Project Title	Monolithic MOFs for enhanced cryo-adsorbed hydrogen storage
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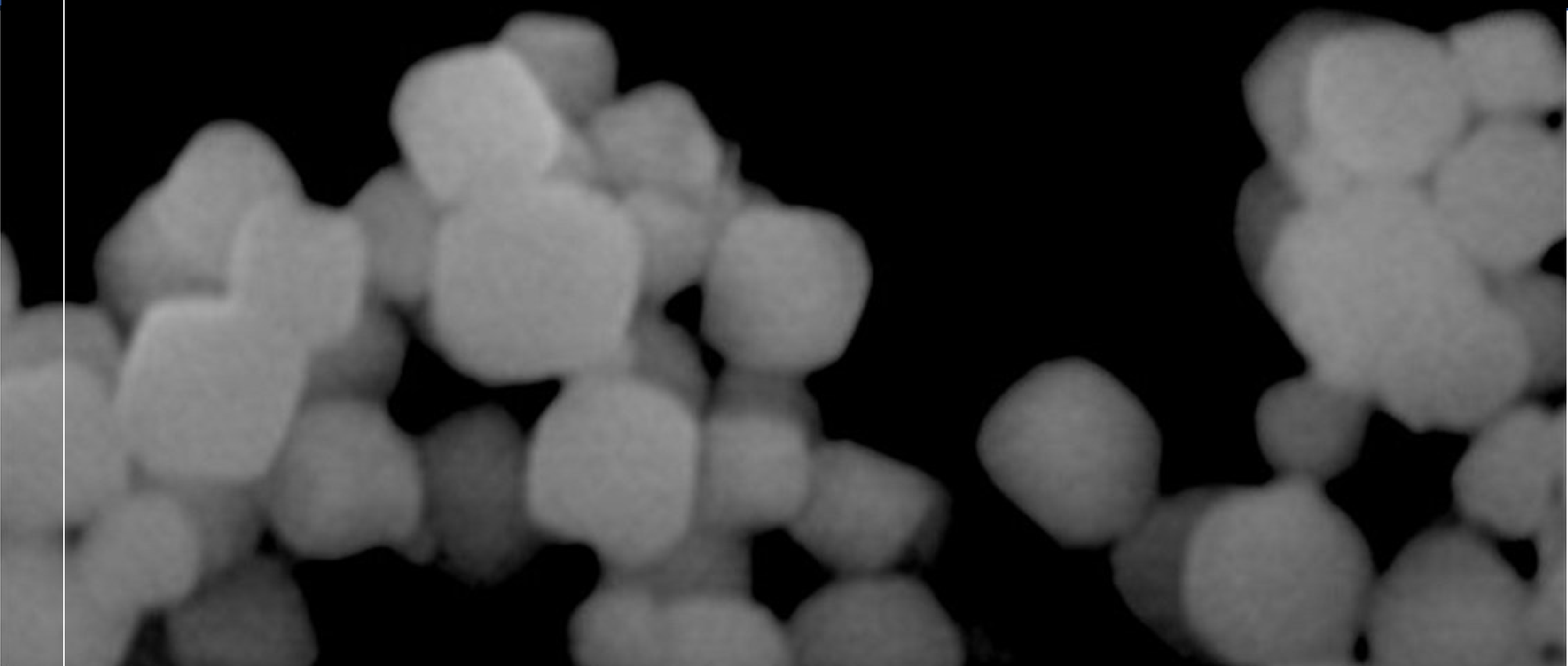
immaterial



Document Summary

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Executive Summary

As a signatory to the Paris Agreement in 2015, the UK has a legally binding obligation to limit global warming well below 2 °C above pre-industrial levels, and is targeting an increase of less than 1.5 °C. The UK government set out further legislation in 2019 committing the UK to a 100% reduction of greenhouse gas emissions by 2050, known as Net Zero. In order to reach this target, society must revolutionise the technologies and processes currently in use.

Hydrogen will play an important role in the decarbonisation of multiple sectors, including industrial, power, heat, and transportation. Current hydrogen demand is predominantly from industrial applications, including ammonia and fuel refining. The use of hydrogen for vehicular transportation presently makes up less than 2% of the global hydrogen market. Forecasting shows that hydrogen use in vehicles should experience the most rapid growth in the coming two decades, however, it is essential that new technologies in this sector are developed to enable this increased demand.

The most significant challenge in creating the hydrogen economy is the development of cost-effective, safe, and environmentally friendly hydrogen storage and transportation methods. A range of on-board storage options exist for the transportation sector, including compressed (gaseous), cryogenic (liquid), cryo-compressed, and chemisorption (chemical storage in hydrides or LOHCs). There are substantial limitations with each of these technologies.

Physisorption – using porous materials to soak up hydrogen and store it at greater volume with reduced pressure - is widely acknowledged to have the potential to overcome these limitations subject to suitable porous materials being developed. The UK, through Immaterial and Cambridge University, is a world-leader in cutting-edge porous materials with the potential to enable this entirely new and highly beneficial type of hydrogen storage. This project aims to demonstrate the viability of a novel materials-based hydrogen storage technology known as cryo-adsorbed. This project focusses on developing cryo-adsorbed technology for on-board fuel storage applications including bus, train, HGV, forklift, and small-scale marine.

In this feasibility study Immaterial set-out to understand how metal-organic frameworks built on its patented ‘monolith’ platform would perform in a real-world system, and whether this would enable significant value propositions for its target markets. Immaterial developed new monolith materials and these have been demonstrated to have world-record breaking storage capacities of 59g/L under benign storage conditions, whilst also being exceptionally robust. Immaterial has developed computational models and system designs using standard multiphysics techniques to ascertain that its cryo-adsorbed system will enable volumetric capacities that are ~40% higher than using 700 bar and more than double 350 bar storage. Due to relatively low pressures used (<100bar), this will enable the use of conformal tanks enabling ideal use of vehicle real-estate.

Immaterial has engaged companies throughout the ecosystem and validated the significance and value of the technology. It has onboarded a range of partners with clear intent to support development and deployment of the technology if it can be proven. The next step will be to build a demonstration unit – a first of a kind monolith-enabled cryo-adsorbed conformal fuel tank that will be installed on a bus, with the demo overseen by OEMs from a range of transport sectors.

Glossary of Terms & Abbreviations

bar	metric unit of pressure equivalent to 100,000 Pa
BET	Brunauer-Emmett-Teller
BETSI	Brunauer-Emmett-Teller Surface Identification
BSOG	Bus Service Operators Grant
CO_2e	carbon dioxide equivalents
DOE	US Department of Energy
e-fuel	synthetic fuel manufactured with carbon capture
EU	European Union
EU Horizon	The EU’s key funding programme for R&D
FCEV	Fuel cell electric vehicle
GCMC	Grand canonical Monte Carlo
Gen	generation
$H_{2(g)}$	Gaseous hydrogen
$H_{2(l)}$	Liquid hydrogen
HGV	Heavy Goods Vehicle
HPVA	High Pressure Volumetric Analyzer
HTS	High-throughput screening
kWh	kilowatt-hour
LOHC	Liquid Organic Hydrogen Carrier
LHV	Lower Heating Value
m-MOF	monolithic Metal-Organic Framework
mbar	millibar
MO	Monitoring Officer
MLI	multi-layered insulation
MOF	Metal Organic Framework
$MtCO_2e$	megaton carbon dioxide equivalent
NCC	National Composites Centre
NIST	National Institute of Standards and Technology
NLDFT	Non-Local Density Functional Theory
NPV	Net Present Value
NREL	National Renewable Energy Laboratory
OEM	Original Equipment Manufacturer
p.a.	per annum
P&ID	Piping and Instrumentation Diagram
Pa	Pascal
PSD	Particle Size Distribution
PXRD	Powder X-Ray Diffraction
rpm	revolutions per minute
SWOT	Strength, Weakness, Opportunity, Threat
t	ton (metric)
TCO	Total Cost of Ownership
TWh	terawatt-hour
WP	work package

Contents

1 Project Overview

1.1 Introduction

Cryo-adsorbed technology has been considered one of the most promising concepts for tackling the intractable problem of low cost, high volume, ergonomic storage of hydrogen for many years. This type of storage uses benign conditions to store hydrogen in a condensed (adsorbed) phase using ultra-porous materials that soak up gas like a sponge soaks up water. Unlike other materials-based solutions this is a physical, not a chemical condensation, and does not require significant energy to return hydrogen to gas phase. It utilises Van der Waals forces, making no changes to the chemistry of hydrogen thus retaining its purity. Immaterial, a Cambridge spin-out, is a world leader in cutting-edge porous materials called metal-organic frameworks (MOFs) and has unique technology – monolithic MOFs - that is enabling this new type of storage for the first time with global implications. The US Department of Energy has been funding cryo-adsorbed technology development although before now, no materials were able to achieve target performance. The significance of Immaterial's cryo-adsorbed technology is well understood.

Immaterial is applying this technology as a new type of fuel tank for transport applications including rail, HGV, bus, forklift, and small marine. In these applications, volume (range) is of critical importance as is total cost of ownership. Immaterial's cryo-adsorbed technology enables more than double the volumetric performance of the current technology in use (350 bar) whilst using conformal (non-cylindrical) tanks, that are lower cost, and cost less to refuel.

The value propositions enabled by Immaterial's technology resonate throughout the value chain. Immaterial has brought together a group of thirty partners, each of which clearly perceives this value from different perspectives – transport OEMs, fleet operators, tank design, hydrogen refuelling infrastructure, energy companies, safety, and specialist technologists from global materials science.

In phase 1 Immaterial set out to develop a computational fluid dynamics model of a cryo-adsorbed system enabled by Immaterial's technology, leading to an initial demonstrator design and technoeconomic model; and to develop and optimise second generation materials with improved performance. The focus of phase 2 will be to demonstrate the technology in the real world through integration with a hydrogen bus, and the demonstration will be overseen by representatives from other transport sectors.

The project builds a unique skills base in the UK and will contribute significantly to the UK's hydrogen and high value manufacturing economies. The pathway to commercialisation is clear with Immaterial and its key partners planning vehicle programmes with companies from each of the target sectors if successful. Immaterial is working with a world leader in cryo hydrogen technology and an existing manufacturer of conformal cryo tanks – a long term partnership for roll-out is envisaged.

1.2 Technical Background

1.2.1 Adsorption and porous materials

Adsorption is the accumulation of a thin layer of gas or liquid molecules (blue) onto the surface of a solid (red/grey), driven by electrostatic attraction. It can be thought of as “forced condensation” as the adsorbed layer behaves like a liquid. Just as in a standard liquid/vapour system, the process is reversible, and the ratio in each phase is determined by the conditions: high pressures and low temperatures favour adsorption, while low pressures and high temperatures favour desorption. Adsorption occurs on any solid surface but is much more significant in porous materials such as zeolites or activated carbons as they have considerably more accessible surface area.

