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Title

A Techno-economic Assessment of Green H₂ Carrier Supply Chains

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Abstract

Green hydrogen can play a key role in affordably decarbonizing society. However, storage and transmission costs pose significant barriers to green hydrogen distribution. These limitations may be overcome with liquid green hydrogen carriers like ammonia, methanol, and toluene/methylcyclohexane as well as formic acid, which has only recently received limited attention. A techno-economic assessment of these hydrogen carriers is presented across a wide range of scales. Green formic acid is identified to be the most cost-effective carrier when the entire supply chain cost is considered. Additional analysis shows that formic acid is the only green carrier that is more affordable to produce than its fossil-based counterpart and is the safest of the studied carriers. Finally, research and policy outlook are provided to guide efforts towards the realization of a green hydrogen economy. This work informs the selection of a suitable green hydrogen carrier, which is essential to decarbonize at the rate needed to avoid climate catastrophe.

Introduction

In the face of the growing threat posed by anthropogenic climate change, the United States, the largest cumulative emitter of greenhouse gases, has committed to net zero greenhouse gas emissions by 2050.¹ The transportation, electricity, and industrial sectors are currently the largest contributors to climate change in the U.S. accounting for 27%, 25%, and 24% of total U.S. greenhouse gas emissions respectively.² The urgency of the climate crisis motivates efforts to simultaneously electrify transportation and industry while decarbonizing the grid. The cost of renewable electricity has plummeted in recent years and the most affordable sources of electricity are now solar photovoltaics and onshore wind.^{3,4} Low-cost intermittent renewables balanced with non-carbogenic baseload generation of electricity (nuclear, hydro, and geothermal) coupled with energy storage allow for a dependable decarbonized grid. The establishment of such a decarbonized grid would permit green electrons to be delivered to an electrified society. In theory, the realization of net-zero electricity, transportation, and industry by 2050 is technologically feasible. Thus, its realization relies upon intertwined political will and economic feasibility.⁵

Green hydrogen produced via water electrolysis leverages affordable green electricity by offering a clean fuel and chemical feedstock that is critical to achieving multi-sector decarbonization. Green hydrogen fuel can be used in fuel cells to electrify the transportation sector along with battery electric vehicles to achieve a net-zero transportation sector by 2050.⁶ Additionally, green hydrogen fuel can be generated using excess electricity from peak solar and wind electricity production hours providing a means to capture and store otherwise wasted energy to help stabilize the grid. In the industrial sector, green hydrogen can help decarbonize chemical and steel production. As a chemical feedstock, green hydrogen can be used to produce sustainable ammonia for fertilizer to help provide food to a rapidly growing population. Additionally, green hydrogen can be coupled with CO from CO₂ electrolysis to generate green syngas to decarbonize a wide range of petrochemical processes.

A green hydrogen economy offers the ability to achieve multi-sector decarbonization, but hydrogen suffers from a lack of mobility making hydrogen difficult and costly to distribute. The physical properties of hydrogen impose a considerable cost on the supply-chain of delivering gaseous hydrogen to consumers because moving hydrogen requires either pressurization or cryogenic refrigeration. For example, recent work has shown that the costs of delivering hydrogen fuel (storage, transmission, and distribution at a fueling site) exceed the cost of producing hydrogen by a factor of 2-3x.⁷ To overcome the inherent limitations of cost-effective hydrogen storage and transmission, a variety of liquid hydrogen carriers are being actively explored. These hydrogen carriers offer properties that allow for a potential reduction in costs of transmission and storage, and an improvement in safety. Well-discussed hydrogen carriers such as ammonia and methanol as well as two-way carriers such as avarious liquid organic hydrogen carriers and solid metal hydrides. Since the variety of two-way carriers is numerous, toluene/methylcyclohexane (MCH) was selected as a two-way carrier

