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Review

A Comprehensive Review of Liquid Organic Hydrogen Carriers: Typology, Energy Efficiency, Life Cycle Assessment, and Techno-Economic Analyses

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Abstract

This paper presents a holistic review of Liquid Organic Hydrogen Carriers (LOHCs), focusing on typology, energy efficiency, techno-economic analyses (TEAs), and life cycle assessments (LCAs). Initially, the study categorizes various LOHC systems documented in existing literature, outlining their chemical structures, catalysts, properties, and main applications. This survey aims to provide a comprehensive understanding of LOHC varieties, making it easier to compare across different types. Next, we explore the efficiency of LOHC systems by reviewing hydrogenation and dehydrogenation energy requirements, catalyst behavior, heat-management constraints, product-separation needs, and net energy storage capabilities. This review also includes reaction stoichiometries, recent catalyst and reactor developments, catalyst-deactivation mechanisms, and heat-integration options for high-temperature dehydrogenation. Finally, our investigation offers a detailed evaluation of TEA and LCA for LOHC systems found in the literature. By exploring economic feasibility and environmental impact, this study presents a complete picture of the sustainability of LOHC deployment. It includes assessments of life-cycle carbon emissions, levelized cost, supply-chain configuration, carrier recyclability, infrastructure compatibility, renewable-electricity capacity factors, and heat-recovery assumptions. Our findings aim to contribute to hydrogen storage and transport research by identifying the most important technical, economic, and environmental trade-offs for LOHC systems. By addressing gaps in recent literature, TEA comparability, and LCA coverage, this paper seeks to advance the development of LOHC technologies and support their broader adoption in a green and sustainable energy landscape.

Keywords: Liquid Organic Hydrogen Carriers (LOHC); toluene/MCH; life cycle assessment; techno-economic analysis; hydrogen energy

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1. Introduction

Hydrogen has emerged as a promising alternative for achieving decarbonization targets, primarily because it produces no greenhouse gas emissions and can be sourced from various methods [1]. Its application in transportation and various industrial sectors

is expanding, highlighting its environmental benefits [2–4]. However, significant technological challenges persist in the transportation and storage of hydrogen, especially over long distances [5,6]. For short-range transport, gaseous hydrogen is moved using tube trailers, whereas vacuum-insulated liquid tankers are employed for longer distances [7–9]. Key issues include the energy-intensive liquefaction process, high power consumption, and boil-off gas during transport [10,11]. In terms of storage, hydrogen is kept on a small scale in compressed gas within pressure vessels, medium scale in underground storage, and on a large scale within geologic formations like salt caverns, though the availability of such caverns often poses a challenge [12–14].

Producing hydrogen cost-effectively and managing its distribution remain challenging [15,16]. Hydrogen's low volumetric density presents challenges in both its liquefied form and when compressed to high pressures [17]. The costs associated with compression, both in terms of capital and energy requirements, are substantial, necessitating the transportation of hydrogen in its liquid state at temperatures below −253 °C [18]. Moreover, vacuum-insulated liquid tankers that transport significant amounts of hydrogen over extended distances face additional challenges [9,19]. The liquefaction process demands a large amount of energy—over 10 kWh per kg, equivalent to more than 30% of hydrogen's energy content—alongside losses from boil-off gas during transportation [10,11]. These transportation methods are technologically complex, require a strong emphasis on safety, and demand a significant financial investment to establish a large-scale distribution infrastructure [20]. To address these challenges, recent research has explored alternative hydrogen carriers such as ammonia, methanol, and toluene/methylcyclohexane. These carriers have shown potential in overcoming many of the existing obstacles associated with hydrogen transportation and storage [21–25].

Synthesized from natural gas, ammonia (NH_3) is primarily utilized in agriculture as a fertilizer [26]. Over the next few years, it is anticipated that ammonia production capacity will increase by six percent, with the largest facilities capable of producing up to 2700 tons per day [27]. Although the production of ammonia for transportation and its conversion back to hydrogen are energy-intensive processes, the existing infrastructure for its handling and shipping is robust [28]. The primary advantages of ammonia include its high hydrogen content and the potential for its production using renewable energy sources [29].

Serving as an industrial raw material, methanol (CH_3OH) is integral to producing a broad spectrum of chemicals, including solvents, adhesives, plastics, and fuels [30–32]. Its consumption is primarily driven by the demand for formaldehyde, alternative fuels like gasoline blending, and the synthesis of other chemical byproducts. In recent years, the capacity of methanol production facilities has expanded, with the development of larger plants now considered technically feasible (up to 10,000 metric tons per day) [33].

Toluene, a byproduct of petroleum, is primarily used as a precursor for other chemicals, a solvent for paints, and as an octane booster in gasoline. In comparison to ammonia and methanol, toluene is produced on a smaller scale and has modest growth projections [34,35].

Liquid Organic Hydrogen Carriers (LOHCs) are organic molecules capable of reversible hydrogenation and dehydrogenation, effectively releasing hydrogen. They maintain a liquid state at ambient temperature and pressure, ensuring efficient hydrogen storage without losses. Their resemblance to oil enables straightforward integration with existing petroleum infrastructure, fostering increased research into LOHCs aimed at pinpointing the most suitable candidates for hydrogen storage and transport [36–39]. Notable LOHCs include cyclic hydrocarbons such as benzene/cyclohexane, toluene/methylcyclohexane (MCH), naphthalene/decalin, biphenyl/bicyclohexyl, and dibenzyltoluene (DBT)/perhydro-dibenzyltoluene. These chemicals are widely used industrially, with benzene and toluene alone reaching a global production nearing 50 million

metric tons annually [1]. The hydrogen storage capacity of these hydrocarbons typically ranges from 6 to 8 wt%, with the energy demand for their hydrogenation and dehydrogenation processes averaging between 62 and 69 kJ/mol H_2 [40,41].