1.2.2 Metal-organic frameworks (MOFs)

Metal-organic frameworks are a class of ultra-porous materials formed from metal ions (spheres) and organic linkers (cuboids). They have modular structures which can be tailored by switching either the metal or the linker with thousands of alternatives. This means properties such as pore size, surface chemistry and stability can be fine-tuned with a freedom not available to other porous materials. They also have the largest surface areas of any material; 1,000-8,000 m2/g vs. 200-800 m2/g for zeolites and silicas [1-3]. This combination of high surface area and tailorable surface chemistry means their adsorptive capacity is considerably higher while at the same time having lower energy requirements to regenerate (desorb) the material.

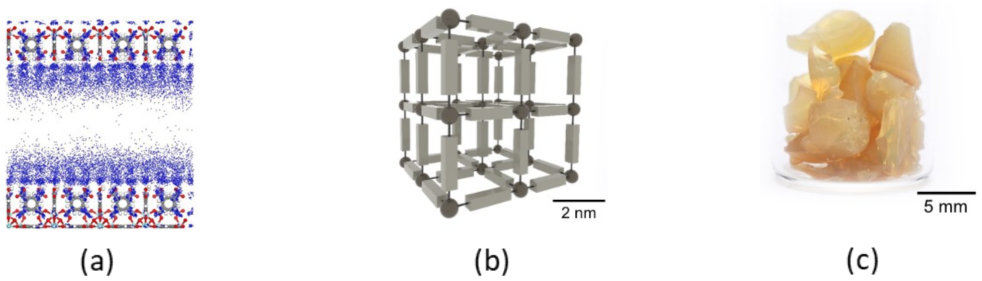

Figure 1(a): Adsorption, (b): Metal-organic framework, (c): the monolith

1.2.3 Cryo-adsorbed hydrogen storage

Cryo-adsorbed hydrogen uses a porous material to store hydrogen at high energy densities, under considerably milder conditions (~80K, <100 bar) than other storage technologies including compressed (350 or 700 bar), cryo-compressed (40-80K, 350-500 bar), and liquid (20K, 1-10 bar). The milder conditions improve safety, technoeconomics, and ergonomics (conformal tank shapes) making cryo-adsorption a highly sought-after solution [4-6] and an enabler for conversion to hydrogen in a range of transport applications.

Metal-organic frameworks (MOFs) are the leading materials choice for cryo-adsorbed hydrogen storage and are named specifically in the HySupply Category 3 competition scope. The development of cryo-adsorbed systems has been championed by the US Department of Energy (DOE), who have funded extensive research into the technology over the past decade [5-14]. Their system-level work has identified the volumetric storage capacity of the porous material as the most important limiting factor in the viability of cryo-adsorption [15-17].

1.2.4 The monolith

MOFs demonstrate excellent potential in a wide range of gas storage and separation applications, however industrial deployment to-date has been limited. The primary reason for this is that existing synthesis techniques produce fine powders, which pack poorly and are unsuited to any application involving a flow of gas. Powders can be bound or pelletised, but binders block pores, occupy mass and volume, and hinder mass transfer in and out of the pellet, often to the point that many performance benefits are erased.

Immaterial's unique, patented technology produces MOFs as crystalline "monoliths". Not only do these overcome the pelletisation problem, but they are also far denser, offering triple the volumetric performance of the native powder [18-23], with gravimetric uptake unchanged. The particle size distribution of the monolith crystals can be controlled to maximise bed packing, with just a 7% void fraction recently demonstrated [23]. The monolith platform technology can be applied to any of the 100,000 known MOF materials, enhancing well-researched materials that have been considered and developed for hydrogen storage.

Our generation 1 monolithic materials demonstrated world-leading volumetric capacity, reaching storage capacities of 45 g/L at 25 bar and 77K. This is already a 22% enhancement over the DOE conceptual (not peer reviewed) record of 37 g/L at 100 bar [9], and exceeds the current EU Horizon's MOF hydrogen target of 40 g/L [24]. This was confirmed by the DOE's own validation lab at NREL. Our generation 2 monolithic materials developed during phase 1 have demonstrated further improvement, reaching storage capacities of 59 g/L at 100 bar and 77K, a 59% enhancement over the DOE record. As such, Immaterial's cryo-adsorbed technology more than doubles the volumetric capacity of 350 bar storage, whilst using conformal tanks at considerably lower pressures. Monolithic MOFs offer a step-change in the volumetric capacity - the single most important system metric - and serve as a key enabling technology for cryo-adsorbed hydrogen.

1.3 Project outline & objectives

Immaterial's critical Phase 1 objectives were a) to understand how metal-organic frameworks built on its patented 'monolith' platform would perform in a real-world system, b) whether this would enable significant value propositions for its target markets, c) understand performance and our ability to tune performance using our optimisation toolbox, d) tune synthesis conditions for low-cost benign production. All objectives have been achieved. Phase 1 has proven the feasibility of Immaterial's monolith-enhanced MOF-based cryo-adsorbed hydrogen storage technology. The storage tank modelled using industry standard computational fluid dynamics software has identified very promising performance at the system level. This model was used as the basis for an initial demonstrator design for a 6 kgH_2 storage tank to be tested in a double deck bus with one of our commercial partners. In parallel to this, generation 2 materials were optimised to further improve storage capacity and robustness, and a high-level technoeconomic analysis was conducted.

Phase 2 involves the detailed design, build and testing of the demonstrator unit in conjunction with research and commercial partners. A more detailed technoeconomic analysis will be completed to ensure the route to market is well understood and to maximise the rollout potential of the technology. In doing so, phase 2 aims to address all five targets of HySupply2:

- Reduce costs of hydrogen supply – through lower refuelling cost.
- Increase carbon saving potential – by enabling hydrogen in hard-to-decarbonise sectors.
- Develop novel technologies to increase market competition – by enabling prized cryo-adsorbed storage.
- Knowledge building to inform policy development – through Immaterial's ecosystem network and advisory board.
- Develop the knowledge and skills required to meet net zero – by transferring the knowledge already developed in the US into the UK supply chain.

Success in phase 2 will significantly advance the state-of-the-art, enabling a novel storage technology with major technoeconomic and safety improvements over existing systems. These outcomes have the potential to constitute an important component of the phased transition towards a low-carbon economy and help meet the UK's net zero emissions target by 2050.

2 Material Optimisation

2.1 Material characterisation

Dynamic behaviour of adsorbent materials includes kinetics, thermal conductivity, specific heat capacity and heat of adsorption. In this section, we described these terms for our monoliths.

2.1.1 Hydrogen Uptake

H_2 adsorption uptake at 77 K and 100 bar of our 1st (MOF-15, MOF-17) and 2nd (MOF-18) generation monoliths shows 45 and 59 g/L, respectively, exceeding the DOE targets (42 g/L at 77 K and 100 bar), and showing world-leading volumetric capacity. These are indeed the highest values reported to date for conformed, shaped porous solids, and represent a significant improvement over any previously reported experimental values.

2.1.2 Robustness and stability

We tested the robustness of our monoliths by using a vortex shaker to simulate the vibrations that our materials will be exposed to in real life. Also, we have done consecutive adsorption-desorption experiments to check the stability of the materials upon H_2 adsorption. Both 1st and 2nd generation monolithic materials performed well on robustness and stability tests, not showing any dusting or mass loss after the intense vibration test.

2.1.3 Specific heat capacity

The specific heat capacity is a function of the adsorption temperature and typically increases with the temperature. We collected the specific heat capacity of MOF-15 between 60 and 300 K from literature.

2.2 Material optimisation and new candidate selection

2.2.1 Material selection

We computationally simulated the performance of 3,000 experimentally synthesized MOFs for hydrogen storage. We conducted a high-throughput screening (HTS) using grand canonical Monte Carlo (GCMC) simulations at four pressures (5, 25, 50, and 100 bar) and five temperatures of (77, 160, 198, 233, and 298 K). This allowed us to understand the properties-performance landscape of hydrogen adsorption in porous MOFs and to select candidates for monolith synthesis. We selected MOF-15 and MOF-17 as 1st Gen materials due to their high porosity and outstanding volumetric performance. MOF-17 monoliths were synthesised and produced a BET area of 2500 m^2 g^{-1} and a density of $\rho b = 0.80$ g cm^{-3} (yield: 85%). Regular synthesis uses corrosive metal salts in toxic solvents. We replaced these chemicals with benign alternatives and optimised the syntheses. This resulted in scalable, cost efficient and environmentally friendly synthesis pathways. MOF-15 monoliths produced by a green synthesis resulted a BET area of 1600 m^2 g^{-1}, being very similar to previously reported values. The monoliths displayed a high density of $\rho b = 0.85$ g cm^{-3} and a reaction yield of 90%.

Our generation 2 material (MOF-18) was selected following the computational HTS screening due to its high potential for H_2 storage. Traditionally, MOF-18 is synthesised using a toxic solvent. We replaced the use of this solvent with a water-modulator-based process. We chose to divide the water-based synthesis into two steps: i) cluster synthesis and ii) MOF synthesis. MOF-18 monoliths produced by this green synthesis resulted a BET area of 2130 m^2 g^{-1}, being very similar to the product synthesised in ethanol. The monoliths displayed a density of ρb = 0.82 g cm^{-3} and a reaction yield of 95%.

2.2.2 Gen 1 & 2 synthesis optimisation

For all materials, we tried to change the common procedure into green and cost-effective processes. Hence, the selection of metal source and solvent is very critical. Making drastic changes to general procedures requires several optimisations on precursor concentration, reaction time, modulator concentration and reaction temperature to produce an optimum material with large porosity, high density, and reaction yield. In this section, we described the optimisation of 1st generation and 2nd generation materials.

2.2.3 Thermal conductivity enhancement

MOFs, due to their large porosity, have low thermal conductivity. We incorporated graphene nanoplatelets-MOF composites to increase the MOF thermal conductivity. As a proof-of-concept, we added 5 and 10 w/w% of graphene to the 1st generation material. By comparing our results with literature reports, we expect to improve the thermal conductivity up to 5 W/m-K.

2.2.4 Robustness and stability optimisation

We described the robustness test for our monoliths by using vortex and consecutive adsorption-desorption experiments to check the stability of the materials. We also compared the results with the products synthesised by common methods. The results showed that our optimised materials have better robustness and stability than the ones synthesised through common procedures.

