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Research Article

Elias Andraos[1], Guido Merino[1], Maximilian Ritter[2]

[1]Department of Chemistry, McGill University, Montreal, QC, Canada
[2]Berufskolleg Hilden des Kreises Mettmann, Am Holterhöfchen 34, 40724 Hilden, Germany

Eco-Audit of MOFs as H_2 Storage Materials for Vehicle Applications, Using Novel Refueling Model

Keywords

Metal-organic framework, Ni-MOF-74, hydrogen storage, fuel cell vehicles, vehicular hydrogen storage, exergy

Email Correspondence

elias.andraos@mail.mcgill.ca

Abstract

Metal-organic frameworks (MOFs) are a heavily researched candidate for fuel-cell electric vehicle (FCEV) hydrogen storage. However, little analysis has been done on the environmental impact of potential MOF vehicles compared to established alternative vehicles, such as compressed hydrogen or battery-electric vehicles. In this work, a preliminary eco-audit was conducted for a FCEV using an MOF hydrogen storage system based the best current MOF Ni_2(*m*-dobdc) (Ni-MOF-74). (1) Cost and environmental impact analyses were performed for both the production and use phases of an MOF-FCEV. The cost and environmental impact of MOF production was compared to that of Lithium Nickel Manganese Cobalt Oxide (LiNMCO) batteries, the current state-of-the-art for BEVs. (2) Environmental impact was assessed using embodied energy estimates based on reported values for LiNMCO BEVs. These highlighted MOF vehicles as a competitor to current renewable energy vehicle technologies. For the use phase, a hydrogen refueling station that produces hydrogen onsite by proton exchange membrane (PEM) electrolysis from grid electricity was compared to an equivalent population of battery electric vehicles (BEVs) charged at distributed recharging stations. FCEVs using the proposed refueling model were able to compete with BEVs both in terms of electricity CO_2 footprint and cost in the simulated solar-dominated Californian grid, but not in the hydro- and nuclear-heavy Ontario grid.

Introduction

Hydrogen has received much attention as a renewable vehicle fuel due to its high specific energy and potentially low footprint of production. (3) The main challenge facing its application as a vehicle fuel is its low volumetric density. Current applications use either heavily compressed (350-700 bar) or cryogenic hydrogen, both of which come with a heavy energy penalty. (4) Even the theoretical minimum thermodynamic values for intense compression or liquefaction are a significant fraction of the specific energy of hydrogen, making possible alternatives to simple physical storage systems attractive. Chemical approaches to increase the energy density of hydrogen broadly fall into 4 categories: hydrogenation of organic molecules, synthesis of hydrogen-rich small molecules, metal hydrides, or adsorption. (5) Adsorption-based storage systems, as depicted in Figure 1, rely on the adsorption-desorption equilibrium to lower the gaseous pressure of H_2. In a material with a high surface area and a low skeletal volume, this can increase the possible volumetric density of the gas compared to empty space at the same pressure. Current candidates for adsorption-based hydrogen systems for fuel cell electric vehicles (FCEV) include graphene, multi-walled carbon nanotubes (MWCNTs), and metal-organic frameworks (MOFs). (6)

MOFs

MOFs have been examined as a hydrogen storage solution since the discovery of hydrogen physisorption in MOF-5 in 2003. (7) MOFs are excellent candidates for hydrogen storage by physisorption as they have exceptionally high specific surface areas (up to 2900 m^2/g, compared to 805 m^2/g for MWCNTs). (8) For on-board storage, the volumetric capacity is of greater concern than the gravimetric capacity, but the densities of MOFs and other adsorptive media are similar enough to make the surface area per weight a reasonable proxy. Additionally, MOFs are more thermally stable than carbon nanotubes and other high-surface area materials. (6)

MOFs are a class of material which form highly organized one-, two- or most commonly three-dimensional structures comprised of metal ions or clusters coordinated to organic ligands. MOFs are extremely porous due to the coordination geometry around the metal and the shape of the organic linker. The high variability in the cluster or linkage selection for MOF synthesis allows for the control of its characteristics, such as the quantity of available adsorption sites. (9) These properties make MOFs an attractive candidate for hydrogen storage via adsorption. Fine control over energies of adsorption and desorption is needed to provide both high H_2 bonding at high pressures as well as fast H_2 release at low pressures. (10) Additionally, the wide range of combinations of potential metals and organic ligands allows for a variety of methods for synthesis, making scale-up for industrial production easier.