In addition to identifying suitable LOHCs, extensive techno-economic assessments (TEAs) of the hydrogen transport value chain have been conducted. These assessments include scenarios such as long-distance harbor-to-harbor hydrogen transport and road hydrogen transport. However, due to varying methodologies and assumptions, results across these studies are not directly comparable. The primary focus of these assessments is to establish the economic feasibility of organic carriers for hydrogen transport, with less emphasis on the technical evaluation of hydrogenation and dehydrogenation stages from an engineering viewpoint. For instance, studies have specifically examined LOHCs like DBT in road transport contexts [21], and others such as DBT, toluene, methanol, and N-ethylcarbazole in harbor-to-harbor scenarios [24,42]. Additionally, flexible hydrogen supply chain models for different road transport scenarios have been analyzed, focusing particularly on DBT [43]. Recent studies also include harbor-to-harbor transport evaluations [6,44,45]. Recent work has also expanded the LOHC candidate space to include bio-derived carriers for reversible hydrogen storage [46]. Despite these advances, significant gaps remain, especially concerning the energy efficiency of LOHCs, TEAs, and particularly life cycle assessments (LCAs) [24,47–49].

Contribution

This paper provides a detailed review of LOHCs, with emphasis on Toluene/MCH while also comparing DBT-based systems, N-ethylcarbazole, formic acid, methanol, and ammonia as hydrogen-carrier options. It categorizes LOHC systems from existing literature, describing chemical structures, catalysts, properties, and applications, thereby enhancing the understanding and comparison of different LOHC types. The study delves into energy efficiency, particularly the energy requirements for hydrogenation and dehydrogenation processes, heat integration, catalyst durability, separation, and overall energy storage capabilities. Furthermore, TEA and LCA studies are reviewed to evaluate economic viability and environmental impacts, with a particular focus on identifying current gaps. This review discusses reaction stoichiometry, high-power-density reactor concepts, renewable-electricity capacity factor in the levelized cost of H_2 (LCOH) calculations, infrastructure compatibility, oxygen by-product credits, heat recovery, and LCA impact categories beyond greenhouse-gas emissions. These analyses provide insights into hydrogen storage and transport, aiming to propel the development of LOHC technologies for broader adoption in sustainable energy initiatives, thereby benefiting researchers, policymakers, and industry stakeholders.

2. Typology of Liquid Organic Hydrogen Carriers

LOHCs are organic compound pairs that enable hydrogen storage in the liquid phase through chemical bonding, allowing for its subsequent recovery [37]. The fundamental concept of LOHC technology was initially evaluated using the benzene/cyclohexane system [50]. Since then, various carriers have been studied, including aliphatic compounds (such as methanol and formic acid), single-ring aromatics (like toluene), multi-ring aromatics (such as naphthalene and dibenzyltoluene), and nitrogen heterocycle aromatics (such as N-ethyl carbazole and phenazine) [51].

LOHCs represent an innovative approach to hydrogen storage and transportation, addressing the challenges associated with traditional methods. LOHCs involve the chemical binding of hydrogen molecules to liquid organic compounds, facilitating safer and more efficient storage and transportation over long distances.

The operation of LOHC systems is based on the reversible hydrogenation and dehydrogenation of organic compounds [37]. During hydrogenation, hydrogen is chemically bonded to the carrier molecule in a storage facility, converting the LOHC to its hydrogen-rich form. For hydrogen release, the dehydrogenation process reverses this chemical reaction, releasing pure hydrogen gas that can be utilized in various applications, including fuel cells for clean energy [47].

Table 1 summarizes representative reversible hydrogen storage/release reactions for the main carrier systems discussed in this review. Including the reaction stoichiometry is useful because the gravimetric hydrogen capacity, heat duty, and separation requirement are directly linked to the number of hydrogen molecules stored per carrier molecule.

Table 1. Representative hydrogen storage/release reactions for selected hydrogen carriers. The forward direction corresponds to hydrogenation or hydrogen storage, while the reverse direction corresponds to hydrogen release. Nominal H_2 capacities are reported from the literature [52–54].

Carrier Pair	Representative Reaction	Nominal H_2 Capacity
Toluene/MCH	$C_7H_8 + 3H_2 \rightleftharpoons C_7H_{14}$	6.2 wt%
Benzene/cyclohexane	$C_6H_6 + 3H_2 \rightleftharpoons C_6H_{12}$	7.2 wt%
Naphthalene/decalin	$C_{10}H_8 + 5H_2 \rightleftharpoons C_{10}H_{18}$	7.3 wt%
DBT/perhydro-DBT	$C_{21}H_{20} + 9H_2 \rightleftharpoons C_{21}H_{38}$	6.2 wt%
N-ethylcarbazole/perhydro-NEC	$C_{14}H_{13}N + 6H_2 \rightleftharpoons C_{14}H_{25}N$	5.8 wt%
CO_2/formic acid	$CO_2 + H_2 \rightleftharpoons HCOOH$	4.4 wt%

2.1. Technology Review

LOHCs offer a compelling solution for the storage and transport of hydrogen, a clean energy carrier with the potential to play a significant role in the global transition to sustainable energy systems. Below, we explore various types of LOHC systems, each with its own set of advantages and challenges.

