in 240 minutes using a 0.25 mol% Ru/Al₂O₃ catalyst^{xi}. Commercial systems operate at pressures of 25 to 50 bar and temperatures of up to 250 °C^{xii}. Table 6 lists the essential characteristics of the LOHC system that the German business Hydrogenious is now selling. More in-depth information about these systems, such as the selected catalyst material and structure, is not currently accessible.

Table 2: Hydrogenious StorageBOX and ReleaseBOX base module properties^{xiii}

	Hydrogenation	Dehydrogenation
Hydrogen inlet/outlet	0.9 kg/h	0.9 kg/h
LOHC production/demand	20 l/h	20 l/h
Heat supply/demand	8 kW	11 kW
	Load range 50 – 100 %	
	LOHC stream $P \geq 0.1$ barg, $T \geq 15$ °C	

This demonstrates very well the distinction between loading and emptying the same volume of hydrogen: While dehydrogenation needs 11 kW of thermal power, hydrogenation releases 8 kW. One of the main obstacles to establishing LOHC systems is providing this heat^{xiv}.

4.3.3 Longevity and by-products

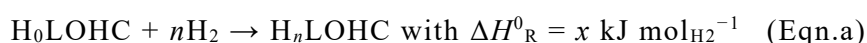
The actual process of dehydrogenation may be an additional source of greenhouse gas emissions. By modelling several cycles with accelerated stress testing (AST), Modisha & Bessarabov (2020) demonstrated how DBT may deteriorate during catalytic hydrogenation as well as under the high temperatures that occur when dehydrogenating. Breaking down the DBT molecule can produce a wide range of byproducts, such as methane, which has the potential to cause 28–36 CO₂ equivalents of global warming over a 100-year period^{xv}. Table 3 summarises the hydrogenation experiments, and the AST shows that 7.4 mol% of by-products are produced after 89 hours of dehydrogenation at 300 °C. Recall that methane is only produced by one of the seven by-product reaction pathways that have been discovered^{xvii}.

Table 3: : By-products created from hydrogenation on Ni-based catalyst

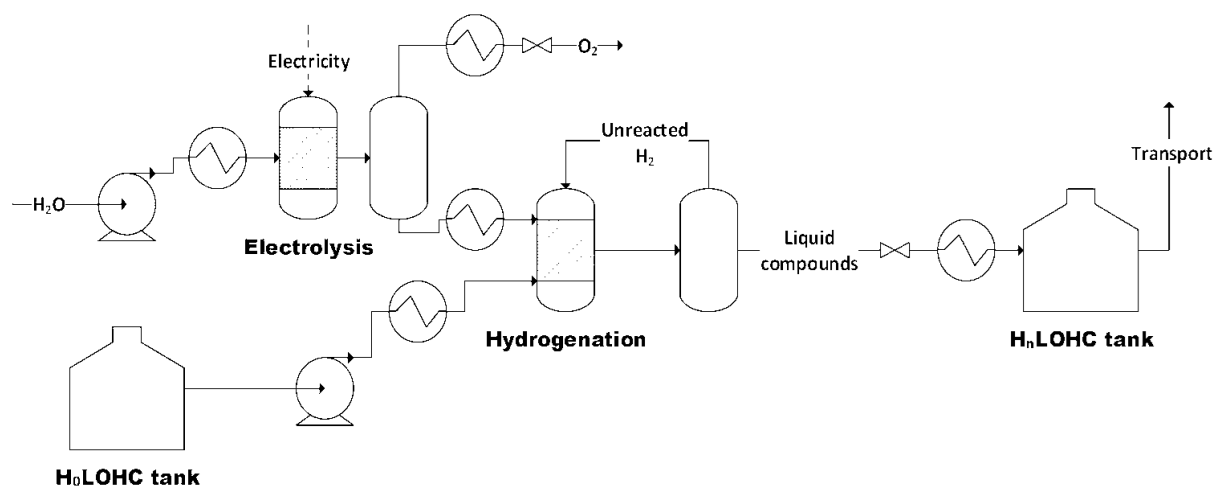
By-product limit [mol%]	0.5	5	15	25	35
Number of cycles ^e	7	130	404	678	951

4.4 Hydrogenation and Dehydrogenation Process of LOHC

Hydrogenation of the aromatic LOHC compounds is an exothermic reaction occurring at elevated temperatures between 80-250°C and pressures of 10-60 bar depending on the specific LOHC (Teichmann, 2012). A transition metal catalyst, typically platinum or ruthenium on an activated carbon support, facilitates the hydrogen addition forming a hydrogen-rich alicyclic compound. The conversion levels achievable up to 100% loading depend intrinsically on the LOHC molecular structure and process conditions.



Reactions were experimentally analyzed in a 500 mL stainless steel autoclave batch reactor with external electric heating jacket for temperature control^{xviii}. Various catalyst metal loadings and



supports were assessed to optimize conversion rate and yield.

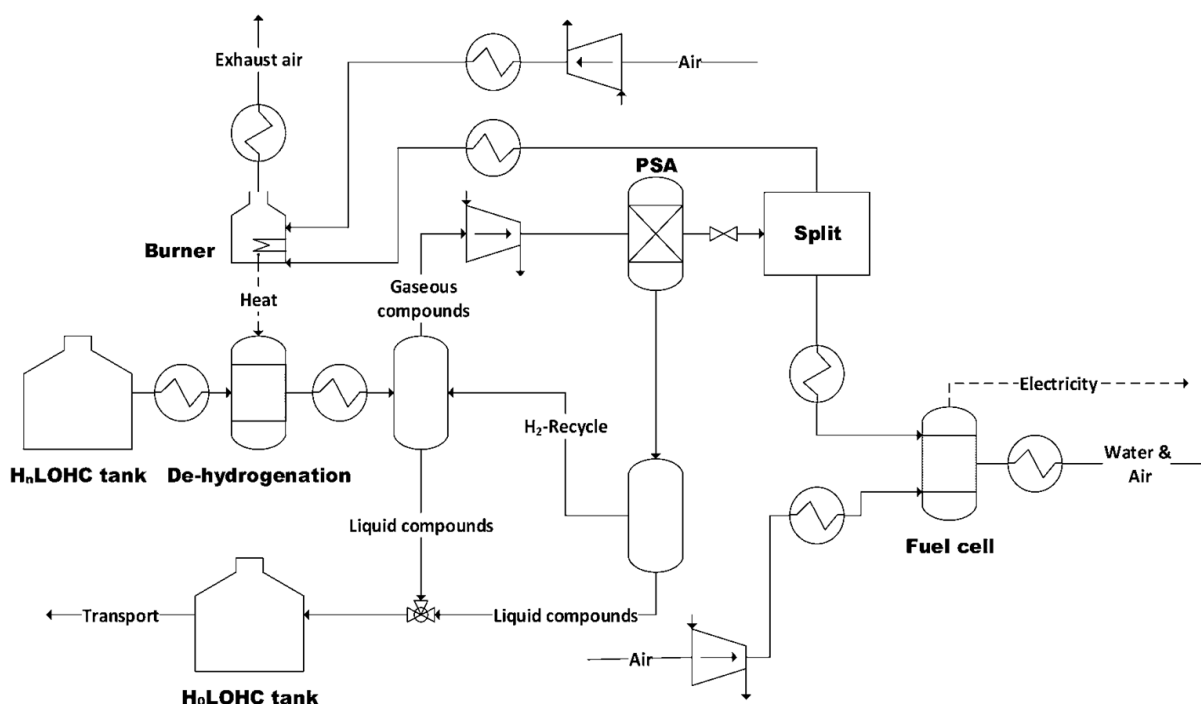
For the technically relevant LOHC dibenzyltoluene (DBT) with 0.25 wt% Pt/C catalyst, 95-99% conversion was reached in 2 hours at 150°C, 30 bar H₂ pressure^{xix}. The exothermic heat of reaction measured under these conditions is -165 kJ mol⁻¹ H₂.