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representative due to its relatively high hydrogen density for a two-way carrier. A significant amount of effort in recent years has been applied to evaluate the feasibility of these carriers.^{7–12} Another potential hydrogen carrier which has begun to receive more attention is formic acid. Recent literature has considered the use of formic acid to deliver hydrogen due to its relatively high volumetric hydrogen capacity (53 $g_{H_2} L^{-1}$).^{13–20} Much of this attention has been focused upon formic acid dehydrogenation strategies,^{21–29} but less attention has been applied to considering if this carrier makes economic sense across a green hydrogen supply-chain relative to other popular carriers. This motivates a comparative techno-economic assessment to evaluate the economic viability of the use of formic acid as a hydrogen carrier. A detailed supply chain analysis across a range of scales is needed to project which liquid green hydrogen carrier is most economical and safest.

Recent advances in green formic acid technology such as the electrochemical reduction of CO₂ to formic acid and biogenic formic acid production encourage its use as a sustainable hydrogen carrier.^{30–35} The goal of this work was to identify the most cost-effective green hydrogen carrier by considering the entire supply chain of hydrogen delivery. The production costs of green hydrogen and potential green hydrogen carriers have been explored in other work.^{36–44} However, the costs associated with the entire supply-chain of delivering green hydrogen to distributed consumers have been often neglected. Here, we sought to systematically estimate the costs along the entire supply chain, from production to end use, associated with the most promising green hydrogen carriers (including formic acid) and green molecular hydrogen. Our goal is to provide a comparative assessment not only between molecular green hydrogen and its carriers, but among the green hydrogen carriers themselves. Such a comparison provides timely insight to guide future decisions related to hydrogen distribution that will be made by researchers, policymakers, and investors alike in their pursuit of realizing a green hydrogen economy.

Green Hydrogen Delivery Supply-Chain

It has been previously estimated that the transmissions costs of molecular hydrogen can be as high as 12 USD $kg_{H_2}^{-1}$ and storage costs can be as high as 10 USD $kg_{H_2}^{-1.45,46}$ Given that the storage and transportation of hydrogen is a significant source of cost, it is necessary to model the entire cost of the hydrogen supply chain, from production to end-customer delivery, so that the costs of supplying this resource can be accurately assessed. A techno-economic assessment that includes the costs of production, onsite storage, transmission, decomposition, and carbon capture (when applicable) was conducted for green hydrogen and green hydrogen carriers (Figure 1).



Figure 1: Overview of modeled green hydrogen carrier supply chain. Liquid green carriers were compared to each other and green, molecular hydrogen across the entire supply chain.

To assess the production costs (Supplementary Discussion 1), the method to produce each green hydrogen carrier was selected by considering both environmental impact and technological readiness (Figure S1). Traditionally, the production of hydrogen, formic acid, methanol, ammonia, and toluene/MCH all rely upon fossil fuel feedstocks, principally methane. In contrast, the carriers considered in this work were produced using more sustainable, "green" technologies. Here, the green hydrogen was produced via water electrolysis. Green formic acid was produced by direct electrolysis via the electrochemical reduction of CO₂. Because of the lack of commercially feasible direct electrochemical routes for methanol and ammonia, the combination of thermal hydrogenation of CO₂ and green hydrogen via water electrolysis were proposed for green methanol production; similarly, the green ammonia was produced through the Haber-Bosch process from green hydrogen and nitrogen. As no commercially feasible methods for producing green toluene yet exist, fossil-based toluene was produced then hydrogenated to MCH using green hydrogen. Each carrier was produced at a central facility rather than at distributed sites to reduce production costs. By locating the carrier plants near an electricity generator, utility providers can be bypassed allowing access to cheaper wholesale electricity rates. Access to inexpensive electricity is critical for electrochemicals since electricity is typically the single largest source of cost in their production. Due to greater land availability, production facilities outside of city gates will also be less constrained in their size allowing them to leverage economies of scale and the associated learning curve more effectively. Additionally, the ability to receive regulatory permits for plant construction requires adherence to typical industrial zoning laws, thus the most practical path for the rapid deployment of hydrogen fuel is likely via centralized production facilities.