1. **Toluene (TOL)/Methylcyclohexane (MCH) System:** TOL/MCH is one of the most extensively studied LOHC systems, where toluene acts as the hydrogen-lean form. Toluene is a colorless, water-insoluble liquid that is advantageous for long-distance and overseas transport due to its liquid state and low kinematic viscosity, which facilitates easy pumping [37,52,55]. The TOL/MCH pair is formed by adding a methyl radical to benzene, resulting in a hydrogen storage capacity of 6.2 wt%, which meets the targets from the hydrogen and fuel cell technologies office (HFTO) in the U.S. Department of Energy (DOE) [56], while also reducing toxicity and increasing the liquid temperature range [53,57]. The limit of dehydrogenation of MCH is 95%, providing a storage capacity of 5.9 wt% and an energy density of 1.6 kWh/L [52]. Toluene's market price and its established use in the chemical industry, where it is produced through catalytic reforming and pyrolytic cracking, further enhance its attractiveness as a hydrogen carrier [55,57,58].

   Hydrogenation of the TOL/MCH system can be catalyzed at temperatures ranging from 150–230 °C and pressures of 0.5–3 bar, using noble metal catalysts such as Pt, Pd, or Ru on an Al_2O_3 support, with zeolites serving as alternative supports [51,59]. The dehydrogenation process, which requires 68.3 kJ/mol H_2, occurs at temperatures between 250–450 °C and is also catalyzed by Pt or Ni on various supports [40,52,60]. Despite these advantages, toluene is believed to be carcinogenic, flammable, and poses environmental risks, while MCH also has safety concerns, such as low ignition temperature and the potential for explosive mixtures at room temperature [52,55,61]. However, TOL/MCH is being utilized by the Chiyoda Corporation to transport low-carbon hydrogen from regions like Australia and the Middle East to Singapore,

with impressive dehydrogenation conversion rates and hydrogen purity achieved during the process [47,62].

2. **N-Ethylcarbazole (H0-NEC)/Perhydro-N-ethylcarbazole (H12-NEC):** Nitrogen-containing heterocyclic compounds, such as H0-NEC, exhibit favorable kinetic and thermodynamic properties, making them promising candidates for LOHCs [37,63]. The presence of nitrogen in these compounds promotes dehydrogenation by weakening surrounding bonds, allowing for lower dehydrogenation temperatures [64,65]. H0-NEC, the first widely studied N-heterocyclic compound, offers a hydrogen storage capacity of 5.8 wt% and an energy density of 2.5 kWh/L [52]. Hydrogenation can be efficiently catalyzed using noble metals or Ni, with Ru showing the highest activity at a 98% selectivity rate [66,67]. Dehydrogenation can occur below 200 °C, and can achieve near-full dehydrogenation below 300 °C with a Pd/CNT catalyst, resulting in 99.99% hydrogen purity [52,53,68]. Despite its potential, H0-NEC has drawbacks, such as a high melting point (69 °C), poor thermal stability above 120 °C, and limited availability due to its production via coal tar distillation, which yields less than 10,000 tonnes annually [36,53,69].
3. **Dibenzyltoluene (H0-DBT)/Perhydro-Dibenzyltoluene (H18-DBT):** H0-DBT is a promising LOHC, widely used as a key component in thermal conductive oil [62]. H0-DBT is noted for its high thermal stability, low toxicity, and safe handling characteristics, thanks to its high boiling point (390 °C) and flash point (200 °C) [70]. The high boiling point also aids in dehydrogenation by reducing the need for hydrogen purification and facilitating quick gas flow [52]. Hydrogenation typically occurs at 150–200 °C and 20–50 bar, using Pt or Ru catalysts on Al_2O_3 supports, while dehydrogenation takes place at 280–320 °C with Pd or Ru catalysts, achieving up to 97% efficiency [52,59,71,72]. However, H0-DBT requires high dehydrogenation energy (65 kJ/mol H_2) and has a slow reaction rate, which necessitates efficient heat management [70,73]. Despite being less toxic than other LOHCs, H0-DBT still presents environmental risks, and developing cost-effective catalysts remains a challenge [52,62].
4. **Formic Acid (FA):** FA is a colorless, corrosive, and water-soluble liquid with potential as a LOHC, particularly through the hydrogenation of carbon dioxide and catalytic dehydrogenation [51,52]. Although CO_2 is abundant, capturing it from the atmosphere is energy-intensive, though it can be captured during hydrogen production. Hydrogenation is exothermic and can be influenced by solvents or bases, while dehydrogenation can be controlled by adjusting pH, temperature, or pressure. However, FA's toxicity, flammability, and corrosiveness present significant handling challenges, and its low storage capacity when solvents are involved diminishes its appeal as a LOHC. Despite these drawbacks, the potential for renewable production makes FA a subject of continued research [52,74].

2.2. Properties

Tables 2–4 present a comprehensive summary of various hydrogen carrier systems discussed in the literature, along with the specific catalysts used in hydrogenation and dehydrogenation processes, which are crucial for the deployment of LOHCs. Table 2 provides an overview of different LOHC systems, detailing their hydrogen storage capacity, operating temperatures for hydrogenation and dehydrogenation, catalysts used, and the cost implications. Notably, systems like TOL/MCH and HO-DBT/H18-DBT highlight the variations in catalyst compatibility and costs, reflecting the balance between performance and economic viability in hydrogen storage technologies. This table emphasizes the broad

spectrum of LOHC applications and their respective efficiencies and costs, providing a snapshot of the current advancements and challenges in hydrogen storage technologies.

Table 2. Summary of discussed hydrogen carriers. Prices are indicative bulk carrier prices and should not be interpreted as directly comparable delivered-hydrogen costs because source year, purity, region, and scale differ among studies.