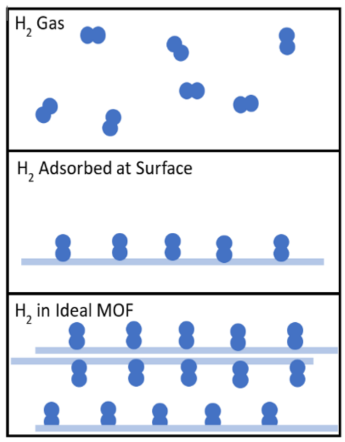

Figure 1. Schematic showing principle behind adsorptive H_2 storage. While it is counterintuitive that more H_2 can be fit into a space also containing an MOF, the lowering of pressure through adsorption allows a significant increase in g H_2/L.

Although MOFs have not yet been commercialized for vehicular gas storage, MOFs are available for other commercial uses and research is being devoted to minimizing the environmental impact of MOF synthesis. Other than solvothermal synthesis in an organic solvent, MOFs have been pre pared by aqueous synthesis (11) and by mechanochemical methods such as liquid-assisted grinding. (12) Although MOFs with high gravimetric capacities have not yet been produced with the latter method, recent advances have been made, such as the use of salt additives to enhance mechanosynthesis. (12) We assume that it will be a comparable method to the current solvothermal synthesis approach and can thus be considered a feasible synthesis method for this preliminary analysis. Current state-of-the-art MOFs achieve gravimetric capacities of up to 10 wt.% and volumetric capacities of up to 40 gH_2/L, at a pressure swing from 5 to 100 bar and a temperature of 77 K. (8)

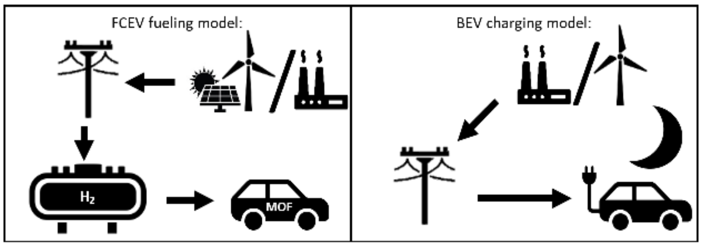

Figure 2. Proposed MOF-FCEV refueling model compared to model of current BEV charging. The low pressure required for MOF-FCEVs compared to traditional FCEVs means that no significant compressionis required between bulk storage and vehicle refueling. This allows complete flexibility in terms of electricity usage times, unlike conventional high-pressure FCEV refueling which requires significant compression shortly before refueling.

Proposed Refueling Model

Due to the thermodynamic efficiency limits of hydrogen production by electrolysis and hydrogen oxidation by fuel cells, even an ideal hydrogen storage solution will not rival the cycle efficiency of a battery system. (13) An advantage of using hydrogen that may make up for this is that it can be stored between its production by electrolysis and used in vehicles, compared to BEVs, which must draw electricity from the grid while charging. Many current electrical grids have a significant share of renewable energy sources but rely on non-renewable energy, instead of energy storage, for times when renewable energy cannot meet demand. In such grids, CO_2 footprint and cost of electricity will vary significantly over timescales as short as hours. Drawing energy from the grid at a time when it is produced with a low carbon footprint before storing this energy may lead to a lower footprint even if more electricity is used overall. Considering that most battery electric vehicles are charged overnight due to long charging time, (14) grids with an abundance of solar energy during the day may be an ideal target for such a FCEV refueling model.

Using MOF vehicle hydrogen storage is crucial to this model, as the lower operational pressures lower the energy requirements of hydrogen preparation. Additionally, current state-of-the-art refueling stations (for 350-700 bar vehicles) keep the majority of their hydrogen at a lower pressure in storage tanks before compressing it into short-term buffer tanks for use, (15) which must draw electricity at the time of demand instead of being able to wait for ideal conditions.

