Liquid Organic Hydrogen Carriers (LOHCs) for Trucking

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1 Motivation:

The costs associated with hydrogen production, distribution, and storage have been studied in detail by our group for the long-haul trucking applications. The results can be found under "Hydrogen: Overview" listed **here** . Our analysis shows that the cost of delivery and refuelling are major contributors to the cost of hydrogen at the gas station. This is primarily because hydrogen needs to be either compressed or liquefied before it can be transported and used as fuel. The predicted hydrogen price for the long-term scenario (2050) is higher than $4/Kg, which is insufficient to out-compete diesel. Therefore, it is clear that we need to develop alternate methods to transport and utilize hydrogen.

2 Background:

Liquid organic hydrogen carriers (LOHCs) are chemicals that can be reversibly hydrogenated or de-hydrogenated to capture and release hydrogen as needed. There are several potential molecules such as methylcyclohexane (MCH), di/mono benzyl toluene (DBT, MBT) which function as LOHCs. The energy density varies for each molecule but is around 1.8 kWh/L. The key advantages motivating the use of LOHCs to transport hydrogen are as follows:

- **Liquid Fuel:** Existing fuel distribution infrastructure has been optimized for room-temperature liquid fuels such as diesel and gasoline. Distribution of hydrogen via LOHCs allows us to take advantage of the existing infrastructure. Given the fast-approaching emission targets, it is important to develop technologies that can be easily scaled. LOHCs don't need a new distribution network which is both expensive and time-consuming build.
- **Easy to store:** LOHCs boast excellent thermal stability and have low vapor pressures. Therefore, it offers a convenient and cheap solution for hydrogen storage. Easier storage would enable local inventories (at gas stations) adding much-needed robustness to the supply chain. Low storage costs also enable long-distance shipments allowing procurement from the most competitive hydrogen sources globally.
- **Availability of LOHCs:** LOHC molecules such as MCH and DBT are commercially manufactured chemicals. They are inexpensive and are already being produced in large volumes, making them conducive to applications such as long-haul trucking.
- **Scientific maturity of the field:** The hydrogenation and de-hydrogenation steps for LOHCs are well studied. Existing literature has identified high activity catalysts and optimized reaction conditions for both steps [3, 4, 8]. Full-scale hydrogen generation plants that utilize LOHC have already been deployed, proving the readiness of the technology for a large-scale commercial application [1, 7].

Based on the advantages listed above, it is clear how LOHCs can help the hydrogen distribution and storage challenge. Currently, the LOHC hydrogenation is performed at a centralized plant, then it is shipped to smaller distribution centers where the dehydrogenation step occurs, releasing hydrogen that is supplied to the end-users. Several techno-economic studies have evaluated this LOHC-based hydrogen supply chain and found it to be competitive against other hydrogen distribution methods, especially for long-range distribution [2, 5]. Despite these benefits, LOHCs are still not competitive enough to replace diesel. The major pain points when it comes to applying LOHCs to long-haul transportation are as follows:

- The highly endothermic dehydrogenation step is a major contributor to total costs. Roughly 30% of the energy content of the hydrogen released from the LOHC is consumed during de-hydrogenation.
- The hydrogen liberated post dehydrogenation must be compressed before it can be used as fuel for trucks. The price of the compressor and ancillary units can cost upwards of US$ 1 million, in addition to the energy cost associated with compressing the hydrogen [2]. The sizeable up-front capital investment required to add hydrogen compressors to existing gas stations, which are often small businesses, is a deterrent to wide scale-acceptance.

3 Project Aims:

3.1 Drive-train Design:

We propose a modified distribution scheme as shown in Figure 1 where the de-hydrogenation step will be performed on the truck.