3 System Development & Modelling

3.1 Model development

At this stage, the cryo-adsorbent storage bed model is numerically developed and validated with experimental tests of MOFs at grams scale to study the dynamic behaviour of the bed for three different geometries followed by developing an initial system design based on the best geometrical design in terms of energy consumption, loading time, volumetric capacity, discharging time and dormancy period. A sensitivity analysis is carried out to study the effect of different operating conditions, packing density, loading, and discharging time. A simplified model is developed to study the effect of scaling up the storage bed for different applications (forklift, buses, trucks, etc.). Based on the obtained results, an initial demonstrator design is developed for the second phase supported with a simplified P&ID. The details of the PFD and P&ID can be found in the test rig section. Before modelling the cryo-adsorbent storage, the following points are considered to minimize the computational cost and obtain the required results in a reasonable storage scale:

The modelling was carried out using 5.6 L storage tank (D = 0.16 m, H = 0.3 m) which is a reasonable scale to extrapolate the results for different demonstrator scale designs.

The storage tank is designed based on obtaining the cooling energy from either a precooled hydrogen gas at 77K or feeding a liquid hydrogen at 22K.

Three H_2 storage tank geometries were investigated, a blank tank, a tank with central feeding tube and a baffled tank.

The working conditions are selected based on the first MOF generation adsorption isotherm during loading and discharging processes.

The average required flow rate to load the tank within three minutes is around 1.5 g/s. This flow rate is set as the base case. This can be controlled for specific applications (bus, train, forklift etc.).

Four baffles are used inside the baffled storage tank to minimize using $H_{2(l)}$ or $H_{2(g)}$ in cooling the adsorbent material from 160 to 80K (average temperature).

3.2 Assumptions, initial conditions, and boundary conditions

The assumptions, initial and boundary conditions are selected based on the real conditions that will be applied in the test rig and demonstrator designs. These assumptions and conditions can be summarised as follows:

a. Local thermal equilibrium condition between hydrogen gas/liquid and solid phase. This means that the temperature of solid adsorbent material is identical with the temperature of the gas between the voids. This assumption is valid with the selected hydrogen flow velocities through the bed [25].

b. The heat losses are based on using multi-layered insulation (MLI) in a vacuum chamber which provides a heat loss of 1.2 W/m^2. This value is obtained under a cryogenic condition [26] which will be illustrated in point (d).

c. The storage tank consists of four layers (these layers are summarized on one layer in the simulation) of:
    i. innermost: 2 mm of low-density polyethylene (thermal conductivity: 0.39 W/m-K) – this is optional but helps in insulation as well as avoiding leakage.
    ii. 4 mm of aluminium vessel wall. This thickness is selected after studying the stress analysis at the given operating conditions.
    iii. multi-layer insulation – aluminized Mylar separated by low-conductive spacers (thermal conductivity 0.0001 W/m-K) with a vacuum chamber. The total thickness is 20+5 mm.

d. Initial conditions: 5 bar, 160K. The initial conditions are based on assuming that the storage tank has just finished the discharging process and has less than 5% of hydrogen, so that the first-generation MOF material requires a temperature of 160K and pressure of 5 bar to be regenerated.

e. Hydrogen flow rate is based on increasing the pressure from 5 bar to 25 bar within 60 seconds. This assumption can be changed to be based on a fixed flow rate.

f. After reaching 25 bar, the hydrogen feeding is adjusted to keep a constant pressure inside the tank.

g. The outlet flowrate is initially 0 m/s and then increases to 9 m/s after 10 seconds.

h. Pressure drop inside the tank is calculated based on spherical 1 mm pellets of adsorbent material with a shape factor of 1. More data about the effect of the packing density on the pressure drop can be found in the packing report (WP2).

3.3 Dynamic bed behaviour and sensitivity analysis

3.3.1 Justification of selecting the bed height

As mentioned earlier, a storage tank with a diameter of 160 mm and height of 300 mm is considered as the base case for this study. This is due to the geometrical study that was investigated in a blank tank using different diameters and heights.

To cool down the adsorbent material from 160K to 100K, 90K and 85K, the required amount of recycled hydrogen is studied as a function of the bed height as shown in Figure 2. The 'coolant' gas referred to here is H_2 gas recycled by flow-through cooling and is retained and returned to the refuelling system. Prior to further system optimisation (see below), to cool down the material to 100K, 546g of coolant gas is required to adsorb 82.2g (546/82.2 = 6.6 times) at a bed height of 200 mm, while only 307g (3.7 times) is required using a bed height of 650mm. To cool down the material to 85K, 2080 g of coolant gas is required to adsorb 98.5g of hydrogen (2080/98.5 = 21 times) using 200mm cylinder height. This amount is reduced to 1190g using 650 mm cylinder height (1190/98.5 = 12.1 times).

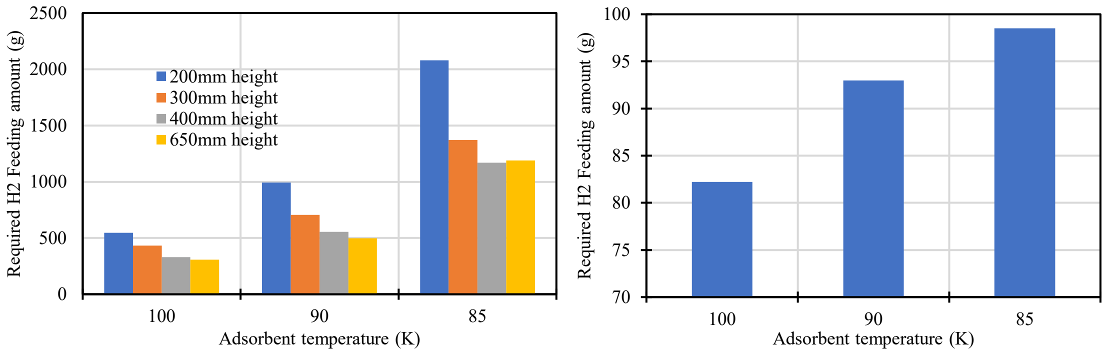

Figure 2: The required amount of hydrogen gas and the volumetric capacity of the hydrogen storage at different adsorbent material temperature

Increasing the bed height has a negative impact on the dormancy period wherein the outer surface area of the bed is increased which ultimately increases the heat losses in the storage tank. Based on the selected insulation (heat loss = 1.2 W/m^2), the heat losses are 0.28, 0.24, 0.22 and 0.21W using a bed height of 650, 400, 300 and 200mm, respectively. Therefore, the bed height between 650 mm and 200 mm should be considered. Thus, the base case is selected to be a bed height of 300 mm to balance between the required H_2 coolant and the boil-off rate.

3.3.2 Selecting the best cryo-adsorbed geometrical design

Figure 3 summarizes the temperature and hydrogen uptake during the loading process using different geometrical designs fed with hydrogen gas. It is clearly shown that the hydrogen tank with baffles is the best design in terms of requiring less hydrogen to cool down the bed since all the geometrical designs are fed with the same flow rate. Thus, when the tank is cooled to the required temperature faster than the others, it requires less hydrogen.

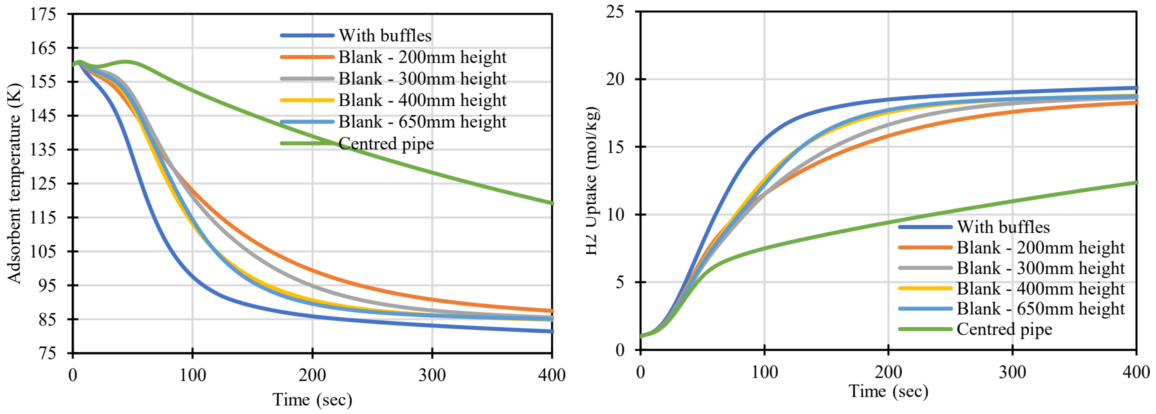

Figure 3: Summary of different geometrical design during the loading process using hydrogen gas

3.3.3 Feeding with $H_{2(g)}$ at 77K and different flow rate

Different flowrates are considered to check how the temperature distribution is affected with time. The boundary conditions are shown in Figure 4. The pressure increases from 5 to 25 bar in 60 seconds. The outlet velocity is adjusted to maintain 25 bar inside the tank after 60 seconds. Two different velocities are considered: 3 m/s and 9 m/s.

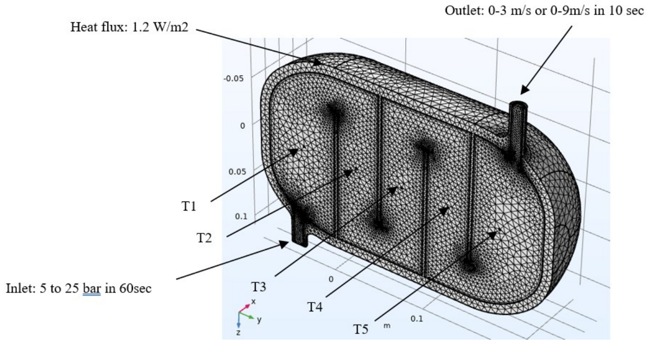

Figure 4: Boundary conditions

At outlet velocity of 9 m/s with a feeding temperature of 77K and initial material temperature of 160K, the maximum temperature in the tank is equal to 175K after 50 seconds as shown in Figure 5. The maximum temperature is observed near to the outlet of the tank (at T5). This means that the generated heat from adsorption and compression is much higher than the rejected heat (Heat lost from the system as a result of feeding $H_{2(g)}$), thus the temperature becomes higher than the initial condition (160K). After getting the peak temperature, a significant drop in temperature is observed in which no generated heat due to compression is found since the pressure inside the tank is maintained at 25 bar after 60 seconds of loading. The generated heat due to adsorption also starts to drop after hitting 25 bar in the tank since the material starts to be saturated with H_2. This is due to the fast adsorption kinetics between H_2 and MOF material. With a lower flow rate (slower outlet velocity (3 m/s)), the peak temperature inside the tank reaches higher than 180K. Therefore, it is important to maintain the flow rate at a certain level to avoid having a significant increase in the temperature during pressure building inside the tank.