Ni_2(dobdc) cost. (16) This calculation was done considering two different synthesis methods for the MOF: liquid assisted grinding (LAG) and solvothermal. The total weight of MOF needed to adsorb the assumed 5.6 kg of H_2 for a full vehicle tank was determined by the reported 2.2 wt % hydrogen storage capacity of Ni_2(*m*-dobdc). (16) The cost of a storage system using MOFs as hydrogen storage was previously modeled. (18) To incorporate the cost of the MOF material estimated in this report to the production cost of the storage system, the price for the material was replaced by the calculated production cost of the required Ni_2(*m*-dobdc) to yield the total storage system cost. The hydrogen storage system must be attached to a fuel cell to complete the power supply system of the MOF-FCEV. In this case, a proton exchange membrane (PEM) fuel cell of 80 kW for light duty vehicles was assumed to be the fuel cell of choice as this technology is currently used for on-road light-duty vehicles and is considered by literature to estimate future fuel cell system production and manufacturing costs. (19) To complete the total production cost of a MOF-FCEV, an additional cost of $22,352 (CAD) was assumed for other auto parts (including heating, ventilation, braking system, etc) and mark-up percentages for the power supply production, marketing, warranty and profit costs taken from literature. (19) The calculated cost for the MOF-FCEV was compared to the production cost of a current LiNMCO battery electric vehicle of same power as the MOF-FCEV fuel cell based on costs calculated by Berckmans et al. (Table 1), which include profit margins of production. (20) Furthermore, the MOF-FCEV was compared to a FCEV for which the total cost was calculated following the same assumptions as the MOF-FCEV, where the cost of the MOF storage system was replaced with that for a type 4 compressed hydrogen storage system. The compressed hydrogen storage system is used by the literature for cost projections of future light-duty fuel cell vehicles. (18)

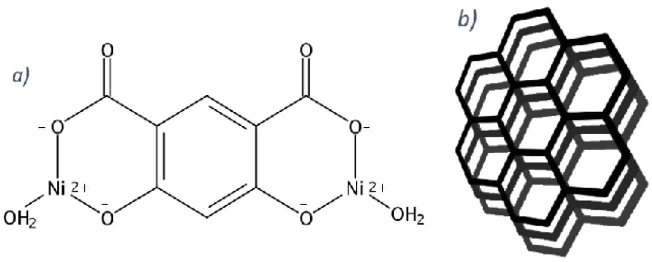

Figure 3. a) Nickel metal clusters coordinated to the organic linker (H_4(m-dobdc)) which constitute the Ni-MOF-74. The clusters are coordinated in three directions to form b) hexagonal sheets that stack vertically with noncovalent interactions.

	Value	Unit
Production rate for vehicle components	500 000	Systems/year
PEM Fuel cell efficiency(19)	0.6	kWh/kWh
Electric vehicle efficiency(19)	0.3	kWh/km
PEM Fuel Cell cost rate for 80 kW low duty vehicle(17)	45	$USD/kW
mark up factor for power supply production(17)	1.17	
mark up factor for Marketing /warranty and profit(17)	1.29	
Lithium ion BEV cost of production (from NMC BEV)(18)	466	$/kWh

Table 1. Key assumed values used for the calculation of the total cost of production of the various power supplies for electric vehicles.

Methods

Production Model

The production cost of a fuel cell electric vehicle with MOFs as hydrogen storage (MOF-FCEV) was estimated by the sum of literature and estimated production costs for the separate vehicle components constituting an MOF-FCEV. The production cost of the MOF material needed was modeled for the best current MOF (1) Ni_2(*m*-dobdc) (Figure 3) by calculating the factor relating the literature values for Mg_2(dobdc) (Mg-MOF-74) MOF cost (16) to the Mg_2(*m*-dobdc) cost (17) and applying it to the

To assess the energetic impact of MOF-FCEV production, an estimation on the total embodied energy of production of a MOF-FCEV power supply (i.e: the MOF storage system and the PEM fuel cell) was conducted. The embodied energy of production for the MOF material was determined by exergy approximation, using literature values for the MOF embodied energy to attempt an estimate of the embodied energy for the specific best current MOF Ni_2(*m*-dobdc). (21)