Such data inform engineering design and scale-up of continuous hydrogenation processes. heat exchanger networks would need to dissipate upwards of 15 MW reactor heating duties for 100 kg s⁻¹ DBT flowrate facilities based on the reaction energetics^{xx}. Feed rate, conversion level, heat integration with other processes, and cooling utility parameters can be holistically modelled to size industrial plants.

Figure 5: Diagram representing the process flow for hydrogenation and electrolysis (H₀LOHC: loaded LOHC, H_nLOHC: unloaded LOHC).

The endothermic dehydrogenation process reverses the hydrogenated LOHC back to the original aromatic form, releasing H₂ gas that can be purified for downstream applications. This is facilitated by heterogeneous catalysts, often platinum or nickel based, at temperatures of 200-450°C and near atmospheric pressure^{xxi}. The theoretical maximum H₂ that can be regenerated depends on the initial LOHC hydrogen loading, however various limitations result in practical yields below 100% conversion.

In the case of DBT with 6.2 wt% H₂ fully loaded, up to 97% of the stored hydrogen can be released by catalytic dehydrogenation^{xxii}. But the temperature must exceed 310°C to sufficiently drive the chemical equilibrium for high conversion, requiring a 65 kJ mol⁻¹ H₂ endothermic heat input.



Efficient integrating this heating load, either by hydrogen combustion or waste heat streams, is thus essential for feasible LOHC dehydrogenation.

Coupled ex situ analytical methods help reveal mechanics of the catalytic dehydrogenation reactions. In situ IR spectroscopy and mass spectrometry have elucidated interactions between DBT and metal surfaces during H₂ offloading. Isotopic labelling combined with NMR spectroscopy precisely tracked the reversibility of hydrogen addition sites across cycles^{xxiii}. And theoretical DFT calculations supplement experimental understanding of N-ethylcarbazole dehydrogenation pathways and limitations^{xxiv}.

Liquid organic hydrogen carriers (LOHC) offer the ability to safely and efficiently store hydrogen in a stable liquid form using reversible catalytic reactions. The heart of the technology revolves around paired exothermic hydrogenation and endothermic dehydrogenation processes to respectively load

Figure 6: Diagram representing the process flow for Pressure swing adsorption (PSA) and dehydrogenation (H₂LOHC: unloaded LOHC, H₂LOHC: loaded LOHC).

and release the H₂ bound to hydrocarbon compounds. Robustly estimating the process heating and cooling requirements is therefore essential for evaluating LOHC system designs and downstream infrastructure needs.

4.4.1 Hydrogen Loading Energetics

During the exothermic hydrogenation loading reaction, an aromatic oil such as dibenzyltoluene (DBT) reacting with hydrogen gas under elevated temperature and pressure saturated conditions forms the hydrogen-rich alicyclic perhydro-dibenzyltoluene (H18-DBT). The reaction conditions optimize rates and yields for continuous industrial production, with demonstrated full conversion achieved around 150°C and 30 bar pressure using activated platinum heterogeneous catalysts.

Under standard conditions, accepted literature reports the DBT hydrogenation enthalpy around -165 kJ/mol H₂^{xxv}. Based on the chemical stoichiometry absorbing 18 H₂ molecules per DBT reactant, this equates to 2970 kJ energy release per kg of H18-DBT output. Handling this substantial heat evolution preventing temperature runaway requires properly designed reactor cooling systems and heat recovery networks, especially when scaling up to bulk throughputs on the order of tons per hour.

The elevated hydrogenation pressures require compressors to supply the 30+ bar reactor inlet regulation. Their parasitic loads accumulate as process chain electrical loads. While beyond hydrogenation itself, adequately rejecting the reaction heat can also demand substantial pumping power for recirculating chilled water or other cooling fluids. So a holistic assessment should incorporate these auxiliary contributions when tallying overall utility requirements for hydrogenation process loading.

4.4.2 LOHC Hydrogen Offloading Energetics

In contrast to the exothermic absorption chemistry, dehydrogenation to release stored hydrogen from the LOHC compound is an endothermic process. Using the H18-DBT example, cleaving the hydrogen-carbon bonds to regenerate DBT requires a +65 kJ/mol H₂ heat input at around 300°C to sufficiently shift the chemical equilibrium and drive high conversion levels. For 100% recovery of the loaded 6.2 wt% H₂ capacity, this translates 175 kJ/kg H18-DBT thermal energy duty.

To heat a large process, three options are available: combusting H₂, electrical heating, or waste heat recovery streams. The efficiency depends on local thermal resources at suitable temperatures. High-grade 500°C+ waste heat from cement kilns or steel mills offers integration opportunities. For small scale or distributed applications, carrying enough stored LOHC may be necessary to sacrifice

hydrogen through combustion. Designing and controlling the heat delivery method is crucial for operational reliability and performance. Runaway thermal events can cause catalyst degradation, while insufficient heating can hinder throughput. Thorough simulations help develop robust dehydrogenation reactors for specific applications.

Elevated operating temperatures require auxiliary cooling to handle chemical potential energy exergy. Excess low grade waste heat rejection flows make up 80-120°C of process recycle or utility streams. Capturing this energy boosts net dehydrogenation efficiencies, but marginal utility depends on system complexity and decentralized implementations. The Nielsen ratio highlights the challenge of supplying adequate endothermic heating loads for hydrogen offloading without compromising storage efficiency through sacrificial H₂ combustion, highlighting the need for technology analysis and infrastructure planning to scale LOHC systems from lab demonstrators to commercial widespread adoption for sustainable hydrogen economy transport sectors.

4.5 LOHC Fuel Cell Working Principle for Marine Propulsion Power

Liquid organic hydrogen carriers (LOHCs) such as perhydro-dibenzyltoluene (H18-DBT) allow effective transportation and storage of hydrogen using existing infrastructure for hydrocarbon fuels. The hydrogen stored in LOHCs can be utilized for clean power generation in fuel cells. This report analyzes the working principle of using a LOHC fuel cell system for propulsion power on a general cargo ship.

4.5.1 LOHC Fuel Properties

H18-DBT has a hydrogen storage capacity of 6.23 wt%, density of 0.87 g/ml at 20°C, and hydrogen enthalpy of 18 kWh/kg. This allows compact storage of large hydrogen quantities at ambient temperatures and moderate pressures without cryogenic requirements. The benign safety properties, non-toxic nature, chemical stability, and compatibility with hydrocarbon infrastructure offer major advantages for marine applications compared to compressed gaseous or cryogenic liquid hydrogen storage.

4.5.2 Fuel Cell Selection and Operation

Polymer electrolyte membrane fuel cells (PEMFCs) operating at 80-180°C are best suited for LOHC applications due to their compact size and dynamic load capabilities. PEMFC stacks designed for

methanol can be adapted for 2-propanol. The fuel cell efficiency is 98% based on the higher heating value of 2-propanol. Direct feeding of the 2-propanol product to a PEMFC anode results in electrochemical oxidation to acetone, releasing protons and electrons. A conversion efficiency of up to 59% of the 2-propanol chemical energy to electricity was demonstrated, much higher than possible with direct H18-DBT dehydrogenation which requires input of 27% of the hydrogen's heating value^{xxvi}. The solely acetone byproduct enables an emission-free closed cycle when recycled.