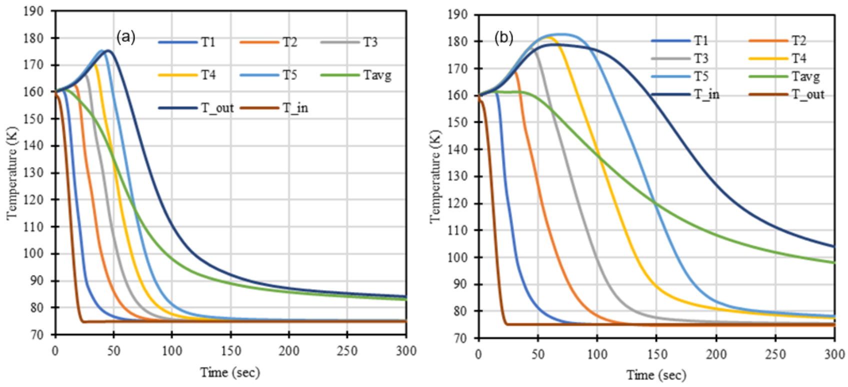

Figure 5: Temperature profile during loading process at (a): outlet velocity of 9 m/s and (b): outlet velocity of 3m/s

3.3.4 Feeding with $H_{2(l)}$ at 22K

In this study, the tank is fed with $H_{2(l)}$ at 22K with outlet velocity of 9 m/s. The pressure is increased from 5 to 25 bar after 60 seconds then maintained at 25 bar for the rest of the loading process. Figure 6 shows the temperature profile at different loading times. The phase change is considered at any temperature higher than 30K. By reaching to the critical pressure (13 bar) during the loading process, there is no heat source due to evaporation, as the fluid is considered in a supercritical phase. To simplify the model and avoid having a sudden change in the H_2 properties between the liquid and gas phases before the supercritical region, a transition period between the phases is considered. The transition period is between 30K and 40K, in which 100% is converted to gas at 40K. It is shown that after 90 seconds, most of the tank temperature is varied between 20K to 90K which provides an average temperature of less than the required (80K).

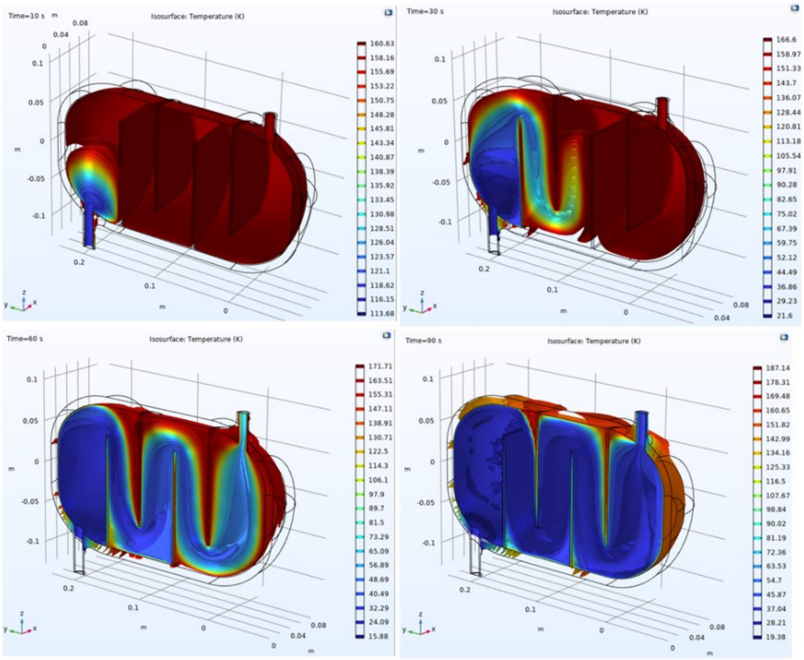

Figure 6: Temperature profile during loading the tank with $H_{2(l)}$ after 10, 30, 60 and 90 seconds

Figure 7 shows the generated/rejected heat during loading $H_{2(l)}$ inside the tank. If we consider the area under the curve as the total energy, it is observed that the rejected heat from the evaporation process is around 1.2 the generated heat from the compression. Thus, less cooling is required to cool down the adsorbent bed.

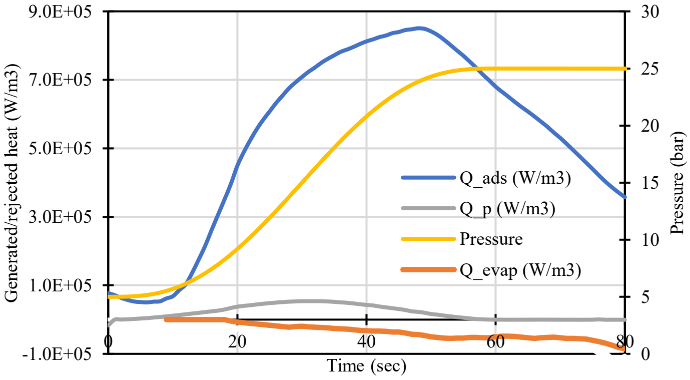

Figure 7. Generated/rejected heat during loading $H_{2(l)}$

3.3.5 Unloading/ discharging process

Discharging the adsorbed hydrogen without using an external heat source is one of the critical advantages in this design which has been proven in Figure 8. The pressure is firstly decreased from 25 to 5 bar within 60 seconds which is the first stage of the discharging process. This causes a temperature reduction from 80 to 62K due to the expansion. Since the expansion process produces cooling to the adsorbent material which increases the volumetric capacity of the material, only 10% of the stored hydrogen is discharged during the expansion process. Then, the discharged amount of hydrogen in the first stage is heated by a heat exchanger with the ambient temperature and recirculated to the tank with an inlet temperature of 250K. Any desorbed amount of hydrogen is recirculated to the tank for 180 seconds (three stages each one in 60 seconds) until the adsorbent material is regenerated by exceeding 160K at a constant pressure (5 bar). The desorption process can be studied also based on the application (the vehicle consumption rate), which is controlled at variable or constant flow rate to the feed the fuel cell in the vehicle.

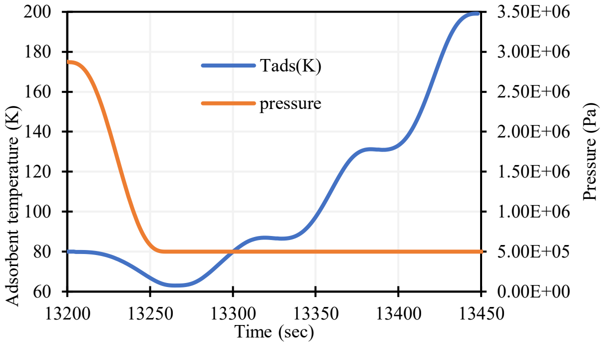

Figure 8: Discharging/unloading process

3.3.6 Boil off during dormancy period

To study the boil off during the dormancy period, a specific application should be considered which is mainly based on the external surface area of the storage tank. After considering the required amount of H_2 for different applications such as forklift, single and double decker buses, train etc. the boil off percentage and temperature inside the tank are calculated from a simplified 2D-axisymmetric model to study a larger computational domain. These calculations are based on the required surface area for each tank assuming a cylindrical shape. The boil-off percentage significantly decreases when larger scale is used such as single and double decker buses which is only less than 0.7% every day with a daily temperature increase of only 1.5K. This heat loss is based on using multi-layer insulation with vacuum that can provide a loss of 1.2 W/m2.

3.4 Initial system and phase 2 demonstrator design

3.4.1 The key metrics of the system scale

Based on the modelling results that are carried out in section 2, an initial system design for the second phase is suggested for a specific application. A simplified 2D axisymmetric model is studied to investigate the key metrics of applying the cryo-adsorption storage for the following applications: forklift, single decker bus, double decker bus, coach and train-single carriage. In this study, the height to the diameter ratio of the tank varies between 1.8 to 2.3 to maintain the same temperature distributions with the storage bed that is studied in section 2 during the loading and discharging processes. In addition to the studied working conditions (loading pressure: 25 bar using the first MOF generation), two more conditions are included. The second one is by applying a pressure of 100 bar during the loading process using the same MOF generation (first MOF generation), while the third one is by applying this pressure using the second MOF generation. Despite the very low working capacity (volumetric uptake between two different pressures) when the pressure increases from 25 bar to 100 bar using the first MOF generation, the overall H_2 volumetric capacity increases since the bulk gas density between the pellets (voids) increases. However, the gravimetric capacity of the system is affected as the higher pressure requires thicker wall. To minimise the weight of the storage tank, the vessel wall is made of aluminium instead of steel or stainless-steel. On the other hand, when the second MOF generation is used at 100 bar, the working capacity increases dramatically when the pressure increases from 25 bar to 100 bar based on the working capacity that is provided in WP2.

Volumetric capacity, gravimetric capacity, loading time, dormancy period, boil-off rate, required energy and required liquid hydrogen are the key metrics included in this study. Note: the loading time can be decreased based on the available flow rate that can feed the storage system in the fuel station without having a significant impact on the required liquid hydrogen.

3.4.2 Demonstrator/system design

The single decker bus was picked as a suggestion for the demonstrator design. The storage tank shape is changed to fit with the available space on the top of the bus as well as the aerodynamic force. More baffles are added to the storage tank to ensure having similar superficial velocity profile to the cylindrical shape. The detailed system equipment is shown in the test rig report. More detail and modifications will be added to the list of equipment in the submission for the second stage of the project. Since developing the below design, our partner has proposed that we build the demonstrator for their double decker bus and so this design will change before submitting Phase 2. The liquid/gas hydrogen loading process is illustrated in the P&ID. During the loading process of liquid hydrogen, a liquid pump will feed the baffled storage tank. The discharged gas hydrogen from the tank will be recycled using a blower and mixed with the main feeding stream to feed it again to the storage system until getting an average temperature of 80K inside the tank. The same process is applied when gas hydrogen is fed to the storage tank. During the discharging process, the pressure is firstly reduced and then the bed heated up using the waste heat from the fuel cell of the bus and is recycled using a blower to heat up the adsorption tank based on the required hydrogen to generate the required flow rate and pressure to the powertrain. More details about the control philosophy are provided in the test rig report. Modifications will be included in the submission for the second phase of the project.

4 Technoeconomic Assessment

A first technoeconomic analysis of Immaterial's monolithic MOF-based cryo-adsorbed hydrogen storage technology has been conducted. Our technology was benchmarked against a counterfactual technology, 350 bar compressed, selected as the currently preferred on-board hydrogen storage technology in all the targeted applications. 700 bar storage is not used by partners in the project.

The analysis confirmed that Immaterial's hydrogen storage technology has the potential to offer:

- Considerably lower pressure requirements than the counterfactual, improving safety risk and reducing limitations on design and reducing cost of the tank.
- Substantially lower OPEX utilising liquid hydrogen infrastructure
- Significant economic and environmental benefits that could be realised in the UK economy over the lifetime of operation, providing significant returns, substantial job creation, clean energy, and sustainable hydrogen storage.
- Key direct environmental benefits are low energy, low-cost refuelling
- Key indirect environmental benefits are enabling conversion of hard to convert markets to hydrogen through lower TCO and >2X the range: volume ratio.