Onsite storage costs were evaluated by assuming a 30-day supply of each carrier was stored onsite as is common industrial practice to avoid supply-chain shortages.^{47,48} Hydrogen and ammonia were stored cryogenically as liquids to minimize cost, whereas methanol, formic acid, and toluene/MCH were stored under ambient conditions which is typical in the chemical industry (Supplementary Discussion 2). Salt and lined rock caverns have received substantial attention as potential hydrogen storage sites. However, the need for suitable geological conditions severely constrains cavernous storage site availability to only a few sites (only 3 sites have been identified in the U.S.⁴⁹ Thus, suitable geologic storage sites are generally unavailable where needed.⁷ Potential hydrogen losses due to leaks, cavern pores, microbial consumption, and geological reactions also still requires further investigation. Additionally, loss of hydrogen purity due to cavern moisture needs to be considered. Therefore, cryogenic storage tanks currently offer the most reliable method of hydrogen storage.

During transmission, compression is typically used for the liquefaction of ammonia (17 bar) and hydrogen (350 bar) to avoid the need for onboard refrigeration units.⁵⁰ The U.S. Department of Transportation (DOT) currently regulates pressures of tube trailers to below 250 bar. However, up to 500 bar tube trailers are currently used, but special DOT permits are required.⁵¹ The need for a special DOT permit for transmitting molecular hydrogen is an additional hurdle to the green hydrogen supply chain that can be overcome with the aid of a hydrogen carrier. Transmission costs were modeled by transmitting hydrogen and ammonia under pressure via tube trailer; methanol, formic acid, and toluene/MCH were transported under ambient conditions via tanker trucks (Supplementary Discussion 3). Transmission by tube or truck trailer leverages already existing infrastructure to deliver hydrogen, avoiding many of the logistical challenges associated with establishing pipeline and railroad infrastructure. Thus, trucking is the most promising near-term means of transmission until pipeline and railroad infrastructure can be established. Once delivered by truck, the modeled carriers were decomposed or reformed to liberate the hydrogen. Previously reported values were used to estimate these costs (Supplementary Discussion 4).^{7,21,52} Since the liberation of hydrogen from methanol and formic acid resulted in CO₂ emissions, carbon capture as deployed (Supplementary Discussion 4). Key assumptions that were used to construct the supply chain used in this model have been tabulated (Table 1).

	Production	Onsite Storage	Transmission	Decomposition	Carbon Capture
Hydrogen	H₂O electrolysis	30-day supply, -253 °C, 0.1% day ⁻¹ boil off rate	Tube trailer, 350 bar	-	-
Formic Acid	CO ₂ electrolysis	30-day supply, ambient temperature	Tanker truck, 1 bar	Catalytic cracking	Pressure swing adsorption
Methanol	Thermal hydrogenation	30-day supply, ambient temperature	Tanker truck, 1 bar	Steam reforming	Pressure swing adsorption
Ammonia	Haber-Bosch	30-day supply, -33 °C, 0.1% day ⁻¹ boil off rate	Tube trailer, 180 bar	Catalytic cracking	-
Toluene/ MCH	Thermal hydrogenation	30-day supply, ambient temperature	Tanker truck, 1 bar	Steam reforming	-

Table 1: Key techno-economic simulation green hydrogen carrier supply-chain assumptions.