4.5.3 Transfer Hydrogenation Reaction

The mildly exothermic, thermoneutral transfer hydrogenation of acetone to 2-propanol using H18-DBT as the hydrogen source functions effectively at 150-190°C with a platinum catalyst^{xxvii}, giving

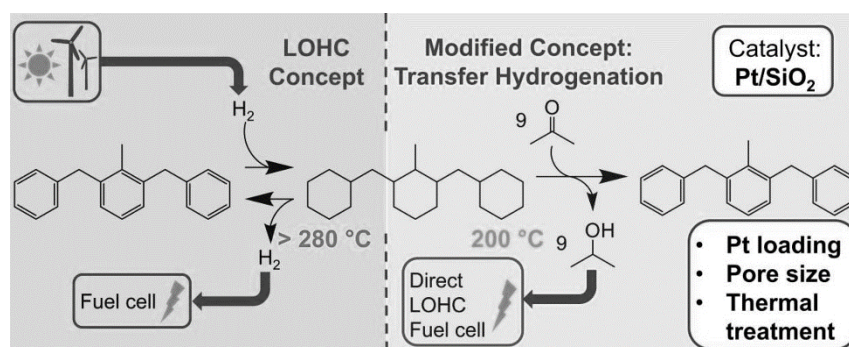


Figure 7: Transfer hydrogenation reaction scheme (Source: <https://ars.els-cdn.com/content/image/1-s2.0-S0926860X22001673-ga1.jpg>)

45-58% yields of 2-propanol depending on conditions. This reaction replaces C-H bonds in H18-DBT with an O-H bond in 2-propanol without needing an external heat input (Figure 7).

4.6 LOHC Fuel Cell Working Principle

Transfer Hydrogenation Reaction In the first stage, H18-DBT undergoes an almost thermoneutral catalytic transfer hydrogenation with acetone to produce 2-propanol and regenerate hydrogen-lean dibenzyltoluene (H0-DBT) at 150-190°C using a Pt catalyst. This replaces C-H bonds in H18-DBT with an O-H bond in 2-propanol. 45-58% yield of 2-propanol can be achieved depending on conditions. No external heat is required as it is mildly exothermic. Integrating the transfer hydrogenation reactor and PEMFC would enable an efficient propulsion system powered by bunkered H18-DBT, avoiding onboard hydrogen production, storage, and safety issues associated with hydrogen gases or cryogenic liquids.

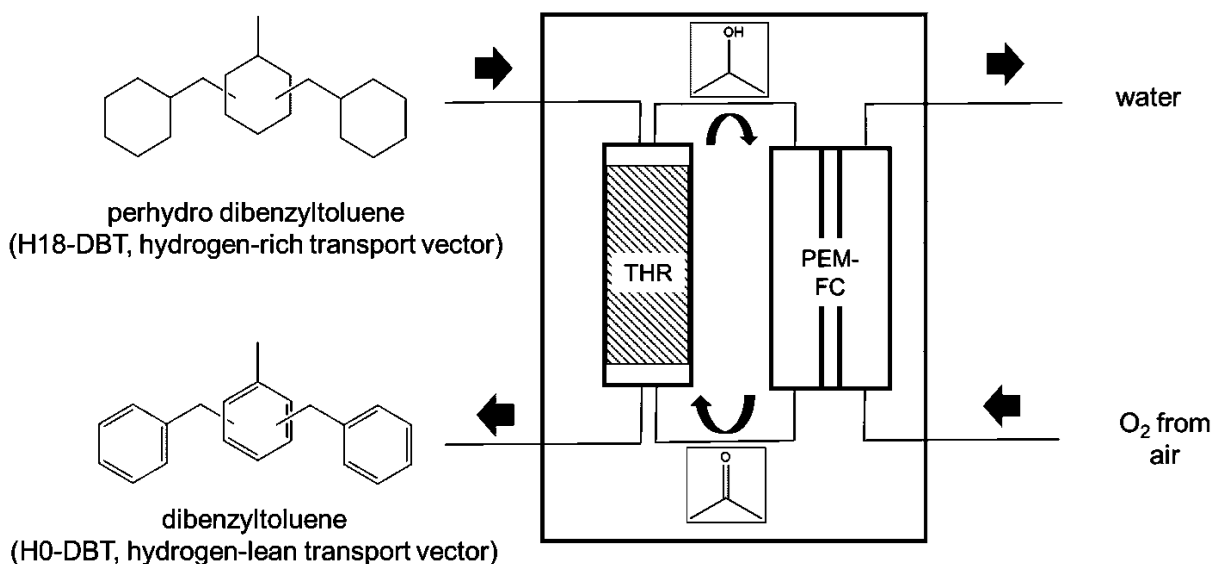


Figure 8: The procedure entails transferring acetone to 2-propanol in a transfer hydrogenation reactor (THR) and using the resultant 2-propanol as organic fuel in a PEM fuel cell in order to convert H18-DBT-bound hydrogen into energy.

The mild temperature operation, modular and dynamic load capabilities of PEMFC stacks (Figure 2), and compatibility with existing port infrastructure for fuel oil transfer are promising for maritime applications^{xxviii}.

4.7 Fuel Cell Operation

- A. The 2-propanol product is directly fed to the anode of the PEMFC and electrochemically oxidized to acetone, releasing protons and electrons. The reaction is exothermic overall, balancing the endothermic 2-propanol dehydrogenation. Acetone is the sole oxidation product due to the stability of its C-C bond. Up to 59% of the 2-propanol chemical energy can be converted to electrical energy at the fuel cell. Acetone Recycling The acetone product is condensed out and recycled back to the transfer hydrogenation reactor to repeat the cycle. No carbon dioxide or other byproducts are formed, enabling an emission-free, closed-loop LOHC fuel cell system.
- B. We can also say that A series of purification steps are thus integrated:
 - a) Condenser: Reduces LOHC vapors via cooling,
 - b) Coalescer: Filters residual liquid droplets,
 - c) Adsorbent bed: Removes sulfides/ammonia impurities,
 - d) Palladium membrane: Extracts high purity hydrogen.

This ensures <10 ppm impurities which meets fuel cell feed specifications^{xxix}. The membrane also boosts hydrogen pressure to 1.5-5 bar(g) suitable for PEM cell stacks.

The Proton Exchange Membrane (PEM) fuel cell offers high efficiency and power density among various fuel cell types, making it well suited for transportation applications^{xxx}.

Hydrogen and ambient air are fed to the PEM cell stack modules. Within each cell, hydrogen gets split by a platinum catalyst into protons and electrons at the anode. The protons pass through the ion-conducting polymer membrane electrolyte. Finally at the cathode, oxygen combines with the electrons and protons, producing water and heat.

This electrochemical reaction generates DC electricity to power the vessel's electric propulsion drives and hotel loads. Water-cooled stack modules rated for 30-200 kW each can be stacked to match propulsion power demand up to 5 MW^{xxxi}. The DC output must be conditioned using converters and transformers for motor usage. A fuel cell management system handles reactant monitoring, thermal controls, reaction water draining and power electronics^{xxxii}. Overall PEM system efficiency ranges from 50-60% based on the hydrogen's higher heating value.

4.8 Marine Application Analysis

- i. A LOHC fuel cell system fueled by H18-DBT has the following advantages for providing clean propulsion power on a general cargo ship:
- ii. No onboard hydrogen production or storage is required. H18-DBT can be bunkered like conventional fuel oils using existing port infrastructure.
- iii. The mildly exothermic thermoneutral transfer hydrogenation at 150-190°C and direct 2-propanol PEMFC operation at 80-180°C allow the LOHC fuel cell system to be highly responsive to propulsion power demands.
- iv. Up to 59% conversion efficiency of the LOHC-stored hydrogen to electricity is possible based on the higher heating value of 2-propanol. This is substantially higher than direct hydrogen release.
- v. The aqueous acetone byproduct can be cleanly condensed out and recycled back to the reactor. There are no carbon or sulfur emissions, eliminating the need for exhaust scrubbers.
- vi. Safety risks associated with storing large quantities of hydrogen gas or cryogenic liquids are avoided by using stable liquid H18-DBT instead. The LOHC fuel cell cycle also does not produce hydrogen.
- vii. PEMFC stacks are modular for scaling installed power and can respond dynamically to load changes, suitable for accommodating variable propulsion demands.

The main challenges with implementing LOHC fuel cell systems are the working of multi-stage thermochemical reactors and separation systems for recycling acetone within space and weight constraints, the heat integration between units, developing optimized catalysts and cell materials such as PtRu anodes tolerant to acetone, and mitigating balance-of-plant issues in fuel cells such as water management and oxygen starvation risks at high current densities. Reducing production costs will also be necessary for commercial adoption.