4.1 Benefits and barriers

Immaterial's hydrogen storage technology (monolith enhanced cryo-adsorbed hydrogen storage) is advantaged to address on-board storage in many major transportation/mobility segments. Inherent advantages of the technology include high volumetric capacity whilst avoiding the extremes of conditions required for established hydrogen storage systems. In turn, this allows greater flexibility in system designs that address key challenges in dormancy, refuelling, and form factor which in turn impacts ergonomic design.

Strengths

- Milder operating conditions allow simpler and safer operation vs incumbent storage tech.
- Volumetric performance benefits vs compressed storage incl. conformal designs
- Physisorbent process is totally reversible and well suited to high purity gas storage and cycling

Weaknesses

- Development risks for early TRL technology
- Need of cryogenic temperatures to maximise storage capacity
- Current materials have a slight gravimetric penalty relative to incumbent storage tech.

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Opportunities

- Drivers for adoption show strong synergies across fleet operators (HGV, rail, bus etc.)
- Ongoing development can unlock further performance advantages
- In turn, further application areas may come into scope

Threats

- Infrastructure develops around incumbent storage tech.
- Non-hydrogen energy vector(s) preferred in all transport applications

Figure 9: SWOT analysis of Immaterial's monolith enhanced cryo-adsorption storage technology, summarising the benefits and barriers investigated in phase 1 through technical investigations and ecosystem engagement

The techno-economics for the target transport segments must be viewed through a total cost of ownership (TCO) lens. This contrasts a lot with the early work for on-board hydrogen storage systems which focused on light duty vehicles where the direct vehicle costs (e.g., the on-board fuel storage system) are central to driving vehicle sales and total cost of ownership sits secondarily – a key reason why 700 bar storage is used in LDVs and 350 bar is used in working vehicles. Cost estimates from previous demonstrators by the US Department of Energy (DOE) showed comparable costs to other physical storage systems for cryo-adsorbed systems [27,28]. These analyses also highlighted refuelling as an important part of the $/kg hydrogen costs. Building on these insights have informed improvements created in this project. Namely;

a) Lower operating pressures have enabled reduced tank costs and allowed for more flexible tank designs. All OEM partners have confirmed the value of these conformal tanks in terms of package design envelope and vehicle balancing,
b) Superior heat management has improved refuelling efficiency and system costs, and
c) The monolith form and ongoing MOF development has unlocked more of the underlying potential of this technology.

These improvements are progressing key TCO factors that are important to the fleet owners and operators as well. Such factors include the vehicle real estate that needs to be dedicated to the fuel storage system, productive operating time otherwise lost to refuelling, space required at refuelling stations and risks posed by maximum credible events. Figure 10 provides a high-level qualitative assessment of these key TCO factors against the incumbent hydrogen storage technology as a counterfactual for the target segments (350 bar compressed hydrogen storage). This leads into a detailed discussion and assessment of each of the factors and the benefits and barriers associated with Immaterial's cryo-adsorbed technology.

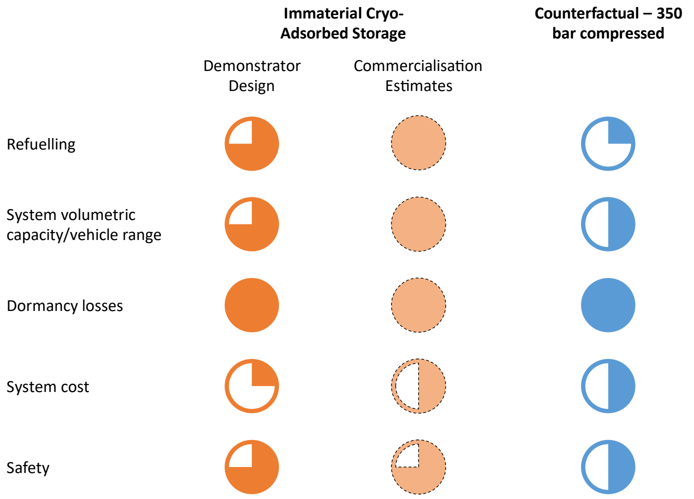

Figure 10: Comparison of Immaterial's cryo-adsorbed technology as characterised through phase 1 demonstrator design and commercialisation estimates against 350 bar compressed storage as a counterfactual for hydrogen storage in target segments, across key TCO factors

4.1.1 Refuelling

Unlike petrol or diesel, hydrogen fuel source and distribution technology have a major impact on overall cost. For 700 bar compressed hydrogen supplied by tube trailer, for example, just ~15% of today's pump price is hydrogen production, while delivery and refuelling (compression) comprise ~35% and ~50%, respectively [29]. Compressors offer limited economies of scale with increasing capacity [29]. In contrast, liquid hydrogen supplied stations can handle faster, more scalable fills [30], with versatility to support all refuelling options at the refuelling station. Based on Immaterial's discussions with advisory board members developing hydrogen refuelling infrastructure, fleet operators, and broader industry trends [31], many organisations are working towards liquid hydrogen playing a leading role in transmission and distribution.

Cryo-adsorbed hydrogen is most effective in the context of a liquid hydrogen supply chain. The low pressures and moderate temperatures can effectively use the energy (and capital) already priced into liquefaction at a central terminal, with simplified infrastructure and reduced cost at the pump. Analysis by the DOE Hydrogen and Fuel Cells program showed that liquid hydrogen-fed cryo-adsorbed storage offered a 36% reduction in refuelling cost (excluding the supplied fuel price) vs. conventional 700 bar compressed hydrogen, and similar improvements against liquid hydrogen-fed compressed and cryo-compressed hydrogen [29]. 350 bar compressed hydrogen was not considered in this analysis but would have a similar cost profile to 700 bar with respect to refuelling costs. The refuelling energetics cost 50% of the counterfactual 350 bar, equivalent to 4% of energetic value of the energy stored. The UK net-zero strategy estimates of 20-40 TWh for transportation is worth 0.8-1.6 TWh to the UK annually. At the current UK emission profile for electricity production, this equates to a reduction of 150-300 $MtCO_2e$ p.a.

The reduction in refuelling cost must be balanced against the cost of the fuel itself, which is different for compressed and liquid hydrogen. This difference depends on the supply chain: analysis by Lawrence Berkeley National Laboratory found that in their base case – 50 tonnes/day supply and separate transmission and distribution networks – liquid hydrogen adds $1.00-1.50/kg over compressed hydrogen in tube trailers. However, liquid hydrogen offers superior scalability and cost is reduced considerably at larger scales or when transmission and distribution are combined [32]. In a scenario where high-purity hydrogen has its own transmission and distribution grid, this would need to be reassessed.

For light-duty vehicles, this 36% reduction in refuelling cost ($0.69/$kgH_2$) may or may not offset the cost of liquid hydrogen, depending on scenario. For medium/heavy-duty vehicles, however, liquid-fed refuelling offers drastic benefits. Because high-capacity compressors scale poorly, liquid-fed refuelling offers a $2-4/$kgH_2$ advantage [30]. This advantage is especially important because – unlike LDVs, which are dominated by vehicle cost – the levelized cost of driving MHDVs is extremely sensitive to fuel cost.

Brighton and Hove Council are opening the UK's first $H_{2(l)}$ bus refuelling site in Crawley this November. At present, $H_{2(l)}$ is only used for transport and bulk storage. The sunk cooling energy for cryogenic temperatures are lost as the hydrogen is compressed to 350 bar for on-board storage.

Looking at refuelling costs through the energy costs is important. This is summarised in Table 1 below where green hydrogen production has been taken as a standardised and idealised starting point. Energy costs for cooling, compression and conversion have been taken from current market-leading processes and expressed in kWh per kilogram of hydrogen or fuel in the case of e-fuel and as a proportion of the value of the energy stored. The latter providing a fairer comparison for the e-fuel to hydrogen. As techno-economics of distribution and stationary storage are driving a move to liquid hydrogen distribution in many segments, Immaterial's energy efficiency has been expressed where that initial liquefaction is considered a sunk cost. This provides a more relevant comparison to other on-board storage technologies such as the 350 bar counterfactual.

Table 1: Energy efficiency from green hydrogen production (<20 bar) through to storage technologies. Values for Immaterial's technology are from initial models and ranges reflect the use of different MOFs.

Hydrogen storage tech:	**Immaterial Cryo-adsorbed** **($H_{2(l)}$ sunk cost in distribution)**	**350 bar compression**	**700 bar compression**	**e-fuel**	**LOHC***	**Liquid**
Energy required to store	1 – 1.6 kWh/kg(H_2)	3 kWh/kg(H_2)	4.3 kWh/kg(H_2)	6.5 kWh/kg(fuel)	+12 kWh/kg(H_2)	7 kWh/kg(H_2)
Energy required to store/total energy stored	3 - 5%	9%	13%	50%	+36%	21%

*thermal energy required for dehydrogenation – other energetic costs may be required to prepare liberated hydrogen for use (e.g. purification or compression

Immaterial's refuelling technology works in a scenario where the sunk energy cost of liquefaction is used to provide the cooling required for cryo-adsorbed storage. The only additional energetic cost comes from the proportion of hydrogen that is required as a coolant and subsequently used for vehicles requiring 350 bar on-board storage.

Whilst cryo-adsorbed on-board storage achieves its greatest techno-economic impact when loaded from $H_{2(l)}$, liquid nitrogen cooling can also be used. From discussions with advisory board members, Immaterial understands that liquid nitrogen could be made cheaply available at hydrogen refuelling stations. This promises an energy efficient refuelling process for cryo-adsorbed storage; however, this has not been modelled within this feasibility study. Importantly, whether we are looking at gaseous or liquid hydrogen refuelling for cryo-adsorbed storage, the possible flexibility in design for refuelling stations and operating conditions for the cryo-adsorbed tank mean that significant cost and energy improvements in refuelling (operational and infrastructural) will be possible from the starting point provided in this feasibility report. At present, availability of $H_{2(l)}$ is considered beneficial but its absence is not necessarily a barrier.

Refuelling time is another important factor for fleet operators. Here, higher pressure refuelling systems scale very poorly (350 or 700 bar) requiring a separate compressor for every vehicle to be refuelled in parallel. In practice, this makes parallel refuelling impractical due to the cost of the compressors and the space required for them. The economic implications for this can only meaningfully be considered with the details of a given fleet and is discussed within the rollout potential.