Exergy estimates the energy needed to produce a material by considering the maximum amount of work required to produce it as the minimum amount of work required to produce the material. (22) In other words, it assumes ideal values for the energy usage in production of a material. Furthermore, exergy calculations for materials assumes the exergy lost during a reaction to be equivalent to Gibbs energy of formation. The calculation needed to determine the total exergy of a material therefore involves summing the exergies of the elements it is comprised of and the Gibbs energy of formation, as seen in Equation 1. (22)

$$b_{cd} = b_c + b_d + \Delta G_{f,cd}$$

Equation 1. Exergy calculation for a material, where b is the exergy value, delta G is the Gibbs energy of formation, and 'c' and 'd' are the elements reacting to produce material 'cd'.

To use exergy as an approximation, the exergy of the same reference MOF used in the cost analysis (Mg-MOF-74) was calculated from literature values (22,23) and related to its literature embodied energy (21) by calculating a correlation factor. We assumed that the synthesis methods for Mg-MOF-74 and Ni-MOF-74 were identical to offer an adequate comparison between embodied energies and exergies of material production. The calculated factor was applied to the exergy value calculated for Ni_2(*m*-dobdc) to obtain an estimated embodied energy of production. To calculate the total embodied energy of the power supply for a MOF-FCEV, the storage system required for MOF was assumed to be comparable to a Type 3 (350 bar) compressed hydrogen storage system. It was compared to a Type 3 system, which includes the fewest undesired components for a hypothetical MOF-FCEV storage system compared to other compressed hydrogen systems. Additionally, the embodied energy required to manufacture the storage system per weight was readily available in literature (see Table 2), which was used to calculate the embodied energy of its production. Furthermore, the embodied energy for production of the PEM fuel cell in the power supply system of the MOF-FCEV was calculated from 'case 3 of production' literature values (see Table 2), which assumes a mix in electricity grid composition going towards production of the PEM fuel cell and 75% recycling of the platinum group metals used in production. (24)

This estimated total embodied energy of production was compared to that of a FCEV power supply made with the same PEM fuel cell as the MOF-FCEV power supply but with a type 4 (700 bar) compressed hydrogen storage system. As previously mentioned, this is the hydrogen storage system used by most literature for cost projections of future light-duty fuel cell vehicles, for which embodied energy values can be seen in Table 2. The MOF-FCEV power supply was also compared to a LiNMCO BEV battery, for which the total embodied energy was calculated using the average embodied energy of manufacturing (Table 2).

	Value	Units
Embodied energy for storage system (Type 3) production(25)	0.138	MJ/kg
Embodied Energy for a Type 4 (700 bar) hydrogen storage tank(25)	16.2	MJ/tank
case 3 estimated PEM embodied energy(24)	744	MJ/kW
LCO embodied energy(26)	320	MJ/kW
Li ion Battery production embodied energy (average)(27)	2318	MJ/kWh
Literature MOF Embodied energy(20)	91300	MJ/ton

Table 2. Key assumed values used for the calculation of the total embodied energy of various power supplies for electric vehicles.

Use Model

As shown in Figure 2, the model used is a refueling station that produces H_2 onsite by electrolysis during peak renewables capacity. H_2 is stored at 100 bar in traditional storage, until it is cooled to 198 K shortly before being filled into vehicle MOF tanks. On-site electrolysis capacity was modelled to be between 1500 and 2000 kW, falling well within a reasonable cost range for a refueling station (using an estimate of $323/kW for mass-produced PEM electrolyzers.) (27) Energy for hydrogen compression and cooling was calculated using tabulated values (28) that assume ideal gas behavior of H_2. Calculated values were compared to values from literature (4) to confirm that this assumption is reasonable over the range of conditions of operation (Table 1). H_2 demand for vehicle refueling was modelled after USA gas station demand data from Nexant Inc. 2008, (29) as reported in Grouset et al. 2018. (30) Battery vehicle charging demand was modelled after Fig 11. from Schey et al. 2012 (digitized using ImageJ). (14) Station tank capacity was modelled after gas station underground tank sizes ranging from 12000-24000 gallons. (31)