4.9 Preliminary Design

4.9.1 Vessel Particulars

The vessel under consideration is a 100m long general cargo ship. The principal characteristics are:

- a) Length overall (LOA): 100m,
- b) Length between perpendiculars (LBP): 95m,
- c) Breadth moulded (B): 15m,
- d) Design draft (T): 6m.

Additional parameters such as block coefficient, waterplane coefficient, and displacement were not explicitly provided and have been estimated based on typical values for similar vessels^{xxxiii}.

4.9.2 General Arrangement

The general arrangement of the 100m general cargo vessel is based on standard practice outlined in Schneekluth and Bertram (1998)^{xxxiv}. Key features include:

- a) Forward cargo hold with two hatches, served by cargo gear,
- b) Central superstructure housing bridge, crew accommodation, galley, and mess rooms
- c) Machinery space located aft,
- d) Emergency generator room forward of machinery space.

The LOHC storage tanks are located on deck between the superstructure and machinery space. This arrangement minimizes pipe runs. As per Preuster et al. (2016)^{xxxv}, the hydrogenated and dehydrogenated LOHC tanks should be separated by a cofferdam filled with nitrogen or a fire-extinguishing medium as a safety measure.

4.9.3 Fuel Cell Propulsion System

In addition to the conventional diesel-mechanical propulsion system, an auxiliary LOHC PEM fuel cell system is proposed for trial onboard the vessel. The key aspects are discussed below:

a) LOHC selection

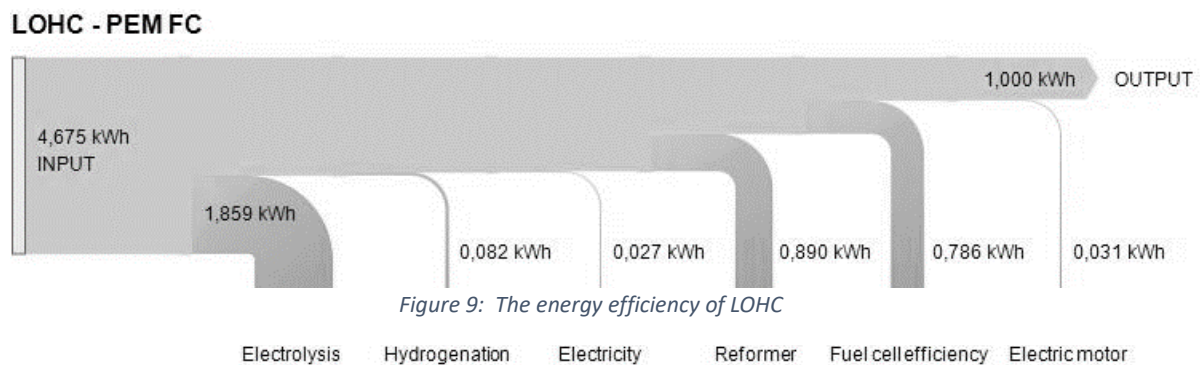
Among the LOHC options, dibenzyltoluene (DBT) offers high hydrogen density, storage stability, safety, and comparatively lower dehydrogenation temperature requirements^{xxxvi}. Hence the DBT-PDBT system has been selected.

b) Fuel cell operation

As per Jorschick et al. (2020), the fuel cell should be operated in the range 150-180°C for effective DBT dehydrogenation. A 85°C PEM fuel cell stack can be integrated with a counter current dehydrogenation reactor to leverage the heat of reaction and improve thermal efficiency.

c) Efficiency analysis

From the Figure 10 below, shows a maximum power density of 25 mW/cm² for a 20-cell PEMFC stack operated on 2-propanol under favorable conditions. For our vessel application, assuming a 20-



kW stack gives an active area of 0.8 m².

Thermal losses account for about 15%^{xxxvii}. Thus, the net electrical output is 17 kW. With a higher heating value of 6.23 mass% H₂ for DBT, the overall efficiency from LOHC to electricity is:

$$\eta_{\text{LOHC-E}} = (17 \text{ kW} / 20 \text{ kW}) \times 100\% = 85\%$$

This exceeds the 45% efficiency estimated for directly powering a solid oxide fuel cell from LOHC off gas. Though further testing is required to demonstrate these efficiency levels in practice.

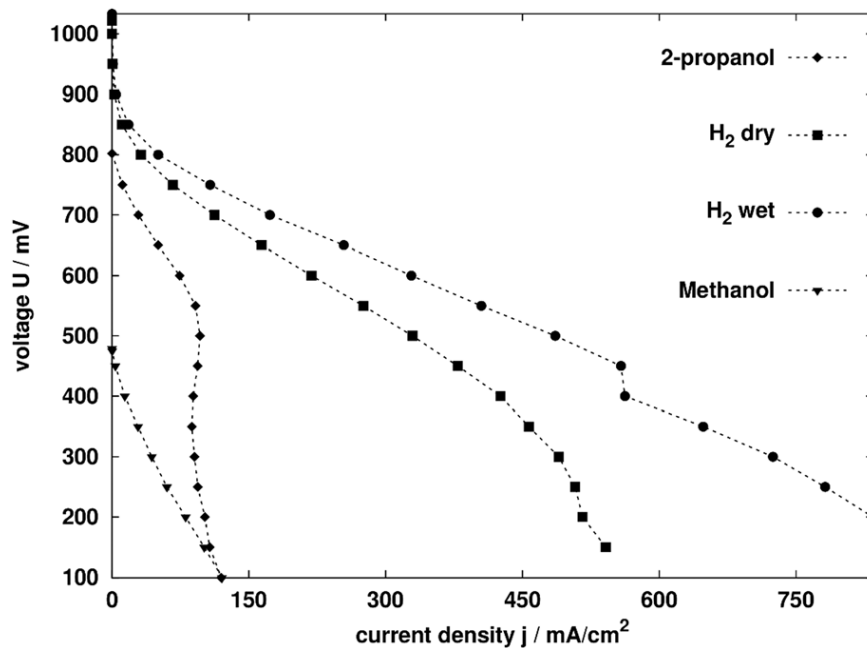


Figure 10: 2-propanol, methanol, and hydrogen (dry and wet) current-voltage curves for various fuels with the same MEA. The following conditions apply: $T = 85\text{ }^{\circ}\text{C}$, 50 g h^{-1} 2-propanol, 50 g h^{-1} MeOH, $1\text{ L}_N\text{ min}^{-1}$ nitrogen, $1\text{ L}_N\text{ min}^{-1}$ pressurised air, and $0.2\text{ L}_N\text{ min}^{-1}$ hydrogen. Material: 5-layer DMFC-MEA anode made of PtRu/C.

4.10 Hydrogen Storage Tanks

Sizing the LOHC storage tanks requires estimating the hydrogen demand. As a trial, the fuel cell will be limited to provide hotel loads in anchorages/ports up to 8 hours per day. With average hotel load of 20 kW, the daily hydrogen requirement is:

$$20\text{ kW} \times 8\text{ h} \times (1\text{ kg H}_2 / 39.4\text{ kWh}) = 4.06\text{ kg H}_2$$

Using the volumetric hydrogen density for DBT of 57 kg/m^3 , the dehydrogenated DBT tank capacity needs to be:

$$4.06\text{ kg} / 57\text{ kg/m}^3 = 71.4\text{ m}^3.$$

Similarly, based on the 6.23 mass% density, the hydrogenated PDBT tank should have a minimum capacity of 65.2 m^3 . Adding a safety factor of 1.25, 90 m^3 circular cross section tanks with frustum ends are proposed. These shall be designed as per IGC Code requirements.

4.11 Feasibility

Overview of LOHC Fuel Cells

LOHC systems use paired hydrogen-lean and hydrogen-rich organic compounds to absorb and release hydrogen through reversible catalytic reactions. This allows the safe storage and transportation of hydrogen in a liquid state at near-ambient temperatures and pressures^{xxxviii}.