4.1.2 System volumetric capacity/vehicle range

Cryo-adsorbed hydrogen offers double the volumetric storage capacity over the counterfactual, at, currently, a small cost to gravimetric capacity (Table 6). Importantly, as the technology development moves to a prototyping stage, cryo-adsorbed storage is expected to offer an even greater volumetric benefit and close the gap on a gravimetric basis as analysis is conducted at the vehicle system/real estate level. The biggest challenge posed by mass of storage systems is the configuration and vehicle balance. By way of examples, some trains have high-mass storage on the roofs of individual carriages, and buses have storage entirely on the rear axle. The modest pressures required for cryo-adsorbed storage allow for conformable tanks which may be packed efficiently within the vehicle real estate. This contrasts to 350 bar vessels which must remain spherical or cylindrical shaped and stored safely away from other vehicle components, requiring further vehicle real estate. Further, the shape constraints of 350 bar vessels frequently requires multiple vessels to be packed within the vehicle real estate to provide the required hydrogen storage capacity. The need for multiple tanks increases the storage system volume and weight relative to the mass of hydrogen stored. This has not been accounted for in Table 2 but offers further advantages to cryo-adsorbed storage over the counterfactual.

Immaterial Cryo-Adsorbed		**Counterfactual – 350 bar**	
g/L	**wt.%**	**g/L**	**wt.%**
37.7	4.2	18	5.5

Table 2: Comparison of typical volumetric and gravimetric capacity of Immaterial's cryo-adsorbed technology at the tank level with a 350 bar vessel for a given mass of hydrogen stored.

4.1.3 Dormancy and waste

All low-temperature systems must consider system warming during use cycles, particularly through periods of dormancy. This alone eliminates liquid hydrogen from on-land transportation applications, as 40% of the stored hydrogen is vented in a typical use cycle [33]. Cryo-adsorbed performs similarly to cryo-compressed for peak hydrogen loss during extended parking, but higher thermal inertia gives more than double the dormancy time before venting occurs. This is an important metric in the context of variable demand for vehicle usage.

This means that cryo-adsorbed storage is a solution in applications where dormancy is a concern.

1. Idle desorption rate is approx. 0.5% per day
2. This is not wasted but will result in a pressure increase
3. Acceptable dormancy is therefore a product of:
    a) the desorption rate,
    b) how full the tank was at time of dormancy,
    c) the difference between the operating pressure and the rated pressure

Cryo-adsorbed technology therefore creates zero waste when operated with some degree of planning. 350 bar storage is also a solution in this scenario as the hydrogen is already at ambient temperatures.

4.1.4 System cost

Total system cost of Immaterial's cryo-adsorbed was estimated and compared to the counterfactual. These cost estimates assume the ancillary components of the two technologies will be the same, and focus on the unique parts of each technology, namely the tank and MOF production costs. Cost estimates were based on a storage tank for a double deck bus, rated at 27 kgH_2 storage capacity. Cost is normalised on a £/kWh to allow comparison across the two technologies. The energy content of hydrogen was taken on a lower heating value (LHV) basis i.e., the LHV of hydrogen is assumed to be 33.3 kWh/kgH_2. Therefore, the total energy content of the full tank is 899.1 kWh.

For a 27 kgH_2 cryo-adsorbed storage tank, the total system weight is 641.0 kg with a volume of 715.7 litres, based off the calculated volumetric and gravimetric storage capacities. The amount of MOF material per tank is estimated to be 286.9 kg from the system modelling analysis. Gen 2 MOF production costs are based on 1000 tons/yr facility (Section 4.2.1), or sufficient material to fill 3500 units/yr. Cost estimates for Type I tanks of height 1.6m, diameter 0.64m and wall thickness 25 mm were estimated using data from commercial partners. Table 3 presents total system cost comparisons of Immaterial's technology versus the counterfactual. Hydrogen production, transportation and refuelling costs are not considered here as these are external to the system.

	Immaterial Cryo-Adsorbed	**Counterfactual - 350 Bar**
Tank costs (£)	£8,000 (Type I)	£20,000 (Type III)
Tank costs (£/kgH_2)	£308/kgH_2	£769/kgH_2
MOF costs (£/kgMOF)	£12.41/kgMOF	n/a
MOF costs (£/kgH_2)	£137/kgH_2	n/a
System cost (£/kgH_2)	£445/kgH_2	£769/kgH_2
System cost (£/kWh)	£13.36/kWh	£23.10/kWh

Table 3: Total system cost estimates for a 27 kgH2 storage tank for Immaterial's cryo-adsorbed using Gen 2 MOF versus 350 bar cryo-compressed storage

The overall system cost for the Immaterial cryo-adsorbed technology is estimated to be £13.36/kWh; 42% lower than the counterfactual. The overall cost for a 27kgH_2 storage tank is approx. £11,560. This is deemed to be well within the price tolerance for early entrance into this market segment as confirmed by our commercial partner. Typically, hydrogen storage tanks in buses make up 15-25% of the overall vehicle cost. In our case, the unique system costs make up only 6% of the estimated £200,000 vehicle cost target for hydrogen buses.

The levelized cost of storage (LCOS) is also considered based on the H_2 loading cost and the capital cost of 27kg of H_2 storage tank. Based on a system cost of £11,560, the tank can be loaded every day with ~90% of its capacity (27kg x 0.9 = 24.3kg) for 20 years based on the life cycle of the MOF material. Thus, the overall amount of the stored H_2 over this period is 24.3*365*20 = 177,390 kg. So, the capital cost over this period is £0.065/kgH_2. On the other hand, the loading cost is calculated based on the required energy for compression and cooling which is provided in table 1 (1.6 kWh/kgH_2). By assuming an electrical efficiency of 80%, the total required electrical energy for the loading process is 2kWh/kgH_2 (£0.4/kgH_2 based on an electricity price of £0.2/kWh). Thus, the LCOS is 0.4+0.065 = £0.465/kgH_2. While in compression storage tank, the cost is £1.6/kgH_2 [34].

4.1.5 Safety

Owing to the much milder conditions, the reliability of a cryo-adsorbed storage solution is expected to be higher than competing technologies once an equivalent level of maturity has been achieved. For similar reasons, maintenance requirements are expected to be lighter. Modest operating conditions allow use of type I hydrogen vessels and puts the technology in an operating window where safety considerations are well understood.

The operating conditions are comparable to systems in widespread use today such as:

- Pressure of 25 – 100 bar for cryo-adsorbed storage is a range that is typical for hydraulic and pneumatic systems that are commonplace in many applications
- Temperature cycling from 80 K to 160 K is similar to those required for liquified natural gas (110 K)

The low-pressure operation of cryo-adsorbed hydrogen (25 - 100 bar) offers a considerable, inherent safety advantage over cryo-compressed and compressed hydrogen systems [35]. In the event of a tank rupture, a cryo-adsorbed system will also vent gas far more slowly than a compressed cylinder at the same pressure due to a) the packed bed impeding gas flow and b) the slower release of gas from inside the porous material, which will continue to get slower due to endothermic desorption.

4.2 Route to market assessment

Future energy storage needs to meet a net-zero energy ecosystem are part of an evolving landscape. Key dependencies include the mix of the production methods and end-uses of low/no carbon electricity, hydrogen, and other energy vectors. The UK is at the forefront of this evolution with the articulation and implementation of its net-zero strategy including the delivery plan for the hydrogen ecosystem as laid out in Figure 11. Hydrogen plays a similar role in other national and regional net-zero strategies (e.g., US, EU), although prioritisation of hydrogen as an energy vector (in terms of timings and breadth of use) reflects local natural resources (e.g. availability of natural gas) and political appetite. This techno-economic assessment does so within the context of the delivery plan laid out by the UK government. Similarities in global net-zero strategies are enough to mean global and export markets can be expected to emerge, whilst the UK provides the lead market for development and deployment of Immaterial’s technology.

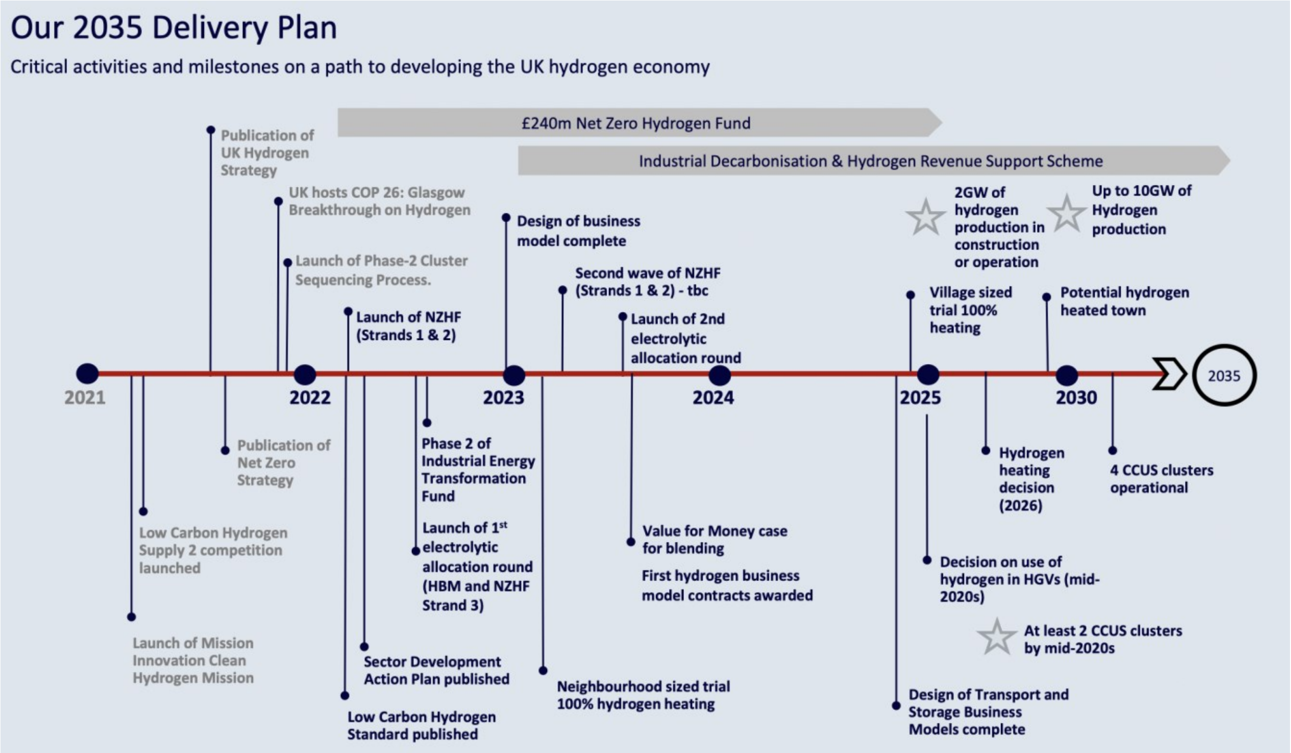

Figure 11: UK delivery plan for the hydrogen economy as set out the UK government in April 2022

Other important milestones in the 2035 delivery plan in assessing the potential of cryo-adsorbed hydrogen storage are the decision on the use of hydrogen in HGVs in the mid-2020s and the aim of 10 GW of hydrogen production in 2030 to be split evenly between green and other low-carbon hydrogen production methods. The scale and method of hydrogen production is important as this makes large-scale production sites likely (e.g. from steam methane reforming) which in turn makes adjacent liquefaction and liquid hydrogen ($H_{2(l)}$) an attractive vector for hydrogen distribution. This has an important implication for Immaterial’s hydrogen storage technology as in this scenario, cryogenic cooling has been priced into the hydrogen value chain prior to the end application, thus reducing cost considerations for cryo-adsorbed hydrogen refuelling.