LOHC System	H_2 Capacity (wt%)	Hyd. Temp (°C)	Dehyd. Temp (°C)	H_2 Storage Catalyst	H_2 Release Catalyst	Price (USD/kg)	Ref.
TOL/MCH	6.2	130–450	200–550	Pd, Ru	Pt, Ni	0.32	[51–53,57,59]
H0-DBT/H18-DBT	6.2	150–200	180–320	Pt, Ru	Pd, Ru	4.29	[52,59,70–72]
H0-NEC/H12-NEC	5.8	150	200–300	Pd, Ru	Pd, Ru	42.85	[52,68,75]
FA	4.4	50–100	50–100	Fe, Re	Fe, Re	N/A *	[52,76–78]
NH_3	17.8	400	TC	Fe	Ni, Ru	1.08	[62,79,80]
CH_3OH	12.1	420	520	Cu	Ir, Pt	N/A *	[52,54]

TC = thermal cracking. * For formic acid and methanol, the cited sources report CO_2 feedstock/distribution costs rather than directly comparable USD/kg carrier prices.

Table 3. Properties of hydrogenation catalysts for different LOHC components [49].

Catalyst	LOHC	Pressure [bar]	Temperature [°C]	Conversion [%]	Time [min]	Ref.
Pt/γ-Al_2O_3	TOL	0.3–1.9	100–250	99.5	1.2	[81]
	DBT	20	150–300	100	n.a	[82]
		40	270–320	100	30	[83]
Ni/Al_2O_3	TOL	15–2.5	120–180	100–25	22–25	[81]

Table 4. Properties of dehydrogenation catalysts for different LOHC components [49].

Catalyst	LOHC	Pressure [bar]	Temperature [°C]	Conversion [%]	Time	Ref.
Pt/γ-Al_2O_3	MCH	1–9	340–380	~100 (1 bar)	225 min	[84]
		1–8	340–379	80–90%		[84]
		1–10	340–380	99%		[85]
Pt/γ-Al_2O_3	H18-DBT	1	250	n.a	n.a	[82]
		2	320	n.a	n.a	[86]
		2	320	81.30%	0.5–5 min	[83]
		1	250–320	~100		[87]
Pt/C	H18-DBT	1	270	97%	3.5 min	[72]
		1	280	97%	2.5 h	[88]
		1	260	55%	2.5 h	[89]
		1	270	69%	4 h	[90]
		1	280	11%	3.45 mL/min/g_{kat}	[88]

Tables 3 and 4 present the specifics of the catalysts used for hydrogenation and dehydrogenation, respectively, providing a detailed comparison of operational conditions such as pressure and temperature ranges, conversion rates, and operation times. These tables highlight the performance characteristics of catalysts like Pt/γ-Al_2O_3 and Ni/Al_2O_3, which are crucial for optimizing the hydrogenation process, as well as Pt/C used in dehydrogenation, demonstrating how different materials and conditions impact the efficiency of hydrogen release from LOHCs. This detailed catalyst data helps in understanding the nuances of each process step, crucial for improving the overall efficiency and feasibility of hydrogen storage systems. Together, these properties not only demonstrate the technical parameters and performance of various catalysts but also underscore the importance of

matching the right catalyst with the appropriate LOHC system to maximize efficiency and minimize environmental impact.

Catalyst durability is a critical engineering issue for high-temperature LOHC dehydrogenation, particularly for perhydro-dibenzyltoluene and perhydro-benzyltoluene systems operated near 270–330 °C. The most common deactivation pathways include carbonaceous deposits from side reactions or over-dehydrogenated intermediates, strong adsorption of aromatic species on Pt-group active sites, sintering or redistribution of metal particles under prolonged thermal exposure, and poisoning by sulfur-, nitrogen-, oxygen-, or halogen-containing impurities in the carrier stream. Recent catalyst-focused reviews and experiments emphasize that activity, selectivity, and stability must be considered simultaneously, because higher temperature can improve conversion but may also accelerate byproduct formation and catalyst aging; recent examples include highly dispersed $Pd/\gamma\text{-}Al_2O_3$ for reversible benzene/cyclohexane conversion and analysis of steric effects in aromatic-hydrocarbon hydrogenation [91–93]. At industrial scale, mitigation strategies include strict LOHC quality-control protocols, upstream purification of the carrier and hydrogen streams, stable metal-support combinations, operation with minimized hot spots, staged or intensified heat supply, and periodic regeneration when coke formation becomes significant.

Fluid properties also influence the choice of infrastructure. TOL/MCH and DBT-based LOHCs are liquids at ambient conditions and can use pumps, tanks, and handling practices similar to liquid-fuel infrastructure, but their viscosity, vapor pressure, flash point, toxicity, and requirement for a return flow of the unloaded carrier must be included in pipeline and logistics design. Methanol is also easily pumped and has mature liquid-fuel logistics, but it is toxic, flammable, miscible with water, and used consumptively when reformed. Ammonia has a high hydrogen mass fraction and existing global infrastructure, yet long-distance transmission requires refrigerated or pressurized handling and careful management of toxicity, odor, and material-compatibility risks. Thus, LOHCs can reduce the need for cryogenic or high-pressure hydrogen transmission, but they transfer part of the engineering burden to carrier circulation, dehydrogenation heat supply, and product purification [48,52,94].

3. Review of LOHC Efficiency

3.1. Hydrogenation, Dehydrogenation, and Supply-Chain Energy Use

The LOHC value chain can be interpreted as a sequence of coupled conversion, storage, transport, heat-integration, and purification steps rather than as independent unit operations. Figure 1 combines the simplified LOHC cycle, the broader logistics chain, and the most energy-intensive process steps in a single schematic. Hydrogen produced from renewable electricity is chemically loaded into the carrier during hydrogenation. The loaded carrier is stored and transported using liquid-fuel-type logistics. Hydrogen is then released in an endothermic dehydrogenation reactor, purified according to end-use requirements, and distributed to the final application, while the hydrogen-lean carrier is returned for reuse.