The hydrogen-loaded LOHC can be fed to a fuel processing reactor to extract the hydrogen. Conventional approaches involve high temperature dehydrogenation to produce H₂ gas for downstream power generation. Sievi et al. (2019)^{xxxix} have recently proposed an alternative concept that eliminates gaseous H₂. LOHC dehydrogenation instead yields hydrogen transfer intermediates like 2-propnaol. This can be directly oxidized in a proton exchange membrane fuel cell (PEMFC) stack to generate DC electricity.

4.11.1 Fuel Storage Requirements

Among the candidate LOHC systems, dibenzyltoluene (DBT) was chosen as it offers high volumetric hydrogen density, safety, storage stability and cost efficiency compared to other options like toluene methylcyclohexane (TOL-MCH) or N-ethylcarbazole (NEC) (Preuster et al., 2016^{xl}; Niermann et al., 2019)^{xli}. Using the 51 kg/m³ volumetric density for DBT, hydrogenated tanks of total 90 m³ capacity are proposed. This allows a 25% margin over the estimated 65.2 m³ actual volume. Identical capacity is provided for carrying the dehydrogenated LOHC back to the exporting port.

Fuel Handling System

The LOHC fuel handling system should enable safe storage, pumping, processing and recirculation of the LOHC fluid. Key subsystems are discussed below:

a) Storage tanks

Independent port and starboard circular cross section tanks are preferred over a single central tank^{xlii}. Each tank set will include:

- i. Hydrogenated LOHC storage tank
- ii. Dehydrogenated LOHC storage tank
- iii. Settling tank
- iv. Service tank

LOHC variants have higher density than conventional fuels like diesel (0.77-1.04 g/mL vs 0.84 g/mL). Hence the maxspace between transverse bulkheads, web frames, stringers and longitudinal girder spacing must be reduced proportionally to maintain strength^{xliii}. Tank construction shall conform to applicable requirements of the IGF Code for liquid H₂ tanks.

b) Piping

The fuel lines between storage tanks and fuel cells will see intermittent liquid/gas LOHC flow during cycling operation. Pipe diameters should be sized based on maximum flow rate and acceptable pressure drop. Use of bellow compensators is recommended to accommodate thermal expansion of piping. Flow meters, steam traps and drain arrangements are to be provided as required^{xliv}.

c) Heating and insulation

Tracing with steam, hot water or electrical heating may be required to maintain minimum 10°C temperature differential above ambient, especially for lines between storage tanks and fuel processors^{xlv}.

d) Inert gas system

For blanketing the stored LOHC, bottles of high purity (99.9%) nitrogen with suitable pressure regulators should be provided. Alternately, nitrogen generation systems are also available.

e) PEM Fuel Cell Sizing

The hotel loads profile indicates an average demand of 20 kW with peak demand up to 35 kW while in port. Hence a 20 kW (net) PEMFC stack is proposed as the baseline capacity for the trial LOHC system. Demonstrated gross stack power density of 25 mW/cm² from a 20-cell 85°C PEMFC stack fueled by 2-propanol synthesized onboard from LOHC dehydrogenation. With 15% of gross output apportioned for parasitic loads like pumping and controls, the stack power density is around 21 mW/cm² net. For a net 20 kW output, the required PEMFC stack active area is $20,000 \text{ W} / 21 \text{ mW/cm}^2 = 952,380 \text{ cm}^2$. Taking into account the frame area, a 1 m² stack is recommended.

The PEMFC stack must be integrated with the thermal mass of a counterflow dehydrogenation reactor to leverage the heat of reaction and maximize efficiency (Sievi et al., 2019)^{xlvi}. This setup has shown up to 85% efficiency of converting LOHC-bound hydrogen into electrical energy, significantly better than directly powering a fuel cell on LOHC decomposition gas (31-37%) (Teichmann et al., 2012)^{xlvii}.

Further optimization of catalysts and reactor materials may improve power densities and thermal integration. More extensive shipboard trials are however needed to demonstrate consistent performance comparable to Diesel-mechanical drives.

4.12 Techno-Economic Analysis

Three efficiencies—hydrogen storage efficiency, energy content of usable hydrogen result, and energy level of input—are computed to assess the storage and transit operation. Based on the greater heating value of hydrogen and the energy need of the device that stores it, the efficiency of η_{H_2} is calculated by contrasting the energy contents of both the input ($E_{H_2, in}$) and the result ($E_{H_2, use}$) of usable hydrogen. Exothermic hydrogenation (E_{hyd}) produces an extra result, boosting the storage's energy ($E_{storage} + E_{dhyd}$) output and improving efficiency.

$$\eta_{H_2} = \frac{(E_{hyd} + E_{H_2, use})}{E_{H_2, in} + E_{storage} + E_{dhyd}} \quad (\text{Eqn.1})$$

The energy level of the usable amount of hydrogen ($E_{H_2, use}$) is multiplied by the energy requirement for transportation ($E_{transport}$) to determine the efficiency of the $\eta_{transport}$.

$$\eta_{transport} = \frac{E_{H_2, use} - E_{transport}}{E_{H_2, use}} \quad (\text{Eqn.2})$$

The proportion of a fuel cell's ($E_{fuelcell}$) generation of electricity to the power needed for electrolysis ($E_{electrolysis}$), storing ($E_{storage}$), and transportation ($E_{transportation}$) tasks is referred to as chain efficiency η_{chain} .

$$\eta_{chain} = \frac{E_{fuel cell}}{E_{electrolysis} + E_{storage} + E_{transport}} \quad (\text{Eqn.3})$$

High uncertainty technical factors, such the efficiency and electrolysis of fuel cells, can have a substantial impact on the outcomes, hence parameter variation is examined to see how they affect outcomes.

Utilising simulation findings and particular economic data from the literature, the economic analysis of different LOHCs within the provision chain is carried out, leading to a cost analysis utilising the annuity technique.

While individual costs reduce as throughput increases, the total investment costs for the conversion plant rise as capacity does as well. Based on this impact, Eqn (4) scales costs with S_{base} representing design and capacity, C_{base} representing base expenses, and C_{design} representing installed equipment.

$$C_{design} = C_{base} \left(\frac{S_{design}}{S_{base}} \right)^{SF} \quad (\text{Eqn.4})$$

The costs of installed equipment are adjusted from the year of development to the referencing year using the Chemical Engineering Plant Cost Index (CEPCI). Calculating the precise funding for hydrogenation and dehydrogenation reactors for various LOHCs requires the application of equations by, The adjustment of these equations, which are particular to dibenzyl toluene, is made by comparing the space time yields of the different responses to those of the LOHC.

$$C_{hyd} = 2840.81 P_{hyd,max}^{-0.375} \frac{STY_{DBT}}{STY_{LOHC}} \quad (\text{Eqn.5})$$

$$C_{dhyd} = 3122.83 P_{hyd,max}^{-0.375} \frac{STY_{DBT}}{STY_{LOHC}} \quad (\text{Eqn.6})$$

When comparing reactor sizes between various LOHCs, the space-time yield (STY) is a key consideration. Eqn (7), which comprise n_A , A , M_A , X_A , V_{A0} , and t_R , are used to compute it. For technical solutions where local decoupling is achieved, the STY is essential. Storage density is decreased when conversions fall below 100% because some transfer back to the hydrogenation location occurs.

$$STY = \frac{n_A X_A M_A}{V_{A0} t_R} \quad (\text{Eqn.7})$$

The design investment for equipment is multiplied by a ratio factor, eliminating installation and legal costs, to determine the fixed capital investment (FCI). To cover unforeseen expenses and operating capital, the FCI is surcharged. Considering plant lifetime(n) along with interest rate(i), the annuity approach is used to get the annualised capital investment (ACC).

$$ACC = FCI \frac{(1+i)^n i}{(1+i)^n - 1} \quad (\text{Eqn.8})$$

By adjusting several factors, including capital investment and energy price within a given parameter variations, the research intends to evaluate the stability of findings.