This project will see a relevant cryo-adsorbed demonstrator in use on a bus. We have validated already that this demonstration will be sufficient for us to move forward with full system prototyping in each of our target sectors, and following Phase 2, we plan to run full scale prototype demos with commercial partners. We also plan to run a prototype with a major HGV OEM. From here, we expect to go into vehicle programmes with each, wherein indicative orders (fixed specifications, system numbers, specific dates) are made and we will enter into strategic procurement. In strategic procurement it is our responsibility to give our customers sufficient oversight and assurance that we will be able to deliver.

To deliver, we plan to work with a leading cryogenic hydrogen technology company. They already have a wealth of highly relevant experience and expertise. Immaterial is already on-track to deliver its first commercial m-MOF factory in Q4 24, and intends to become a major MOF manufacturer, although it is possible it will work with a partner to deliver world scale production in the shortest possible timeframe. It is possible that key partnerships will be cemented via a joint venture.

Key phases are:

- 2023-24 – demonstration (phase 2)
- 2025-26 – muti-platform prototyping, production planning
- 2027-29 – prototyping and vehicle programmes
- 2030 onwards – commercial roll-out

Just as differences exist across the diesel fleets of different transport modes today, the techno-economics of moving to hydrogen is substantially different and will drive differentiated technology across and even within mobility segments. However, where commonalities can be forged, economies of scale will win through. The decision point on hydrogen use in HGVs is likely to be key for many other transport segments due to the sheer number of HGVs and the need for internationally compatible infrastructure for them. This will influence commonalities in technology across the hydrogen ecosystem such as fuel cell design and performance, hydrogen delivery, refuelling infrastructure and on-board storage. Ironically, HGVs will also be one of the most challenging on-land transportation segments to meet the needs of zero emission powertrains (see Figure 12). Much of the technology development in the near-term is likely to occur in other vehicle segments with stronger techno-economics and as this technology matures and becomes more competitive, adapted, and adopted by HGVs.

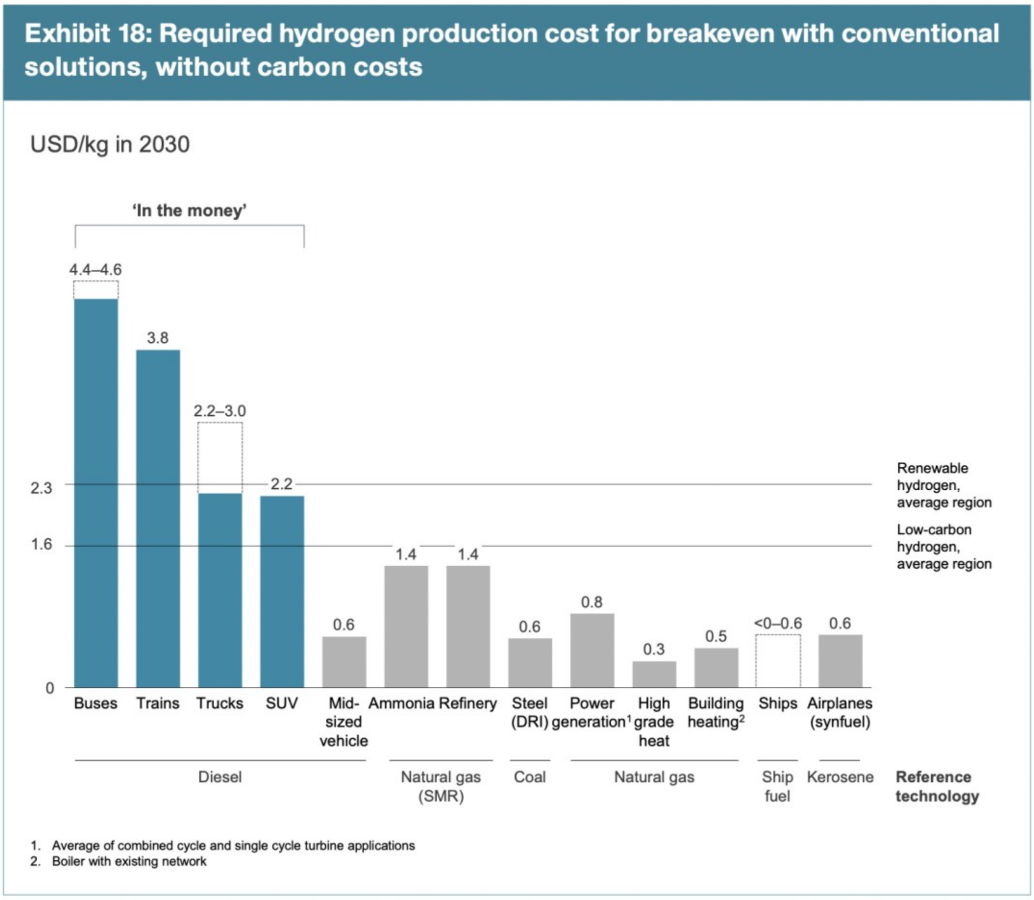

Figure 12: Exhibit 18 taken from "Hydrogen Insights 2021; A perspective on hydrogen investment, market development and cost competitiveness" by the Hydrogen Council and McKinsey and Co. Trucks cover a wide range of heavy-duty vehicles where long-range HGVs are amongst the most challenging to decarbonise.

4.2.1 MOF production and supply-chain

Having production to meet demonstration requirements, vehicle trials and supply chain security demands of vehicle OEMs is essential in facilitating the route to market for cryo-adsorbed storage. The modest operating conditions mean that the vessel can leverage well understood materials and manufacturing techniques. MOFs, however, are still in the early stages of their industrialisation. MOFs are seeing initial commercial uptake with a sale price of ~$20/kg. Immaterial's monolith forming technology is important to the system-level performance. Commercial scale production processes for MOF monoliths are being developed in parallel with our first commercial factory producing monolithic MOFs due to open in 2024. The production process will leverage unit operations already implemented at commercial scale across a range of industries, informing the production cost modelling. Production costs are not expected to vary substantially from one monolithic MOF to another, however, the bill of materials (BoM) for each MOF will become a significant component of the material costs.

Immaterial intends to own the scale-up and production of initial commercial productions of monolithic MOFs. Immaterial's current production capacity is kgs per day. Scale-up work is ongoing from this facility to design and optimise the unit operations and production processes for commercial scale production. Current estimates put the production costs at:

- 100 t p.a. facility, £49.15 per kg
- 1,000 t p.a. facility, £7.41 per kg

Within the current margin of error (± 50%), these estimates are material agnostic. Further economies of scale will be reached as production goes up another order of magnitude. Whilst production facilities at the 10,000s t p.a. are relevant in some of Immaterial's target application areas for hydrogen storage, reducing production costs is no longer a bottleneck for adoption at that point. Further, such estimates lack meaning versus the margins of error from where we are today and so have not been investigated.

The initial assessment of achievable BoM has been summarised below.

	Gen 1		Gen 2	
	Initial	**Ultimate**	**Initial**	**Ultimate**
BoM	£35/kg	£5/kg	£50/kg	£5/kg
Production	£49.15/kg	£7.41/kg	£49.15/kg	£7.41/kg
Total	£74.15/kg	£12.41/kg	£99.15/kg	£12.41/kg

Table 4: Initial and ultimate cost estimates for producing Gen 1 and Gen 2 monolithic MOF materials

Immaterial's supply chain analysis is ongoing. In particular, Immaterial aims to develop closed loop production/use processes as commercial volumes grow. What this entails will depend on the degradation suffered by the MOFs in use. The lowest energy would be reactivation of the framework (such as the removal of contaminants from the surface of the MOF). Physical damage to the framework structure may require reprocessing. If neither reactivation nor reprocessing were possible, the modular nature of MOFs makes them well suited to refining to obtain the original ligands and metal salts, ready to be fed back into the production process.

4.3 Rollout potential

The UK net-zero strategy outlines the major expected use-segments for hydrogen by 2035. Of these, Immaterial's cryo-adsorbed storage technology is currently best suited for serving a range of transportation modes requiring 20-45 TWh of hydrogen storage. Transportation modes best suited to running on hydrogen are mid- to heavy duty up to the extremes of long-range HGV and small marine. Lighter use vehicle categories can have their range and power demands met by batteries. Through discussions with partners, Immaterial understands that even as a liquid, hydrogen will not meet the range and power demands of trans-oceanic shipping, though they remain interested in cryo-adsorbed for smaller vessels. Through discussions with aerospace contacts, Immaterial understands that liquid hydrogen is expected to have a role to play in aviation, starting with short haul flights but the current weight penalty of cryo-adsorbed storage may make this a less attractive option for aviation today. Key target areas are buses, forklift trucks, rail, HGVs, and small maritime. Our partners from each of these sectors will be overseeing the demonstration. These observations are consistent with the UK's hydrogen strategy which in turn builds from the department for transport's "Decarbonising Transport".

The rollout potential for Immaterial's technology includes the US and rest of Europe as export markets with similar adoption timings and priorities. Undoubtedly, further opportunities exist outside of these markets, but these have not been included at this relatively early stage of commercial development.

The greatest chance for success will be achieved by strategically progressing the technology across multiple transportation segments although the greatest value and impact will be achieved by successfully serving the needs of HGVs. Each of these opportunities are aggregate in Table 5. Skilled jobs will be created subject to achieving anticipated roll-out in target markets. Bus ~600, Forklift >200, Rail ~200. Jobs created via the HGV market have not been modelled in Phase 1.

		2030	**2040**	**NPV**
Revenue	Bus	£171m	£1.5bn	£500m
	Forklift	£16m	£574m	£360m
	Rail	£50m	£68m	£51m
	HGV	£2.2bn	£21.6bn	£11.1bn
	Total	**£2.4bn**	**£23.7bn**	**£12bn**
Annual GHG emission reduction ($MtCO_2e$)	Bus	0.01	1.5	
	Forklift	Tbc	Tbc	
	Rail	0.04	0.4	
	HGV	0.06	8.9	
	Total	**0.1**	**10.8**	

Table 5: Revenue and GHG emissions reduction potential of cryo-adsorbed hydrogen in transportation sectors

4.4 Dissemination

Dissemination activities through this feasibility study have been focused on engaging targeted ecosystem partners to form and test insights regarding system and performance targets alongside sharing and discussing updates as the feasibility project has progressed. Immaterial has engaged organisations across a wide range of roles in the ecosystem. Immaterial and its partners at Cambridge are planning to publish a high impact paper on the results attained during Phase 1 – this will be submitted in Q1 2023 and will be publicised. Public dissemination of system-level performance will be subject to physical proof developed in Phase 2 if the project proceeds.