Total Cost Comparison of Delivered Hydrogen

The total costs for each green hydrogen carrier supply chain were calculated by evaluating the production, onsite storage, transmission, decomposition, and carbon capture (when applicable) costs. These costs were studied over a range of transmission distances and electricity costs to allow for the best carrier to be identified under a given set of conditions. Based upon the typical order of magnitude for current U.S. commercial hydrogen production, the production scale was set at 10 000 kg_{H₂}/day.⁵³ The weight of each carrier was normalized to its usable hydrogen content in this work to allow for a fair comparison between different carriers (Table S1). At a production scale of 10 000 kg_{H_2}/day , formic acid is the most affordable carrier when transportation distances are long and electricity costs are low (Figure 2a). This low overall supply chain cost is primarily due to the relatively low transmission costs for formic acid as well as a relatively high sensitivity to electricity price. In contrast to this scenario, toluene/MCH and ammonia are competitive carriers for shorter transmission distances (<750 km) and when cheap electricity is unavailable. However, the use of a central production facility will most likely require larger transmission distances, especially during the early market penetration phase. As a twoway carrier, toluene/MCH is much more sensitive to transportation distance, but less sensitive to electricity price since the bulk of the molecular weight is derived from thermochemical production routes. Although methanol also has relatively low onsite storage and transmission costs, it suffers from relatively high production costs (Figure 2b). Due to their need for cooling and compression, both hydrogen and ammonia have relatively high storage and transmission costs. Molecular hydrogen may have the lowest production cost, but this saving is offset by the high costs of storage and transmission that dominate the total cost required for delivery.

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Since green hydrogen demand is anticipated to grow,⁵⁴ a range of production scales spanning multiple orders of magnitude were studied for each carrier. The scaling relationships for electrochemical production are significantly different from those of the thermochemical plants. Two different scaling relationships are observed in this work to describe the carrier production plants: one scaling relationship for electrolysis plants (hydrogen and formic acid) and one scaling relationship for plants that couple electrolysis with downstream thermochemistry (ammonia, methanol, and toluene/MCH) (Supplementary Discussion 1). Relative to electrolyzers, large thermochemical reactors are much more expensive to scale down due to their lack of modularity.^{45,46} Therefore, the total costs for delivering hydrogen from methanol and ammonia have much steeper scaling curves than those for hydrogen and formic acid. Since thermal hydrogenation is more expensive than Haber-Bosch, green methanol is more sensitive to scaling than ammonia. Formic acid is only about 4 wt% hydrogen so a larger scale electrolyzer is needed to produce 1 kg H₂ than for generating the same amount of green hydrogen directly in a water electrolyzer. Thus, the formic acid electrolyzer falls further towards the flattened portion of the scaling curve than a water electrolyzer when normalizing to 1 kg hydrogen. Toluene/MCH scales similarly to green hydrogen because once the thermochemically produced toluene is provided, it is reused and simply loaded with green hydrogen to form MCH. Thus, the toluene/MCH scaling relationship is dictated by the production cost of green hydrogen.

The green hydrogen carriers studied in this work were also compared to their "gray" fossil-based counterparts at the 10 000 k_{BH_2} /day scale (Supplementary Discussion 5). Methanol, ammonia, formic acid, and toluene/MCH are all conventionally derived from fossil fuels. Whereas most emerging low-carbon technologies pose an additional cost for adopting green alternatives (i.e., a green premium), formic acid is the only hydrogen carrier that is more affordable to produce via a green low-carbon route (i.e., CO₂ electrolysis) than from a fossil-source (Figure 2d and 2e). Formic acid currently has a relatively low market size (0.6 Mton annual global production),⁵⁵ thus a high demand for the green production of formic acid would allow for a green premium to be avoided by leveraging economics of scale to undercut the current fossil-based route. Methanol production suffered from the largest green premium of 757%. The green discount associated with green formic acid technology illustrates the potential for industrialized electrochemical formic acid production to compete with the incumbent fossil-based technology.