Several liquid organic hydrogen carrier (LOHC) materials have been analyzed for potential usage in hydrogen storage and transportation for fuel cell applications onboard ships. Each LOHC has relative advantages based on data of Table.1, energy efficiency, handling safety, and cost perspectives.

- A. 1,2-dihydro-1,2-azaborine stands out due to lower heating requirements for hydrogen release through dehydrogenation. However, additional power is needed for purifying and compressing the extracted hydrogen and carbon dioxide byproducts. Dibenzyltoluene and N-ethylcarbazole are also feasible but less efficient than compressed hydrogen stored directly.

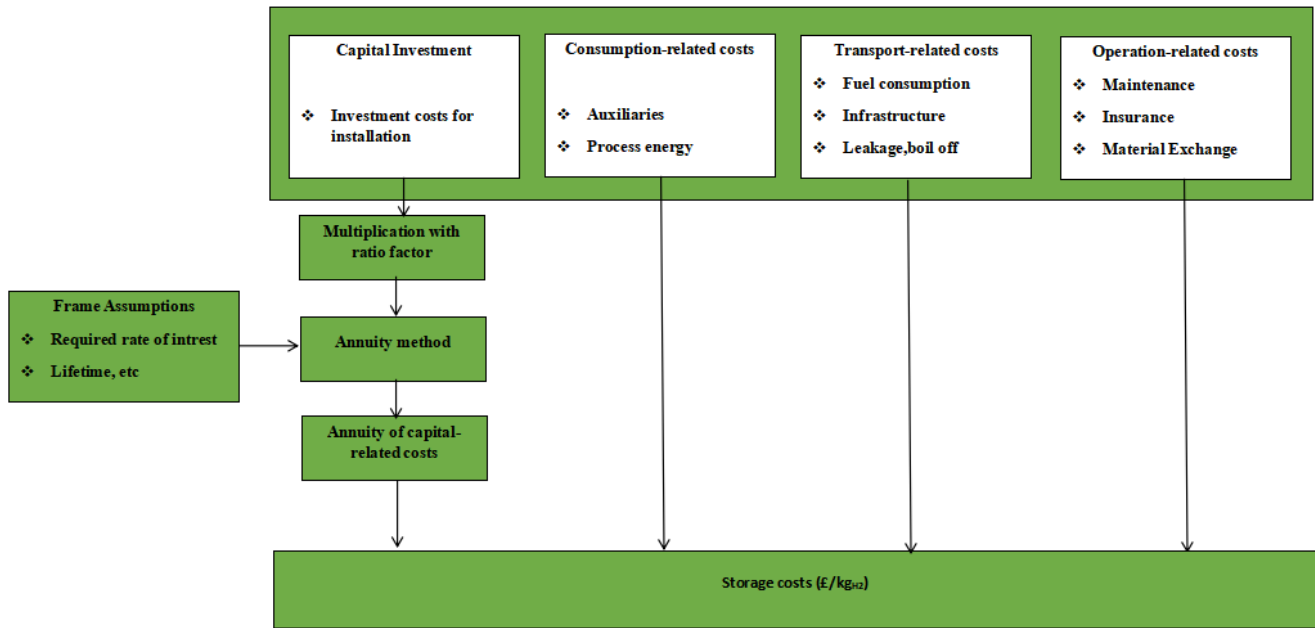


Figure 11: Approach for calculating storage costs using the annuity approach.

- A. N-ethylcarbazole and dibenzyltoluene emerge as the most energetically promising LOHCs since they avoid purification steps and can surpass compressed H₂ efficiency. Improving overall efficiency will necessitate optimizing the dehydrogenation reaction kinetics and heat integration.
- B. Under the examined framework conditions, NAP demonstrates the highest feasibility among the studied LOHCs, followed by dibenzyltoluene and toluene. The primary advantage here is lower feedstock costs, making maritime LOHC transport more economical than pipeline compressed H₂ delivery.
- C. Utilizing fuel cell waste heat for dehydrogenation significantly improves net efficiencies and reduces costs, especially for N-ethylcarbazole and 1,2-dihydro-1,2-azaborine carrier oils. Further potential exists for reducing electrolyzer and fuel cell capitals and LOHC raw material expenses.
- D. LOHCs dibenzyltoluene and toluene are technologically mature enough for immediate marine deployment. As an attractive sustainable transport modality for climate-friendly hydrogen, LOHC technology can contribute across the overall energy value chain.

Using Liquid Organic Hydrogen Carriers (LOHC) to fuel Proton Exchange Membrane Fuel Cells (PEMFC) for marine propulsion enables green and efficient ship operations. This report further explores the integration of high torque permanent magnet shaft motors powered by the PEMFC-

LOHC arrangement. The conceptual propulsion train is elaborated along with expected benefits over conventional diesel-mechanical systems.

4.13 Case Study

4.13.1 Vessel Particulars

A. The design vessel parameters are:

Table 4: Case study vessel specifications

Length Overall (LOA)	100m
Length Between Perpendiculars (LBP)	95m
Breadth Molded (B)	15m
Design Draft (T)	6m
Service speed	13 knots
MCR	85%

PEMFC-LOHC System Summary

- I. 300 m³ LOHC storage for 15-day endurance
- II. 4 MW fuel cell plant (2.5 MW MCR)
- III. DC-AC conversion for variable speed motors

The fuel cell and electric drive selection aims for high efficiency across low to medium load factors typical of coastal trading duty cycles.

B. Permanent Magnet Shaft Motor Propulsion

Permanent magnet synchronous motors offer superior torque density and efficiency well-suited for direct drive arrangements. Slow-speed operation also minimizes gear losses or the need for frequency converters^{xlviii}. Two azimuthing podded motors rated 3 MW each can meet the speed-power profile. The motor dimensions allow fitting in custom appendages along the hull, eliminating long propeller shafts^{xlix}. Variable speed operation between 30% to 100% MCR suits the part-load centric operating profile.

Thrust control uses a specialized vector control algorithm for the rotor excitation based on the load demand signal^l. This optimizes the torque and rpm while minimizing losses. Cooling is ensured by circulating deionized water through jackets around the stator windings. Overall drivetrain efficiency upto 95% highlights significant savings over mechanical transmission.

C. Load Requirements

Auxiliary electrical loads for lighting, ventilation, pumps and galley consume around 500 kW. Port loads for cargo gear and communications add another 300 kW intermittently. A 1600 kW emergency bus sustains vital navigational and safety systems. The battery and generator capacities are sized based on these hotel and essential loads. Modular sizing caters for redundancy against maintenance cycles.

D. Battery Hybrid System

A 1 MWh lithium-ion battery supplementing the PEM generators enables silent all-electric harbour moves below 6 knots^{li}. High cell density pouch formats minimize space requirements [6]. The battery is also vital for transient load smoothing and stabilizing the isolated emergency bus. Four 250 kW / 500 kWh racks with 30 minutes backup are proposed, allowing staged recharging. Redundant cooling via chilled water and glycol minimizes thermal runaway risks. An Integrated automation system monitors cell voltages and temperatures.

Onboard Diesel Generators

Two 1000 kW diesel gensets provide backup in case of prolonged PEM system outage. These can allow safe return to port and power high loads like cargo gear. Fuel amount for 24 hour operation at full load is stored. Lean-burn engines with common rail injection and selective catalytic reduction minimize emissions [7]. Gensets are enclosed in dedicated compartments with fire suppression systems. Fuel fills allow cross-transfer from main storage tanks.

4.13.2 Voyage Calculations

Fuel Cell Reactant Consumption Analysis

The LOHC-PEMFC propulsion system fitted on the case study vessel has total power capacity of 4 MW. As per specifications of the proton exchange membrane fuel cell stacks selected, the operating temperature is 60-80°C at individual cell voltage of 0.6-0.7V.