5 Phase 2 Plan

5.1 Description of the demonstration project

The purpose of Phase 2 is to validate the performance of the MOF-enabled cryo-adsorbed hydrogen storage platform in a demonstrator that will resonate across the target markets, overseen by OEM partners from several sectors. The demonstrators must show sufficient evidence of performance to enable the next steps which will be application-specific prototypes in each of the target sectors. Phase 4 will go into vehicle programmes with OEM partners.

The project has three major milestones – a purpose-built cryo-adsorbed test rig, a prototype storage and fuel cell unit, and finally the representative demonstrator. The aim of the test rig is to validate, at lab scale, the cryo-adsorbed storage concept. The test rig will be an invaluable data gathering device, fitted with sophisticated sensing equipment to gather design data such as capacity, temperature and pressure drop. It will provide the first real-world measurements of filling time, heat transfer, mass transfer, pressure drop, porosity, working capacity, and transient desorption characteristics.

The prototype storage vessel will be built in partnership with a specialist in novel, high quality-control fabrication techniques, which make them an ideal partner for prototyping conformal pressure vessels with advanced monitoring requirements. For example, it's envisioned that the tank, with internal baffles and high-pressure monitoring ports for sensors, may benefit from metallic 3D printing technology. Prototype-scale sensors, refuelling infrastructure, insulated hosing and valve systems will be supplied and developed for the intermediate system with specialist $H_{2(l)}$ componentry experts.

The prototype will be approximately 15 litres, with complex monitoring and attachment to a static vehicle PEM fuel cell test stack. Powering a fuel cell test stack will answer critical questions about fuel delivery, desorption, rate limiting steps and heat transfer. Substantial experience will also be gained on the establishment of equipment peripherals and the health and safety management of a cryo-adsorbed hydrogen system. The information gained from the static vehicle simulator will support the design of the full-scale moving bus technical demonstrator.

The demonstrator itself will be designed for a bus and will be installed on a hydrogen bus prototype. The demonstrator storage system will also be built with specialist partners. The main aim of the demonstrator unit will be the first full-scale functional demonstration of the working concept of cryo-adsorbed hydrogen storage for vehicle fuelling. This will be done in conjunction with the systems integration team at our OEM partner and will also be done according to all regulatory and safety requirements which are relevant. The system will have advanced sensing principally for working capacity and transient filling and discharge characteristics.

Immaterial has confirmed the significance of the planned demonstration with partners from each of the other target sectors. As well as *by invitation* this demo could also be done at other transport trade shows, with the intention of illustrating scalability, synchronicity, and adjacency with sectors like rail, marine, light industrial vehicles, and forklifts.

5.2 Costed development plan

Total project costs for Phase 2 are calculated as **£4,185,565** exclusive of VAT. These costs represent fair market value as they have been calculated as the actual cost to Immaterial without profit. Estimated hours, capital usage and consumables costs are based on past project experience and real data of our running-costs. An overview of costs is provided below. A more detailed version will be included in the full Phase 2 application.

Summary costs are broken down as:

- **Labour:** £1,845,364 (44.1% of total)
- **Overheads:** (up to) £922,682 (22.0%)
- **Materials:** £306,469 (7.3%).
- **Capital usage:** £256,050 (6.1%).
- **Subcontracting:** £845,000 (20.2%).
- **Travel & subsistence:** £10,000 (0.2%)

Total person-days, excluding subcontractors, are 6,537 with the following split:

- **WP1:** Material characterisation: 294 person-days (5%); £132,761 (4%) including subcontractors
- **WP2:** Material optimisation and production scale-up: 1,265 person-days (19%); £506,261 (14%) including subcontractors
- **WP3:** Test rig build and model validation and refinement: 1,082 person-days (17%): £772,417 (21%) including subcontractors
- **WP4:** Prototype design, build and testing**:** 1,320 person-days (20%): £721,667 (20%) including subcontractors
- **WP5:** Demonstrator build and trial: 1,100 person-days (17%); £810,417 (22%) including subcontractors
- **WP6:** Technoeconomic and environmental assessment: 1,054 person-days (16%); £488,727 (13%)
- **WP7:** Project & risk management: 422 person-days (6%); £215,795 (6%)

Detailed phase 2 project plan can be found in the Gantt below.

		23											24											25
		M	A	M	J	J	A	S	O	N	D	J	F	M	A	M	J	J	A	S	O	N	D	J
Monolithic MOFs for cryo-adsorbed hydrogen storage		Q1			Q2			Q3			Q4			Q5			Q6			Q7			Q8	
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
WP1	**Material characterisation** *(Immaterial)*	█	█	█	█	█	█	█	█															
1.1	Robustness and stability analysis	▒	▒	▒	▒	▒	▒																	
1.2	Systematic packing and form factor optimisation	▒	▒	▒	▒	▒	▒	▒	▒															
WP2	**Material optimisation and fabrication scale-up** *(Immaterial)*	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█
2.1	Robustness and stability optimisation	▒	▒	▒	▒	▒	▒	▒	▒															
2.2	Cost assessment and scale-up pathway development	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒			
2.3	Scale-up of lead material	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒
WP3	**Test rig build and model validation & refinement** *(Manchester University)*	█	█	█	█	█	█	█	█	█	█	█	█	▓	▓	▓	▓	▓	▓	▓	▓	▓	▓	▓
3.1	Shop drawing finalised from P1 designs	▒	▒																					
3.2	Component procurement and construction	▒	▒	▒																				
3.3	Experimental work plan	▒	▒	▒	▒	▒	▒																	
3.4	Safety analysis	▒	▒	▒	▒	▒	▒																	
3.5	Test rig trialling and refinement				▒	▒	▒	▒																
3.6	Experimental study						▒	▒	▒	▒	▒													
3.7	Data analysis and model refinement							▒	▒	▒	▒	▒												
3.8	Prototype design data gathering									▒	▒	▒	▒											
3.9	Ongoing *ad hoc* trials												░	░	░	░	░	░	░	░	░	░	░	░
WP4	**Prototype design and build** *(Demaco & Immaterial)*				█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█		
4.1	Engagement of key subcontractors; order long-lead items				▒	▒	▒	▒	▒	▒	▒	▒												
4.2	Establish key design variables and scale-up laws				▒	▒	▒	▒	▒	▒	▒	▒												
4.3	Design of prototype				▒	▒	▒	▒	▒	▒	▒	▒												
4.4	Final shop drawings of prototype and components list										▒	▒												
4.5	Procurement and construction											▒	▒	▒	▒	▒								
4.6	Experimental work plan												▒	▒	▒	▒								
4.7	Safety analysis												▒	▒	▒	▒	▒							
4.8	Prototype trialling and refinement														▒	▒	▒	▒	▒					
4.9	Experimental study																▒	▒	▒	▒	▒	▒		
4.10	Data analysis and model refinement																▒	▒	▒	▒	▒	▒		
4.11	Demonstrator design data gathering																▒	▒	▒	▒	▒	▒		
WP5	**Demonstrator build and trial** *(Alexander Dennis, MTC & Immaterial)*									█	█	█	█	█	█	█	█	█	█	█	█	█	█	█
5.1	Design of bus demonstrator system									▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒			
5.2	Engagement of key subcontractors; order long-lead items															▒	▒	▒	▒	▒	▒			
5.3	Regulatory affairs consultation															▒	▒	▒	▒	▒	▒			
5.2	Third-party safety accreditation																			▒	▒	▒	▒	▒
5.3	Experimental work plan																			▒	▒	▒	▒	▒
5.4	Procurement and construction																			▒	▒	▒	▒	▒
5.5	Production and packing of optimised MOF(s) for trial																						▒	▒
5.6	Experimental study																						▒	▒
5.7	Data analysis and final model refinement																							
5.8	Demonstrator 2.0 design																							
WP6	**Technoeconomic and environmental assessment** *(Immaterial)*	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█
6.1	Stakeholder engagement and dissemination	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒
6.2	Preliminary lifecycle analysis	▒	▒	▒	▒	▒	▒																	
6.3	Comparison with alternative storage technologies										▒	▒	▒							▒	▒	▒		
6.4	Use case evaluation	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒
6.5	Full lifecycle analysis																			▒	▒	▒	▒	▒
WP7	**Project management** *(Immaterial)*	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█	█
7.1	Kick off	▒																						
7.2	Personnel onboarding	▒	▒	▒																				
7.3	Internal communication & project management	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒	▒
7.4	SBRI reporting			▒			▒			▒			▒			▒			▒			▒		▒

6 Conclusions

Immaterial's cryo-adsorbed technology continues to have substantial technology risk as subsystems need to be built for the first time and it has not yet been proven in the real world. The upside potential however is substantial, creating real benefits for each stakeholder in the target ecosystems - low cost, low cost to run, high volume, ergonomic fuel systems that utilise cold temperatures that counterfactual technology is wasting, and can replace expensive compression. Immaterial has engaged key companies throughout this ecosystem and it is clear that these benefits are highly prized, and that the technology is deemed feasible and applicable. Of the transport segments analysed, the technology can enable the decarbonisation of 44% of UK annual emissions by 2040 versus 2019 levels (10.8 $MtCO_2e$) and other segments will become addressable as the technology develops. Further, the refuelling energetics cost 50% of the counterfactual 350 bar, equivalent to 4% of energetic value of the energy stored. Driving such standards across the UK net-zero strategy estimates of 20-40 TWh for transportation is worth 0.8-1.6 TWh to the UK annually. At the current UK emission profile for electricity production, this is a further reduction of 150-300 $MtCO_2e$ p.a.. The export market drives a multi-billion-pound opportunity for a UK-based company to lead in within the current decade. The associated NPV is £12bn creating around 1,000 high tech manufacturing roles, significantly expected to be UK-based. This uptake is driven by substantial cost benefits to fleet operators, often through improved vehicle design, fleet logistics, safety, and reduced infrastructure costs.

Cryo-adsorbed technology concepts are not new - funding has been flowing into cryo-adsorbed in the US, and it is now also the focus of funding in the EU. Immaterial's monolithic MOF technology is the missing link and the enabler for the cryo-adsorbed platform, and the real-world demonstrator will advance the state of the art substantially.

Thanks to the substantial cost benefits of cryo-adsorbed, it can rapidly become the technology of choice in some of the most challenging markets to de-carbonise – enabling and accelerating the switch to hydrogen.

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