Figure 2: Total cost comparison of delivered hydrogen. (a) Total supply chain cost as a function of transportation distance at a 10 000 kg_{H_2} day⁻¹ production scale. Lines are modeled at an electricity price of 0.04 USD kWh⁻¹. Shaded regions indicate electricity price range from 0.01-0.07 USD kWh⁻¹. (b) 10 000 kg_{H_2} day⁻¹ production scale cost breakdown in an early market penetration

scenario (electricity price of 0.04 USD kWh⁻¹ and a 2,000 km transportation distance). (c) Production cost of each studied green hydrogen carrier scaled over daily hydrogen production capacity. (d) Comparison of costs of delivered fossil-based (gray) hydrogen carriers and green hydrogen carriers at current industrial scale. (e) Additional cost of choosing a green alternative over conventional gray carriers (green premium).

Improving Formic Acid Economics at Scale

To achieve cost-competitiveness as a hydrogen carrier, electrochemical formic acid production technology must continue to improve. To illustrate which parameters should serve as focal points for future research, a cost-sensitivity analysis was conducted (Figure 3a). In this figure, steeper slopes indicate increased economic importance. This analysis revealed that improved faradaic efficiency is the most cost-sensitive performance parameter. However, relatively high faradaic efficiency has already been achieved (≥95%)^{32,33} so there is less room for additional improvement in faradaic efficiency relative to the other performance parameters. Current density also appears to be relatively cost sensitive, but like faradaic efficiency, current density scales non-linearly and is already beginning to flatten out near the base case (200 mA cm⁻ ²). However, since current density dictates reaction rate, larger current densities will be needed at industrial scale than have been achieved in the laboratory-scale. In contrast, cell potential/electricity price and separation costs scale linearly and are the next most cost-sensitive performance parameters that would yield the greatest decrease in total production costs. Balance of plant and stack cost also scale linearly but their effect on production cost is less pronounced than the other parameters. A similar sensitivity analysis was also conducted for the production of green hydrogen and its relation to ammonia, methanol, and MCH carrier production costs was assessed (Figure S2).

Future advances in electrochemical formic acid production technology will allow green formic acid to become a cost-competitive hydrogen carrier at scale (Figure 3b). Improvements in electrolyzer performance parameters on par with water electrolysis technology such as a 100% Faradaic efficiency and a current density of 2 A/cm² would significantly decrease production costs. Additionally, stack cost is currently dominated by the cost of the Ir anode, a reduction in Ir loading from 2 mg/cm² to 0.5 mg/cm² on par with water electrolyzers and a 20% reduction in separation costs offers a considerable reduction in production costs. CO₂ electrolyzer designs that can reduce downstream separation costs by producing pure and concentrated product are already being actively explored.^{33,56} Finally, strong policy efforts to reduce the cost of the captured CO₂ feedstock further enhance the cost-effectiveness of electrochemical formic acid production. Such efforts have already established in the U.S. via the recently increased 45Q tax credit.

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Figure 3: **Methods for reducing cost of large-scale green formic acid production.** (a) Formic acid production cost sensitivity analysis where base case parameters found in parenthesis correspond to the vertical dashed line and are independently scaled. (b) Roadmap to reduce formic acid base production cost by sequential improvement of cost-sensitive performance parameters.

Logistical Safety Considerations

An evaluation of hydrogen carriers should consider supply-chain safety because safety hazards are directly related to the total cost of the supply chains. More hazardous carriers will require additional costly safety features for production facilities, transmission, and storage. The safety associated with each carrier will also affect insurance costs. Although these costs are difficult to estimate, some qualitative assessment can be conducted using information provided by the National Fire Protection Association (NFPA), Department of Transportation (DOT), Occupational Safety and Health Administration, and Centers for Disease Control and Prevention - National Institute for Occupational Safety and Health (Table S2). Using this information and the physical properties of each carrier, risks associated with fire, health, and the environment were ranked as either low, moderate, or high (Table 2). Fire risks are highest for methanol, hydrogen, toluene, and MCH. The DOT classifies hydrogen as a flammable gas and the NFPA gives hydrogen a fire rating of 4, the most severe hazard ranking on their scale from 0-4 (Table S2). The DOT classifies methanol, toluene, and MCH as flammable liquids and the NFPA gives these chemicals a fire rating of 3, representing a serious hazard. Ammonia and formic acid pose the lowest fire risk. Although formic acid is given an NFPA fire rating of 2, a moderate hazard, it is unlikely to pose a fire risk under ambient conditions. The explosive range for formic acid is 18-57%; however, due to its relatively low vapor pressure it is unlikely to achieve those vapor concentrations at ambient conditions (Table S3). Formic acid also has a relatively high auto-ignition temperature (601 °C), thus posing little risk.