The largest efficiency penalty typically occurs in the hydrogen-release step. Aromatic LOHC dehydrogenation is strongly endothermic; for common homocyclic systems, reported heat duties are commonly in the range of approximately 62–69 kJ mol^{-1} H_2. Consequently, the practical efficiency of an LOHC pathway depends not only on the thermodynamics of the carrier pair but also on reactor heat transfer, heat-source temperature, product separation, carrier losses, and the number of carrier recirculation cycles.

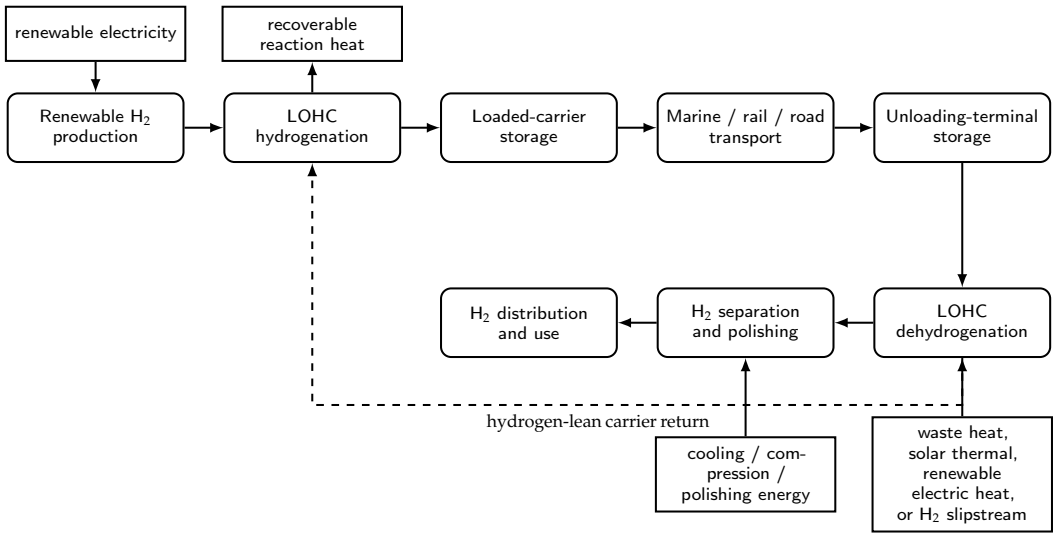


Figure 1. Integrated LOHC supply-chain schematic combining the carrier cycle, logistics, major energy inputs, dehydrogenation heat demand, hydrogen purification, and return of the hydrogen-lean carrier. Solid arrows indicate the main material and energy flows through the LOHC supply chain, while the dashed arrow indicates the return of the hydrogen-lean carrier to the hydrogenation step for reuse. Adapted from [1,48].

3.2. Heat Integration and Intensified Reactor Concepts

Supplying the endothermic heat of dehydrogenation is one of the central engineering challenges for LOHC deployment. At the process level, heat integration can use waste heat from high-temperature industrial processes, solid oxide fuel cells, combustion of a small hydrogen slipstream, concentrated solar thermal heat, electric heating from low-carbon power, or thermal-energy storage. The preferred option depends on the required reactor temperature, heat-transfer coefficient, carrier stability, and whether the final application can accept a reduction in delivered hydrogen when part of the hydrogen is consumed to provide heat. Heat recovery from the exothermic hydrogenation step may also reduce total utility demand when hydrogenation and dehydrogenation are co-located or thermally integrated, but many export/import chains spatially separate these steps, limiting direct heat recovery.

Recent reactor work has focused on increasing dehydrogenation power density by improving heat transfer to the catalytic zone. Inverted fixed-bed and other intensified reactor concepts reduce heat-transfer distances and improve catalyst utilization, thereby addressing one of the practical bottlenecks of conventional packed-bed LOHC dehydrogenation [95,96]. DehyMax-related work on continuous perhydro-benzyltoluene dehydrogenation further illustrates the trend toward compact, high-power-density reactor systems for benzyltoluene-family carriers [46,96]. These intensified concepts may reduce reactor volume and improve transient response, but they also increase the importance of temperature control, pressure-drop management, catalyst stability, and LOHC quality control.

3.3. Hydrogen Purity and Product Separation

Hydrogen purity after dehydrogenation is governed by conversion, gas–liquid disengagement, carrier vapor pressure, byproduct formation, and the separation train. PEM fuel cells generally require high-purity hydrogen, so dehydrogenation systems may require condensation of carrier vapors, demisters, adsorbents, membranes, or catalytic polishing. These operations increase capital cost, auxiliary electricity demand, pressure drop, and heat rejection. Conversely, less intensive separation can reduce energy consumption and cost, but may allow carrier vapors, light hydrocarbons, CO, CO_2, or other impurities to reach

downstream equipment. Thus, there is an inherent engineering trade-off between hydrogen purity, hydrogen recovery, auxiliary energy use, and system complexity. The optimal design depends on whether the hydrogen is used for fuel cells, combustion, refining, ammonia synthesis, or another industrial process.

4. Techno-Economic Analysis (TEA) of LOHC Systems

Techno-economic assessments of LOHC systems differ substantially in their system boundaries, carrier selection, transport distance, energy prices, financing assumptions, and treatment of coproducts and heat recovery. For this reason, LCOH values from different studies should not be compared without first checking whether they include hydrogen production, carrier loading, carrier production or make-up, storage, transport, hydrogen release, purification, distribution, and return transport of the unloaded carrier.