Quantity	Value	Unit
Ideal Energy of Isentropic Compression to 700 bar[1]	2.38	kWh/kgH_2
Real Energy of Compression to 700 bar[1]	2.72 - 7.42	kWh/kgH_2
Ideal Energy of H_2 Liquefaction[1]	3.9	kWh/kgH_2
Ideal Energy of Isothermal Compression to 700 bar[2]	2.25	kWh/kgH_2
Ideal Energy of Isothermal Compression to 100 bar[2]	1.58	kWh/kgH_2
Compressor Pump Efficiency[1]	92	%
Ideal Energy of Isobaric Cooling from 300 to 200 K [2]	0.41	kWh/kgH_2
Total Energy needed for H_2 Preparation before FCEV fueling[2]	2.13	kWh/kgH_2

Table 3. Thermodynamic Calculations for Preparation of H_2 before FCEV fueling. 1) From Gardiner 2009 2) Own calculations, assuming ideal gas. All compression calculations assume H_2 source at 1 bar.

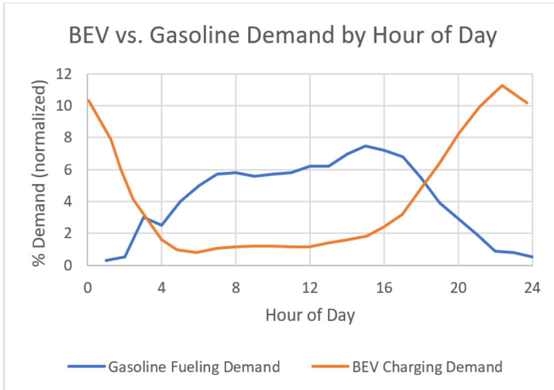

Figure 4. Demand models for gasoline refueling (29,30) and BEV charging. (14)

CO_2 footprint and cost of electricity use were compared using best-case and worst-case numbers for different electricity sources. (32) The compilation of these numbers was provided as class material by Prof. McCalla, and a copy of the table with individual sources can be found in the Supporting Information. CO_2 footprint per kWh was calculated according to Equation 2. Cost per kWh was calculated using estimates for delivered cost of individual electricity types, as actual pricing schemes varied between Ontario and California, and varied by type of consumer.

$$TotalCO_2intensity\left(\frac{kg}{kWh}\right) = CO_2int.fuel\left(\frac{kg}{kWh}\right) + \frac{CO_2int.construction(\frac{kg}{kW})}{plantlifespan(h)*capacityfactor}$$

Equation 2. Total CO_2 intensity as calculated from values in Information Pack.

Geothermal energy was excluded as no estimate for delivered cost was present in the data set. Because hourly averages of the power grid composition lack information about intermittent power sources such as wind (see Figure 4), the model calculated the energy used hour-by-hour over one year using data from 2019 from Ontario and California. (33,34) California is a prime example of an electrical grid with a large percentage of renewables without adequate grid storage, resulting in a large difference in CO_2 footprint across the day. Ontario was chosen as a reference for a more diverse grid, with significant contribution from low-impact nuclear and hydro sources (see SI for raw grid composition data).

The model used to represent the optimization of electricity use by the refueling station was relatively simple. Electricity was drawn from the grid to produce hydrogen if the hourly carbon footprint was lower than the average of the twelve hours before and after. While a real refueling station would not have exact grid composition data available for the future, weather forecasts provide a decent estimate of the amount of wind and solar energy that will be available within 12 hours. Additionally, electricity would be used at suboptimal hours (i.e. when the footprint of energy production is higher) if the station tank reached a minimum threshold. Better performance could be achieved with larger electrolyzer capacity used over a shorter time every day, but this cost-benefit analysis is outside of the scope of this project. Optimization of cost was also considered but losses in carbon footprint made this option unattractive (see model in SI).