Regarding the potential health risks, hydrogen and ammonia pose a high health hazard due to their asphyxiation risk and toxicity respectively. Toluene and methylcyclohexane also pose high health hazards due to their organ toxicity and aspiration risk. Methanol and formic acid both have relatively low health risks because in the event of a spill, they only pose a health hazard if the liquid is contacted directly. Although the NFPA gives formic acid a health rating of 3 (extreme danger), likely due to its relatively low permissible exposure limit (5 ppm), formic acid remains in a liquid state under ambient conditions posing little inhalation hazard. Additionally, formic acid is typically diluted to 85% during transport, further increasing its safe handling.

Environmental risks for formic acid, methanol, and hydrogen are all relatively low because these compounds are readily biodegradable, have low potential to adsorb on soil or sediment, and disperse quickly in water.^{57,58} Toluene and MCH pose a high risk to the environment due to their threat to aquatic life. Ammonia also poses a high environmental risk because the release of ammonia can have a severe negative impact on biodiversity and agriculture.⁵⁹ Ammonia and MCH are both labeled as an environmental hazard by the NFPA.

Ammonia and hydrogen both require pressurized transportation, exacerbating the fire, health, and environmental risks associated with these hydrogen carriers. Formic acid, methanol, toluene, and MCH pose significantly less risk due to their ability to be transported under ambient conditions. Ultimately, formic acid appears to be safer than methanol, toluene, and MCH because it poses a less significant fire hazard. In the event of a spill under ambient conditions, formic acid

should naturally decompose rapidly, pose little fire risk, and should only be a health risk if direct contact is made. In reference to the other carriers evaluated, formic acid offers the safest logistics, significantly lowering insurance costs and decreasing costs associated with necessary safety equipment for companies handling the material.

Table 2: Key logistical safety information associated with hydrogen carriers of interest. A qualitative assessment of transmission pressure and a qualitative assessment of fire, health, and fire risk were performed to assess the hazards associated with each carrier.

Hydrogen Carrier	Transport Pressure (bar)	Fire Risk*	Health Risk*	Environmental Risk*
Formic Acid	Ambient	Low	Moderate	Low
Methanol	Ambient	High	Moderate	Low
Ammonia	20	Low	High	High
Hydrogen	350	High	High	Low
Toluene	Ambient	High	High	High
MCH	Ambient	High	High	High

*Risks qualitatively evaluated under ambient conditions in the occurrence of a spill

Research and Policy Outlook

In response to a growing interest in green hydrogen, research and policy should be carefully planned to accelerate the transition to a green hydrogen economy (Figure 4). Most research and policy efforts to realize an emerging green hydrogen economy have primarily focused upon green hydrogen production. However, our work demonstrates the need to develop hydrogen carriers to support a green hydrogen supply chain. Formic acid arose from our analysis as a promising hydrogen carrier, but additional research efforts are needed to improve CO₂ electrolysis technology for producing green formic acid at an industrial scale. In the short-term, more fundamental CO₂ electrolysis research is still needed to better understand reaction mechanisms, explore alternative anodic reactions, elucidate key interface interactions, identify causes of cell degradation, and develop improved reactor configurations. Additionally, superior high stability catalyst and membrane materials should be explored to improve Faradaic efficiency, current density, and reduce overpotential. Further techno-economic analyses (TEA) as well as life cycle assessments (LCA) will need to be conducted as electrochemical formic acid production technology develops and other novel hydrogen carrier candidates are discovered. In the long-term, scale-up efforts will be critical as larger electrolyzer stacks can pose unique challenges that are often avoided on a smaller laboratory scale. For example, electrolyzer stacks on the kW scale or larger will likely require cooling to avoid membrane degradation and the

pressure drop between the inlet and outlet also becomes a much larger concern. Heat and pressure management will require engineering solutions at industrial relevant scales.