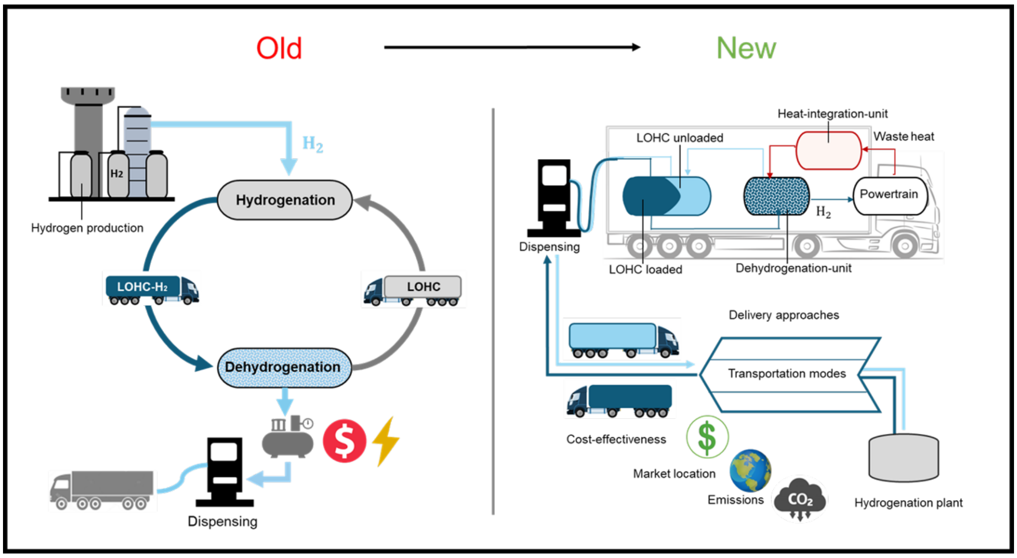

Figure 1: The proposed change in the LOHC supply chain: perform LOHC de-hydrogenation on the truck.

The above-proposed scheme will help address the major pain points discussed before. The new design allows the inclusion of a waste-heat recovery (WHR) loop that can at least partially drive de-hydrogenation, severely reducing the 30% penalty. It completely eliminates the need for compression, as hydrogen is generated onboard. In addition, gas stations and truck drivers will only need to handle liquids, as they already do, making the switch from traditional fossil fuels to LOHCs much easier. LOHC for trucking has only been lightly considered in the existing literature: an experimental prototype built in a lab in 1985 demonstrated a truck can be powered by LOHC, but that prototype had several problems [6]. There have since been several advances in understanding, technology, and computer modeling making us confident in our ability to build a much better powertrain design. There are several choices involved in designing the powertrain which are not only dictated by system efficiency, but also practical considerations such as robustness. A few critical choices are briefly discussed below:

- **Internal combustion engine (ICE) vs Fuel Cell:** Fuel cells have a higher efficiency compared to ICEs when considered as an independent system. However, for this application, we are interested in the overall system efficiency making the choice non-trivial. Combustion engines operate at higher temperatures allowing ICEs to benefit from higher WHR than fuel cells. In addition, fuel cells require high purity hydrogen which might necessitate additional purification steps, reducing overall efficiency. System design requires systematic evaluation of the overall system efficiency for both options.
- **Optimizing operating gears:** Traditional optimization for optimal gears only considers engine efficiency. However, in this case the overall system efficiency is the objective

and it includes WHR. Therefore, we need to consider the temperature of the exhaust while choosing the optimal gears. There maybe potential to have significantly higher exhaust temperatures with minor sacrifices to engine efficiency, thereby improving overall efficiency.

- **WHR system sizing:** Designing a system to extract more waste heat is often more expensive as components such as heat-exchangers have to be larger. Therefore, we see that there is a trade-off between fuel efficiency and cost of drivetrain. The aim is to minimize the total cost of ownership over the 10 year lifetime of the truck. It is an optimization problem where we need to maximize the savings from fuel (operating cost) without making the capital cost to build truck exorbitantly high.

3.2 Technoeconomics:

We will expand our previous study on hydrogen production and distribution methods to include LOHCs. The study will consider the novel drivetrain design proposed in the previous section to calculate the cost of LOHC at the gas station today and in the future. Forecasting hydrogen distribution via LOHCs is significantly different than cryo or compressed hydrogen. For example, as a liquid fuel it has low barrier to adoption which influences the market penetration rates. In addition, we will also evaluate the base case LOHC distribution scheme which involves de-hydrogenation at the gas-station, followed by compression before the hydrogen is used as fuel. The aim is to make a fair comparison amongst all the available hydrogen technologies and help identify a suitable fuel for the future.

References

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