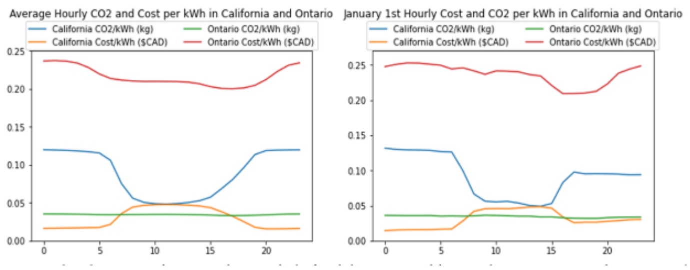

Figure 5. Plots showing CO_2 footprint and cost per kWh of grid electricity in California and Ontario, a) averaged over 2019 and b) for January 1st. Other days showed even larger difference (see SI for raw hourly grid data), but Jan. 1st is shown for transparency. Differences show that simply considering hourly averages is too reductive, as renewable energy sources are not regular, especially in the case of wind energy in Ontario.

Results - Eco-Audit

Production – Cost & Embodied Energy comparison

Based on our assumptions, the results show the financial advantage of producing a MOF-FCEVs. As seen in Figure 6, the total cost of production for an electric vehicle using the best current MOF as hydrogen storage is lower than that for a LiNMCO battery electric vehicle but remains higher than the production cost of a fuel cell electric vehicle with a compressed hydrogen storage system. However, the development of an MOF volumetric hydrogen capacity could lower those costs as it would reduce the amount of tank mass needed and thus offer a competitive alternative to compressed hydrogen.

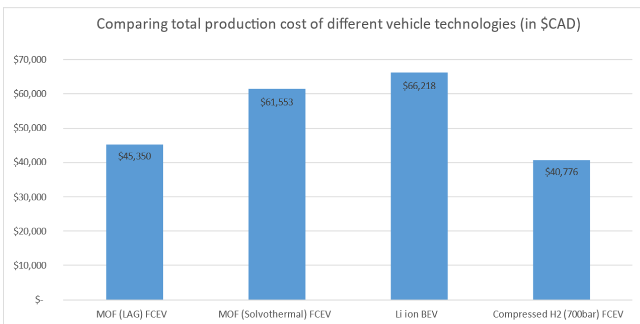

Figure 6. Comparison of the resulting total cost (in $CAD) of vehicle production for different power supply methods and synthesis methods of MOF material.

The total cost of a MOF-FCEV also depends on the synthesis method employed. The most widely used to date for MOF synthesis in MOF research and development is solvothermal synthesis. As seen from Figure 6, the cost of MOF material production increases by roughly $15,000 (CAD) because the synthesis requires expensive organic solvents to dissolve the materials. By modifying the synthesis method to liquid assisted grinding, it was found in literature and demonstrated below that the cost of production greatly lowers because little to no organic solvent is used. (16) Since the development of alternative methods of synthesis promise lower costs in the future, this further confirms the potential of MOF hydrogen storage systems as a competitor to compressed hydrogen fuel cell vehicles.

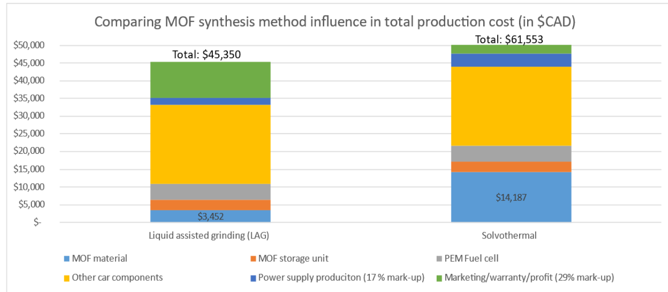

Figure 7. Comparison of the total production costs for two different synthesis methods of the MOF.

The estimated embodied energy of 76 MJ/kg for the $Ni_2(m\text{-dobdc})$ MOF was calculated using the literature embodied energy of 100 MJ/kg for Mg-MOF-74. It was compared to other power supply technologies for electric vehicles to assess the relative environmental impact. As seen in Figure 8, the MOF storage system has a roughly three times lower embodied energy than that of a LiNMCO battery for a battery electric vehicle. Furthermore, the lower embodied energy of Ni-MOF-74 compared to Mg-MOF-74 demonstrates the previously mentioned possibility of developing new MOFs with lower environmental impacts.