4.1. Scope and Cost Drivers

Recent TEA guidance for hydrogen carriers emphasizes that the following parameters should be reported explicitly: hydrogen-carrier production, hydrogen release, carrier recyclability and make-up losses, application sector and scale, infrastructure network, transport distance, geographical position, policy and incentives, oxygen by-product sales, and heat-recovery assumptions [94]. Table 5 summarizes how these parameters affect LOHC economics. Marine transport is only one possible configuration; road, rail, pipeline-compatible liquid transport, and hybrid chains can dominate depending on distance, demand size, and geography.

Table 5. Key parameters that should be considered in TEA of LOHC supply chains, adapted from and synthesized based on prior hydrogen-carrier TEA studies [1,6,24,42].

Parameter	Effect on LCOH and Design Interpretation
Hydrogen production and electrolyzer capacity factor	Often represents one of the largest contributors to LCOH. Lower renewable capacity factors increase the annualized electrolyzer CAPEX per kg H_2 and may underutilize hydrogenation/dehydrogenation assets.
Carrier production, make-up, and recyclability	Carrier losses, degradation, and purification requirements determine make-up cost and environmental burden over repeated cycles.
Hydrogen release and heat source	Dehydrogenation heat demand strongly affects OPEX, emissions, and delivered hydrogen efficiency. Waste heat and heat recovery can reduce cost.
Oxygen by-product credit	Electrolysis produces oxygen; selling or using it can partially offset hydrogen production cost, but market size and location limit the credit.
Infrastructure and transport length	Road, rail, marine, and pipeline-compatible liquid logistics exhibit different scaling behavior, safety constraints, and loading/unloading costs.
Geography and policy	Renewable resource quality, port access, carbon pricing, hydrogen incentives, and safety regulations change the preferred carrier pathway.

4.2. Comparison of TEA Studies

Detailed economic analyses of hydrogen-carrier supply chains, including production, storage, transportation, and distribution, have been conducted over the years. For example, Hurskainen and Ihonen evaluated road transport of hydrogen using DBT-based LOHCs [21]; Niermann et al. compared LOHCs and alternatives for international renewable-hydrogen transport [42]; Raab et al. compared large-scale hydrogen transport using liquid transport media [24]; Papadias et al. evaluated methanol, ammonia, and MCH across production, transmission, decomposition, and storage [6]; Spatolisano et al. analyzed a

detailed TOL/MCH value chain [1]; and Sage et al. reviewed Australian renewable-energy export pathways using LOHCs and competing carriers [48]. These studies confirm that LOHC results are sensitive to the assumed supply-chain boundary and that the same carrier can appear more or less favorable depending on whether hydrogen production, heat supply, distribution, and carrier return are included.

Figure 2 compares the total hydrogen cost breakdown in Australian dollars per kilogram of hydrogen from various techno-economic studies on MCH as an LOHC, including analyses by Autrey et al. [97], Li et al. [98], Niermann et al. [99], Wijayanta et al. [100], and IEA projections for 2030 and 2050 [16]. Across all studies, production costs emerge as the largest contributor to the total cost, with the IEA projections showing a potential reduction in these costs over time due to anticipated technological advancements. While conversion, storage, transport, and release costs are relatively consistent across studies, their proportions vary, with Wijayanta et al. allocating more cost to transport and release. The IEA's 2050 projection highlights significant future cost reductions in storage and release, contrasting with current studies where these remain higher. Overall, while production costs dominate, the distribution of other costs varies, with future projections indicating a trend towards overall cost reduction driven by technological progress.

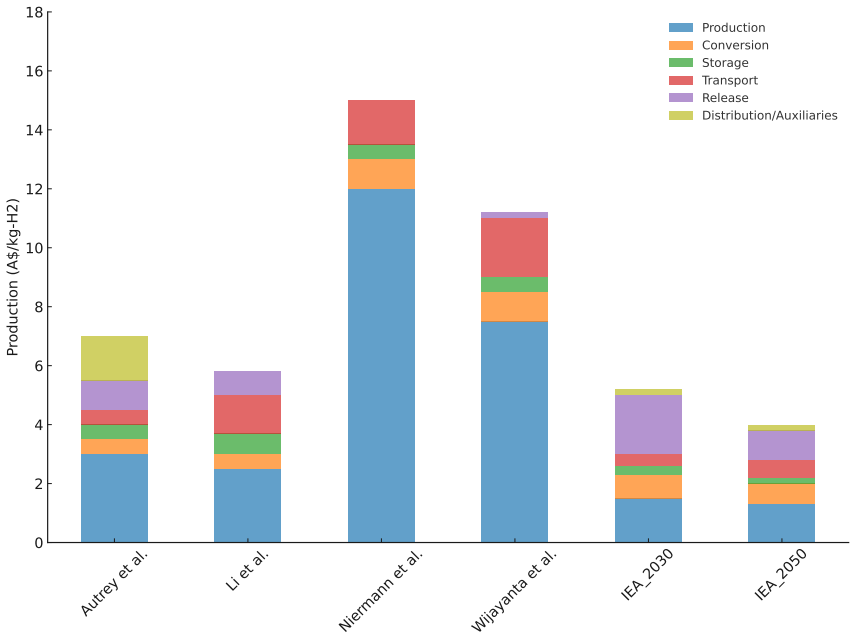
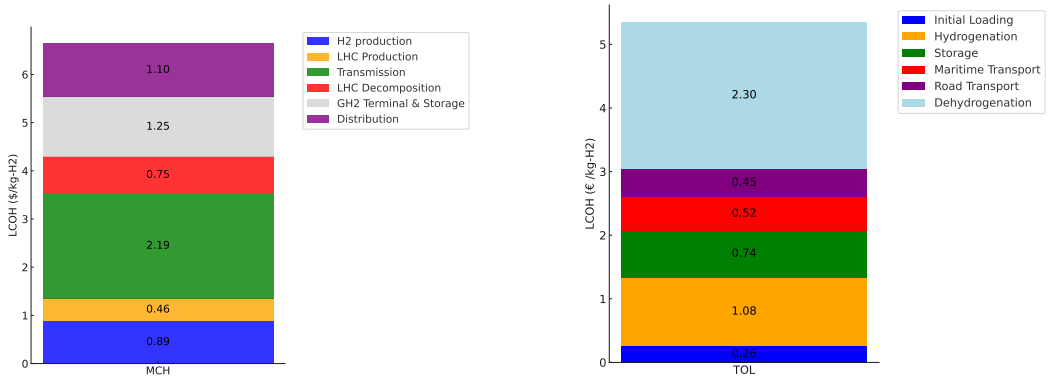