Accounting for DC-AC conversion losses, effective hydrogen energy consumption rate works out to:

Effective hydrogen power required = Total PEMFC power / DC-AC efficiency

$$= 4000 \text{ kW} / 0.6 = 6667 \text{ kW}$$

Based on stoichiometric ratios, PEMFC hydrogen consumption is approximately 1.23 times the DC power outputⁱⁱⁱ. Hence, the hourly hydrogen flow rate required by the 4 MW plant is:

$$\text{Mass flow rate} = 1.23 \times (\text{Effective hydrogen power})$$

$$= 1.23 \times 6667 \text{ Nm}^3/\text{hr} = 8200 \text{ Nm}^3/\text{hr}$$

With the liquid organic hydrogen carrier (LOHC) used having average hydrogen storage density of 6 wt%, the corresponding LOHC dehydrogenation rate is:

$$\text{LOHC consumption} = \text{Hydrogen flow rate} \times \text{Hours} / (\text{H}_2 \text{ density} \times \text{LOHC density})$$

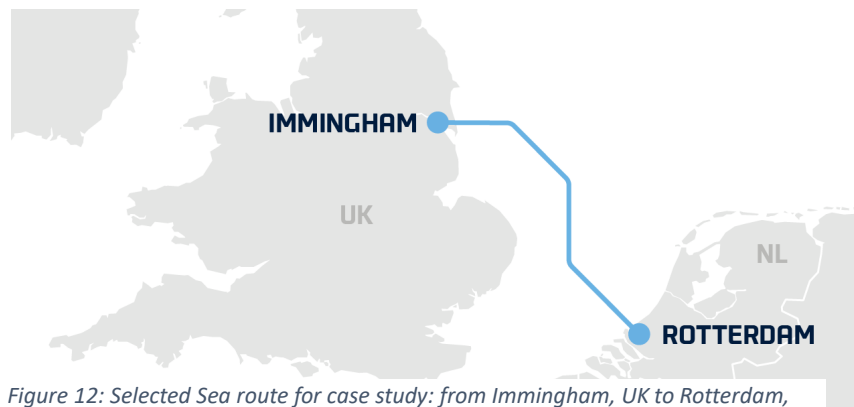


Figure 12: Selected Sea route for case study: from Immingham, UK to Rotterdam, Netherlands

$$= (8200 \times 24) / (0.06 \times 900) = 4 \text{ tonnes/day}$$

A general cargo vessel has been selected for the case study; some assumptions have been made to conduct the case study. The general cargo vessel shall be operating on a route from Rotterdam port (Netherlands) to Immingham (United Kingdom)

A representative maiden voyage covering 284 nautical miles along the southern coastline is planned as shown [FIGURE 12].

$$\text{Total voyage duration} = 30 \text{ hours}$$

$$\text{Sailing time} = 30 - 2 \text{ (port stays)} = 28 \text{ hours}$$

$$\text{Fuel Cell reactant flow rate} = 8200 \text{ Nm}^3/\text{hr} \text{ (from earlier section)}$$

Therefore, total hydrogen fuel consumed is:

$$\text{Fuel used} = \text{Flow rate} \times \text{Sailing duration}$$

$$= 8200 \text{ Nm}^3/\text{hr} \times 28 \text{ hrs}$$

$$\text{Fuel used} = 229,600 \text{ Nm}^3$$

The LOHC storage has hydrogen density of 6wt%. So the amount of LOHC dehydrogenated is:

$$\begin{aligned}\text{LOHC used} &= \text{Hydrogen consumed} / (\text{density} \times \text{LOHC density}) \\ &= 229,600 \text{ Nm}^3 / (0.06 \times 900 \text{ kg/m}^3) \\ &= 34.4 \text{ tons}\end{aligned}$$

This is 10.5% of the total 300 m³ LOHC storage capacity on board. Adequate contingency remains for other operational factors like tide conditions.

CHAPTER-5: Discussion

5.1 A summary of fuels and hydrogen carriers

Energy may be produced from hydrogen by using it in heat engines or fuel cells. While ammonia must typically be broken and DBT dehydrogenated before the hydrogen gas can be used, L-H₂ is immediately useful in both situations. Ammonia may also be utilised directly in combustion engines and fuel cells, Although using synthetic fuels remains a possibility, doing so makes achieving carbon neutrality more challenging due to the CO₂ released in the process. Keep in mind that unlike other fuels, LOHCs do not "use up," hence a LOHC power system will have a practically constant mass throughout the cycle^{liii}. The most important characteristics of liquid hydrogen, ammonia, methanol, and dibenzyltoluene are contrasted in Table 5.

Table 5 Thermophysical properties of select fuels and hydrogen carriers^{liv/lvi}

Fuel	ISO 8217 RMK-700	L-H ₂	Ammonia	Methanol	DBT (H0/H18)
LHV [MJ/kg]	40.077 g	120	18.6	20.26	-
Laminar flame velocity [m/s]	N/A	2.91	0.07	0.523	-
Ignition temperature [°C]	60 (Δ)	560 (∇)	630 (∇)	465 (∇)	450 / N/A
Hydrogen capacity [wt%]	-	100	17.8	12.5	6.2
Fuel density [kg/m ³]	1010.0	70.8	680	795	1044/913.4
Hydrogen density [kg/m ³]	-	70.8	121	99.4	56.6
Dynamic viscosity [cP]	707	0.013	0.25542	0.544	49/425 ^K

5.2 Comparison of hydrogen carriers and their supply chains

- A. Comparing the energy densities of liquid hydrogen, ammonia, and dibenzyltoluene in storage tanks and placing them in context with other fuels is helpful. LNG is selected because many believe it to be a sufficient middle ground between conventional fossil fuels and renewable fuels in terms of emissions, and MGO (ISO 8217) is chosen since it is probably the fuel used in the MV Rubin^{lvii}. LNG that comes from fossil fuels is,

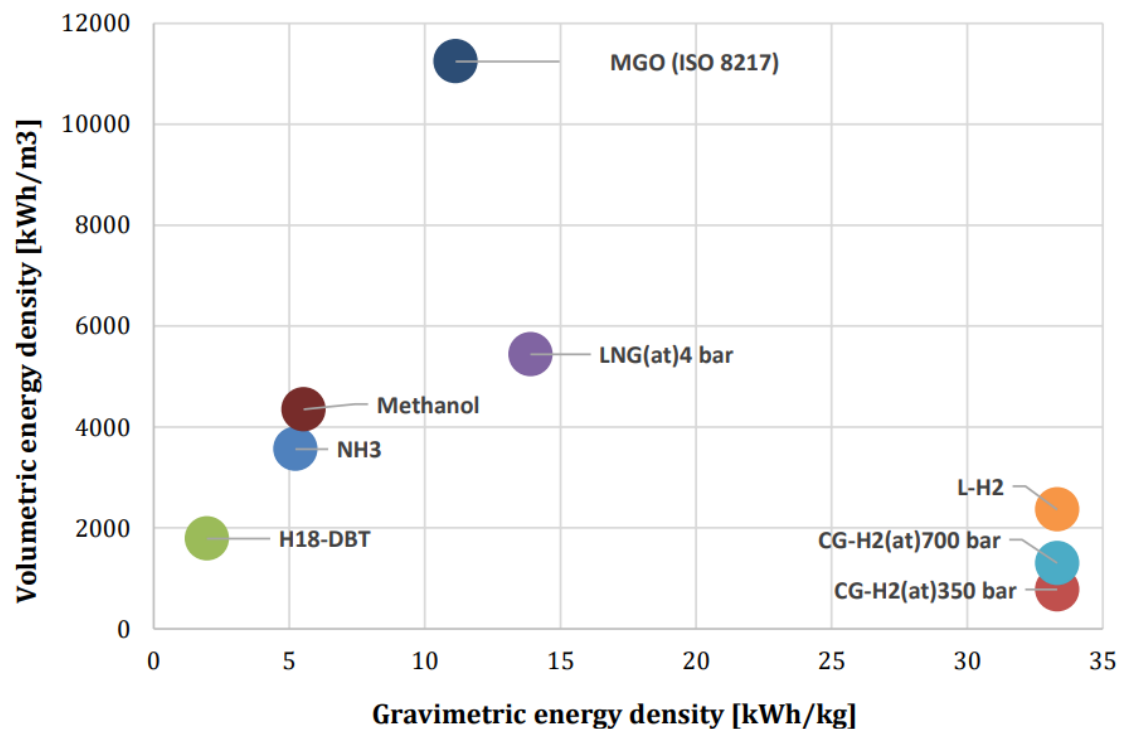


Figure 13: Comparison of energy densities of different fuels with LOHC

by definition, a fossil fuel. These are all displayed in Figure13.