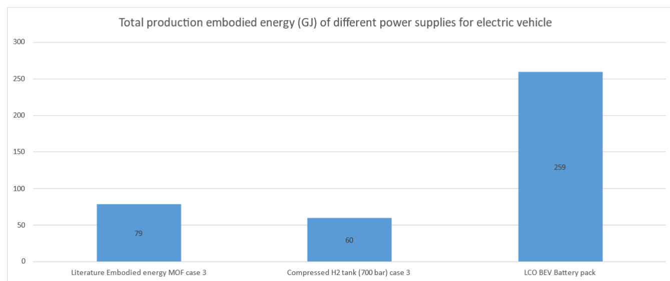

Figure 8. Comparison of the total embodied energy of production of electric vehicles with different power supplies, where the embodied energy for material production for the MOF case was from literature and case 3 denotes the conditions of PEM FC production previously stated.

Like the cost of production results, there is still some modification and optimization needed towards the MOF storage production in order to appropriately compete with current technology. As seen from Figure 9, the MOF material contributes to ~24% of the total embodied energy of production (19 GJ of the total 79 GJ). Therefore, the development of an MOF that would reduce the total mass of the MOF material needed as well as offer a more energy conservative and sustainable synthesis method and increase its viability as an alternative hydrogen storage system for electric vehicles.

Use Phase

The results of refueling model described in the Methods section above are shown in Figure 9. In the solar-dominated Californian grid, MOF-FCEVs can achieve similar carbon footprint values to BEVs, albeit at higher cost (discussed in Limitations below). In Ontario, the fluctuation of renewables, mainly wind, is not enough to make up for the lower efficiency of FCEVs, as shown by both carbon footprint and price.

Based on the cost estimate to produce an MOF-FCEV compared to a BEV and the estimated cost per kilometer driven, we calculated a break-even point of 960,000-740,000 km in California or 310,000 to 150,000 km in Ontario for the LAG-MOF vehicle compared to the BEV vehicle. No lifespan data is available for MOFs for hydrogen storage, but the break-even point for California is well outside of the lifespan of a battery or fuel-cell, Meanwhile, the break-even point for Ontario is approximately equal to or just beyond the lifespan of a battery for a BEV.

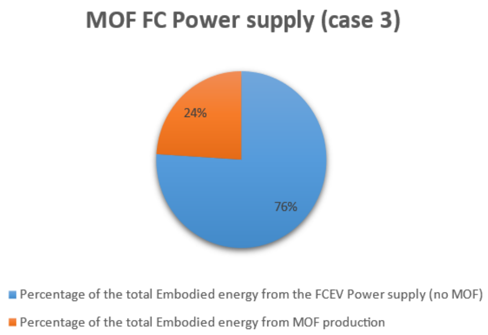

Figure 9. Percentage contribution to the total embodied energy of the fuel cell vehicle power supply by the MOF material.

Comparing the environmental impacts of both the production and use of an MOF-FCEV with a BEV would require additional information, as embodied energy does not translate directly to greenhouse gas emissions. However, based on these separate comparisons of embodied energy of production and CO_2 footprint of use, it is safe to say that MOFs are roughly comparable to BEVs in both production and use phases in terms of cost

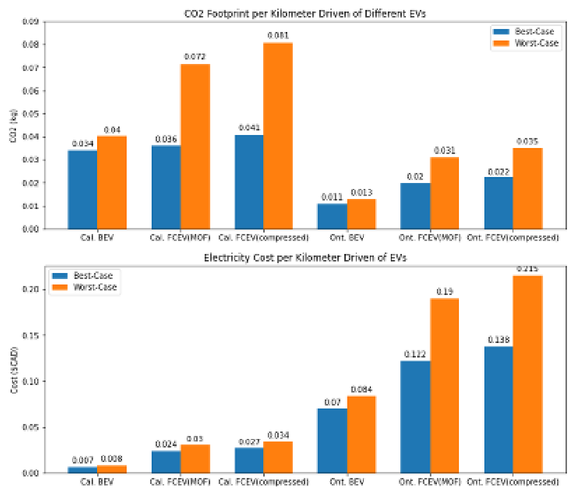

Figure 10. Results of refueling model. FCEV using 700 bar compressed system was added forcomparison, by scaling MOF-FCEV values by factor shown in Table 3. Compressed-H2 FCEV values arelikely underestimated due to the model being tailored towards MOF-FCEVs.

and environmental footprint.