Figure 2. Total hydrogen cost from various techno-economic studies on MCH as an LOHC in Australian dollars per kilogram of hydrogen. The comparison illustrates the sensitivity of LCOH to hydrogen-production cost and to differences in treatment of conversion, storage, transport, release, and auxiliary/distribution costs. Adapted from [16,48,97–100].

In related research, Papadias et al. [6] explored the feasibility of using liquid hydrogen carriers such as methanol, ammonia, and MCH for hydrogen transportation and storage. This study examined the costs and energy requirements associated with the production, transmission, and storage of these carriers via rail and pipeline systems. Using levelized costs, specific energy consumption, and capacity factors for various production plants and transport modes, the findings revealed that producing MCH at a capacity of 350 tpd-H_2 would require a capital expenditure of \$396k per tpd-H_2. As shown in Figure 3a, the levelized cost of H_2 (LCOH) for TOL/MCH is \$6.65 per kg-H_2. The study also noted that methanol and ammonia pipelines could provide cost benefits over hydrogen pipelines for transmission purposes.

Further, Spatolisano et al. [1] assessed the fixed and operating costs for hydrogenation and dehydrogenation processes under different scenarios and cost drivers. The study calculated the LCOH to evaluate the economic feasibility of the LOHC-based value chain. Results indicated a CAPEX of 17.21 million dollars for toluene dehydrogenation, with fixed OPEX of 8.57 million dollars per year for toluene and 9.17 million dollars per year for dibenzyltoluene hydrogenation. Figure 3b shows that the LCOH for TOL/MCH is €5.35 per kg-H_2. The breakdown shows dehydrogenation as the largest single contribution (€2.30 kg^{-1} H_2), followed by hydrogenation (€1.08 kg^{-1} H_2), storage (€0.74 kg^{-1} H_2), maritime transport (€0.52 kg^{-1} H_2), road transport (€0.45 kg^{-1} H_2), and initial loading (€0.26 kg^{-1} H_2). This cost breakdown provides a clearer quantitative comparison of the main contributors to LCOH for the TOL/MCH pathway. Thus, Figure 3 highlights the significant variability in the LCOH even when using the same carrier, such as MCH or TOL. This variation stems from differences in underlying assumptions across different studies, particularly in how the cost components, such as hydrogen production, transport, and dehydrogenation, are calculated.



(**a**) (**b**)

Figure 3. Comparison of different TEAs assessing the LCOH when using TOL and MCH as carriers. The figures illustrate how varying assumptions and methodologies can lead to significant differences in the cost breakdown, highlighting the impact of each cost component on the overall LCOH. (**a**) Levelized cost of H_2 using TOL/MCH as an LOHC considering production, transmission by train, decomposition, storage, and distribution [6]. (**b**) Levelized cost of H_2 using TOL/MCH as an LOHC considering initial loading, hydrogenation, storage, maritime transport, road transport, and dehydrogenation [1].

5. Life Cycle Assessment (LCA) Review

5.1. LCA Scope, Boundaries, and Impact Categories

Studies on liquid organic hydrogen carriers (LOHCs) within the context of life cycle assessments (LCAs) remain relatively scarce in the literature. Wulf et al. [101,102] conducted detailed LCAs on several supply-chain models for delivering hydrogen to refueling stations within a 500 km range, including LOHC transportation and storage. These studies indicate that LOHC pathways can have higher climate impacts than compressed hydrogen systems using cavern storage and pipeline transport, which show the lowest greenhouse-gas (GHG) emissions, approximately 1.5–1.8 kg CO_2-eq kg^{-1} H_2 [101]. Figure 4 displays the climate change impact associated with different stages of using TOL/MCH as a LOHC. The total climate change impact is approximately 6 kg CO_2-eq kg^{-1} H_2, with the largest contribution coming from dehydrogenation.

The LCA evidence base for LOHCs is narrower than the TEA literature and is strongly affected by functional unit, allocation, heat source, electricity mix, carrier make-up, and treatment of the reusable carrier inventory. A rigorous LCA should state whether

the functional unit is kg H_2 delivered, kg H_2 dispensed, MJ of final energy, or a specific end-use service. It should also specify whether hydrogen production, carrier synthesis, catalyst production, terminal infrastructure, return transport of the unloaded carrier, carrier degradation, and end-of-life treatment are included. Without this information, climate impacts reported by different studies may not be directly comparable.