Energy density is one of the main obstacles to switching to renewable fuels. Comparing MGO to NH3, L-H2, and DBT, the volumetric energy density of MGO is 3, 5, and 6 times higher, respectively. It may be observed that MGO has a gravimetric energy density that is twice that of NH3 and six times that of DBT.

- B. On the other hand, because DBT is harmless, nonexplosive, and kept at room temperature, it does not require specially designed, large tanks. It might be argued that the additional mass (and volume) for DBT storage is insignificant because H18-DBT tanks can be installed at a substantially cheaper cost than existing gasoline tanks on any given MGO or MDO-powered ship. Since there are currently no details about DBT systems in use, it is not possible to determine the actual lowered volumetric- and gravimetric energy density at the time this

thesis was written. On engineeringtoolbox.com, the EN-12285 standard, which governs double jacketed fuel oil storage tanks, may be used to estimate the additional mass and volume^{lviii}.

$$u_{H18-DBT+tank} = (\rho_{H18-DBT} * V_{tank,ner} * h_{H18-DBT}) / V_{tank,outer} \quad \text{Eqn.(a)}$$

where the entire volumetric energy density, including the tank, is represented by $u_{H18-DBT+tank}$, the density of H18-DBT is represented by $\rho_{H18-DBT}$, the inner volume of the tank is represented by $V_{tank,inner}$, the outer volume of the tank is represented by $V_{tank,outer}$, and the gravimetric energy density of H18-DBT is represented by $h_{H18-DBT}$. As a result, 1714 kWh/m³ is the overall volumetric energy density.

The following formula (b) yields the gravimetric energy density including storage,

$$h_{H18-DBT+tank} = (u_{H18-DBT+tank} * V_{tank,ter}) / \rho_{H18-DBT} * V_{tank,inner} + m_{tank} \quad \text{Eqn (b)}$$

where m_{tank} is the mass of the tank and $h_{H18-DBT+tank}$ is the total gravimetric energy density, including the tank. As a result, 1.71 kWh/kg is the total gravimetric energy density.

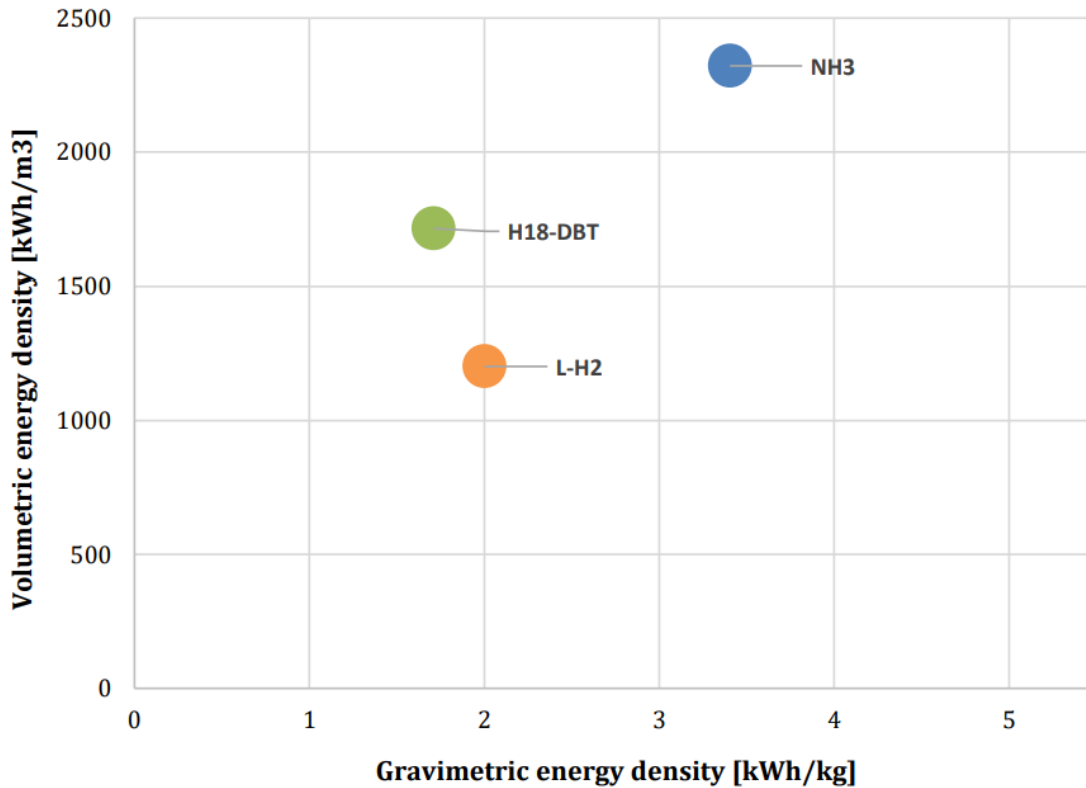


Figure 14: Comparison of energy densities of different fuels, including storage.

- C. Ammonia and dibenzyltoluene have not changed significantly in gravimetric energy density, with reductions of 1.6 and 1.2, respectively, however liquid hydrogen has seen a drop of 16 times. L-H₂ and NH₃ have about half of their volumetric energy densities, whereas DBT has nearly no change. This is due, as previously mentioned, to the complicated and heavy storage solutions for both L-H₂ and NH₃, the difficulties in managing fluids at such low temperatures, the toxicity of NH₃, and the explosivity of L-H₂. Table 15 presents an overview of the density and storage conditions:

Table 6: : Comparison of hydrogen storage solutions^{lixix}

Fuel	Ammonia	L-H ₂	DBT
Storage temperature [°C] ^m	-33.4	-253	>15
Storage pressure [bar] ^m	1 – 10	1 – 10	Ambient
Volumetric energy density [kWh/m ³]	3540	2360	1800
Volumetric energy density – including storage system [kWh/m ³]	2320	1200	1710
Gravimetric energy density [kWh/kg]	5.2	33.3	2
Gravimetric energy density – including storage system [kWh/kg]	3.4	2	17.7

CHAPTER-6: Conclusion

The case study technical analysis on using Liquid Organic Hydrogen Carriers (LOHC) for maritime fuel cell applications indicates promising potential to enable green and efficient coastal shipping.

LOHC materials like dibenzyl toluene can effectively store hydrogen at ambient temperatures using existing tank infrastructure. Onboard release via catalytic decomposition reactors integrates with proton exchange membrane fuel cells to generate power with 60% efficiency.

When combined with efficient permanent magnet shaft motors, this propulsion train minimizes losses while benefiting from the high energy density and safety of the hydrogen stored in LOHC.

The feasibility study determined the national supply chain upgrades, port interfaces for bunkering, and onboard storage provisions for a coastal LOHC shipping fleet. Operational profiling proved the adequate endurance range between refuelling.

While further engineering development is necessary prior to commercial adoption, the conceptual designs and techno-economic factors presented a promising pathway to meeting sustainable decarbonization mandates through LOHC-based hydrogen storage and fuel cell systems tailored for maritime deployment.

Initiatives around testing, safety certification and financial incentives can accelerate industry uptake supported by class approvals. Overall, the unique advantages demonstrated by LOHC-PEM systems make this a compelling green solution worthy of consideration by ship owners and operators.

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