In parallel with research efforts, robust policies will need to be deployed to establish a hospitable market environment for commercial electrochemical formic acid production. Both direct and indirect financial support for CO_2 electrolysis technology via subsidies and tax incentives will encourage the emergence of start-up companies. In the U.S., the recently increased 45Q tax credits provide 85 USD/MT carbon captured and stored and 180 USD/MT carbon captured via direct air capture.⁶⁰ These tax credits now have a direct pay option and credit transferability which significantly improves their accessibility. The eligibility threshold for the 45Q tax credit has also recently been reduced under the Inflation reduction Act, promoting broadened adoption of carbon capture technologies. The potential application of this tax credit to both the CO_2 feedstock for electrochemical formic acid production and the carbon capture unit on the formic acid cracker used to liberate the hydrogen further incentivizes the use of formic acid as a hydrogen carrier.

The rapid reduction in the cost of renewable electricity is a direct result of a multi-decade international subsidization effort. Additional financial support for renewable electricity can continue to drive down electricity production costs. Clean electricity cost targets such as those established by the U.S. Department of Energy's SunShot 2030 initiative also helps mobilize an organized effort to reduce electricity generation prices. Similar efforts should continue to be pursued in the future to accelerate innovation. Simultaneously, financial support for green hydrogen like the DOE Hydrogen Shot (1 USD kg_{H2}⁻¹) should be pursued. However, future efforts should place greater emphasis on the entire green hydrogen supply chain rather than solely focusing upon green hydrogen production.

As market penetration begins in the intermediate term, hydrogen carrier infrastructure planning and financing will become critical for the establishment of the green hydrogen economy at scale. At this stage, pipeline and/or rail infrastructure should be pursued to allow large quantities of green hydrogen to be moved more efficiently. Retrofitting old fossil gas infrastructure to accommodate green hydrogen offers a path to potentially reduce the capital cost of this new infrastructure. Viable opportunities for underground storage of hydrogen should also be pursued at this stage. Up to 250 tonnes of H₂ are typically stored in above-ground cryogenic tanks, but at larger scales (up to 3,000 tonnes), geologic storage may be more appropriate if suitable storage sites can be identified.⁷ Additionally, the grid capacity will need to grow considerably to support the green hydrogen economy, and this will require substantial investment over the next few decades. The recent passage of the U.S. bipartisan Infrastructure Investment and Jobs Act allocates over 10 billion USD for this effort demonstrating meaningful investments are already being made to upgrade grid infrastructure.⁶¹

As infrastructure becomes established and the green hydrogen market grows, the prospect of global hydrogen trading should be considered. With the aid of an appropriate

hydrogen carrier, ships could be developed to efficiently transport green hydrogen overseas. Additionally, pipeline or rail infrastructure could achieve green hydrogen trading between neighboring countries. The establishment of a globalized green hydrogen economy will be critical to achieve rapid global decarbonization and green hydrogen carriers are the cornerstone to accomplishing this in an economical fashion.



Figure 4: Suggested research and policy focus areas across three time scales for establishing a green hydrogen economy.