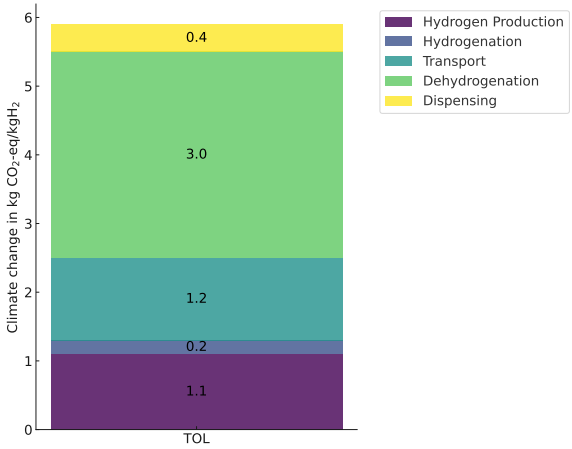


Figure 4. Climate change impact, measured in kg CO_2-equivalent per kg of hydrogen (kg CO_2-eq/kg H_2), associated with different stages of using TOL/MCH as a LOHC. Adapted from [48,101]. The comparison highlights the large contribution of dehydrogenation heat supply and the need to report the energy source used for hydrogen release.

In addition to climate change, future LOHC LCAs should report toxicity, ecotoxicity, photochemical ozone formation, acidification, particulate matter formation, water consumption, resource depletion, land use, and occupational/safety-related indicators. Toxicity and ecotoxicity are especially relevant for aromatic LOHCs such as toluene and DBT derivatives, while water use and electricity mix are critical for electrolytic hydrogen. Conventional oil-derived fuels provide a useful reference point for liquid-fuel logistics, but the comparison must be made carefully because LOHCs are reusable hydrogen carriers whereas petroleum fuels are consumed. Therefore, fossil benchmarks should be used primarily to contextualize transport/storage infrastructure and not as a direct one-to-one comparison unless the same final energy service and system boundary are used [103].

Although LOHCs offer economic advantages, they are among the least environmentally favorable options in some studies due to their significant ecological impact [43]. The majority of greenhouse gas emissions from LOHCs are generated during the energy-intensive dehydrogenation phase, especially when powered by natural gas. However, this environmental impact is notably reduced when hydrogen, renewable electricity, solar thermal heat, waste heat, or other low-carbon heat sources are used for the reaction [101]. When comparing DBT and toluene, differences arise from carrier production, heat and electricity requirements for dehydrogenation, toxicity, and approval constraints for road and maritime transport [48,101].

5.2. LCA Gaps and Comparison with Conventional Technologies

The limited number of directly comparable LOHC LCAs makes it difficult to generalize environmental performance across all carriers and deployment scenarios. For example, a pathway using low-carbon heat for dehydrogenation and high utilization of carrier inventory can have a very different footprint from a pathway using natural gas heat, long return distances, and high carrier losses. Similarly, a comparison with oil-derived liquid fuels must consider that petroleum fuels combine storage medium and energy carrier in one material, whereas LOHC systems separate the hydrogen energy vector from

the reusable organic carrier. The most meaningful comparisons therefore report both a hydrogen-delivery functional unit and, where possible, a final-service functional unit such as delivered useful energy or fuel-cell output.

Recent combined TEA/LCA work on hydrogen delivery options reinforces that no single carrier is universally optimal; performance depends on distance, scale, geography, energy source, and infrastructure availability. LOHC pathways can be attractive when ambient liquid handling, long storage duration, and compatibility with existing logistics are valuable, but their climate benefit requires low-carbon hydrogen production, low-carbon dehydrogenation heat, high carrier recyclability, and careful control of losses and toxic emissions.

6. Conclusions

This comprehensive review of LOHCs underscores their pivotal role in addressing the challenges of hydrogen storage and transport, which are critical to advancing a sustainable energy transition. Our review provides a detailed understanding of various LOHC systems through evaluation of their typologies, reaction chemistry, catalyst behavior, energy efficiencies, TEA, and LCA. The expanded review shows that LOHC feasibility is governed by the coupling between carrier chemistry, heat management, catalyst durability, hydrogen purification, carrier circulation, and infrastructure design. Importantly, while LOHCs offer innovative solutions to hydrogen transport and storage, facilitating easier handling and integration into existing infrastructure, they present considerable challenges in terms of energy requirements for hydrogen release and the environmental impacts associated with their life cycle, particularly when dehydrogenation is powered by non-renewable energy sources.

The TEA within this research has clarified the economic viability of LOHCs, comparing favorably in some contexts to traditional hydrogen storage methods. However, the environmental assessments highlight a critical need for innovation toward reducing the ecological footprint of these systems. Additionally, TEAs can vary significantly depending on the assumptions made, further emphasizing the need for standardized approaches in these analyses. There is also a noticeable lack of comprehensive LCAs, which are essential for a full understanding of the environmental impacts of LOHC technologies.

Future research should therefore focus on improving the analyses related to the energy efficiency of hydrogenation and dehydrogenation processes, with particular attention to estimating energy consumption at different stages of these processes. Priority topics include intensified dehydrogenation reactors, low-deactivation catalysts, carrier quality protocols, heat recovery, waste-heat and renewable-heat integration, separation-energy minimization, oxygen by-product utilization, capacity-factor sensitivity, and standardized TEA/LCA boundaries. Exploring renewable energy sources for these operations will also be crucial in enhancing the overall sustainability of LOHC technologies.

Looking ahead, the potential of LOHCs to contribute to a robust hydrogen economy is evident, yet dependent on concerted efforts in research, policy, and industry collaboration. Continued exploration and optimization of LOHC systems are essential to overcome current limitations and unlock their full potential. This will involve not only technological innovations but also the creation of favorable regulatory frameworks and market incentives to support the deployment of LOHC solutions. By addressing these challenges, LOHCs can play a crucial role in the global shift toward sustainable energy solutions, marking a significant stride in the quest for clean, efficient, and accessible energy storage and transport systems.

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