Conclusions

Potential

We believe our estimates and preliminary calculations show that MOF hydrogen storage systems have the potential to compete with battery systems such as the state-of-the-art LiNMCO battery packs for vehicle energy storage, both in terms of CO_2 footprint and cost. Despite the rough estimates made due to lack of data, our modelling approach can be easily refined when more data becomes available. The MOF considered for this model, Ni_2(m-dobdc), is an already synthesized material, and other MOFs that may be better suited for H_2 storage have already been identified in theoretical work. (8)

One technology that may also greatly improve the competitiveness of MOF-FCEVs is high-pressure electrolysis, which might be able to produce hydrogen at pressures high enough for direct use, which eliminates the need for energy-costly compression. (35) MOF-FCEVs might benefit more from this technology than other FCEVs due to lower pressure requirements.

Limitations

As stated previously, multiple values were estimated due to a lack of available data. For the production phase calculations, the exergy-based estimation of the embodied energy of a MOF-FCEV will need to be investigated further before drawing any conclusive statements. The refueling model proposed in the use phase will also need a more thorough proof of concept and experimental verification. However, we do believe that these estimates are enough to show that MOF-FCEVs are a viable alternative to current BEVs. Of course, battery technologies other than LiNMCO batteries are currently used and are being developed for use in EVs, and these may compare more favourably to MOF-FCEVs.

It should be noted that two limitations in this study present a disadvantage to MOF-FCEV. First, the data set used for CO_2 footprint and delivered cost of various energy sources is slightly outdated because newer comparable numbers could not be found for all types of energy production considered. This caused an overestimation of footprint and cost of some technologies, particularly of solar energy, which disadvantaged the FCEV in our model.

Second, the difference in vehicle space and weight requirements were not considered even though they are significant. Despite the mass density of only 2.2% H_2 in the MOF, the total mass needed for hydrogen storage ranges from 175 to 205 kg, while the BEV requires between 365 and 475 kg of batteries. The volume occupied by the energy storage is also markedly better for the MOF-FCEV, with under 0.2 m^3 needed compared to 0.2 to 0.45 m^3 for a BEV. While neither of these values for the MOF-FCEV include the fuel cell, the difference is large enough to show the advantage of an MOF hydrogen storage system over batteries for vehicle design. Despite these differences, both types of vehicles were modelled as having an efficiency of 0.3 kWh/km. (3) Accounting for this difference may significantly improve the results of the MOF-FCEV.

As mentioned above, no degradation data or estimates are available for MOF hydrogen storage systems, so the fuel cell was taken to be the limiting factor in terms of vehicle lifespan. Vehicle maintenance was also not considered. No end-of-life recovery was considered. Li-ion battery recycling is challenging but under development, while no data on MOF recycling was found.

Outlook

As stated above, we believe our work provides a "back of the envelope" estimate showing that MOF hydrogen storage materials have the potential to compete with other forms of power supplies for electric vehicles. This is not news to any of the researchers working in the MOF gas storage field. However, we believe that the value of this work is to provide a simple set of assumptions and calculations, any of which may be challenged, to stimulate further discussion of real-world applications. We provide sources for all our assumptions and calculations should any reader be interested in performing a similar analysis for a different set of materials or environments. We look forward to more data becoming available about the application of MOFs as vehicular hydrogen storage and we hope that this work can provide a starting point for more refined calculations.

Acknowledgements

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Software Used

Calculations and Figures: Microsoft Excel, Jupyter Notebook
Code and raw data available at https://github.com/EA-chem/MOF-FCEV/tree/original/Github%20version
Image digitization: ImageJ

Image Credits

Figure 2: Own composition from built-in Word icons, Electricity Pole and Power plant from Andrejs Kirma from the Noun Project (Creative Commons License)

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