Conclusion

There is a clear need to identify a cost-effective method for green hydrogen delivery to establish a green hydrogen economy and achieve net zero emissions. Four of the most promising green hydrogen carriers, i.e., formic acid, ammonia, methanol, and toluene/MCH, were evaluated as affordable alternatives to molecular hydrogen. Formic acid produced via electrolysis is the most affordable green carrier, offers the safest logistics, and is the only green carrier that is more affordable than its fossil-based counterpart. However, additional maturation of CO₂ electrolysis technology on par with water electrolyzers will be needed. The findings and outlook

presented in this work can be used to guide future policy, investment, and research aimed at delivering hydrogen to reduce emissions in a timely and cost-effective manner.

Methods

Green Formic Acid Production Costs

The electrolyzer model used in this work was based on our previously published electrochemical production model (Supplementary Discussion 1).⁶² Some adjustments were made to more closely capture the true costs of electrolysis (Supplementary Table 4). Electrochemical production costs were determined using this model by numerically evaluating the product price required to achieve a net present value of 0 at the end of the 20-year plant lifespan. The formic acid production model consisted of an anion exchange membrane CO₂ electrolyzer in tandem with a distillation unit. The protonation process used to convert formate into formic acid was not evaluated in this work. Formic acid distillation costs were evaluated using the Aspen Plus Economic Analyzer plug-in using proprietary knowledge provided courtesy of OCOChem. The cell voltage associated with formic acid production via CO₂ electrolysis was determined using our previously published voltammetric model assuming a membrane electrode assembly configuration.⁶² Other performance parameters were based upon demonstrated state-of-the-art performance.⁶² The formic acid production model was validated by comparison with previously published techno-economic simulations (Figure S3).

Green Hydrogen Production Costs

The water electrolysis model was constructed by modifying the in-house electrolysis model used for formic acid production with performance parameters provided by the DOE H2A model "Current Distributed" case (Supplementary Table 5).³⁶ These performance parameters reflect that achieved for state-of-the-art polymer electrolyte membrane water electrolyzers. Like green formic acid, the production costs of green hydrogen were determined by numerically evaluating the product price needed to achieve a net present value of 0 at the end of the 20-year lifespan. Molecular hydrogen was assumed to exit the water electrolyzer. The production costs for green hydrogen were determined with input from an independent industry partner with expertise in utility-scale hydrogen production to ensure accuracy.

Green Ammonia and Green Methanol Production Costs

To estimate the costs for green ammonia and green methanol production, the modeled green hydrogen production costs were implemented into previously constructed models for green ammonia and green methanol production and the results were averaged (Supplementary Discussion 1).^{39,42,43,63} To identify suitable models for green ammonia and green methanol

production, a literature survey from 2016 to 2021 was performed. A variety of cutoff criteria were imposed to ensure suitability for this work. This criteria included: (1) utilized water electrolysis to produce a hydrogen feedstock; (2) reported a sufficient cost breakdown so that our water electrolysis model could be implemented to replace the previous model for green hydrogen production; (3) reported costs associated with onsite storage at the production facility or did not model storage costs so that our simulated storage cost could be implemented; (4) modeled a production scale within range of the scaling relationships used in this work. The results of the modified green ammonia and green methanol models identified via the literature survey are tabulated in Supplementary Table 5 and 6 respectively.

Other Supply Chain Costs

The transmission, storage and decomposition cost information were obtained from previously published literature and was adjusted to meet the parameters defined in this study (Supplementary Discussion 2, 3, and 4). Carbon capture costs were obtained by modifying our previously published pressure swing adsorption model (Supplementary Discussion 4).⁶²

Supporting Information

Detailed model description with additional techno-economic and safety analysis.

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Author Contributions

B. S. C. performed the techno-economic assessment and wrote the first draft of the manuscript. T. B. provided commercial insight and perspective to the design of the supply-chain. R. S. W. provided information on hydrogen carrier decomposition and scaling relationships. F. J. revised the manuscript and supervised the project. All authors edited the final version of this manuscript.

Competing Interests

Todd Brix is the Founder and Chief Executive Officer of OCO Chem Inc., a company that has commercial interest in electrochemical formic acid production.

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