Sustainable Hydrogen

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Hydrogen for a Sustainable Built Environment

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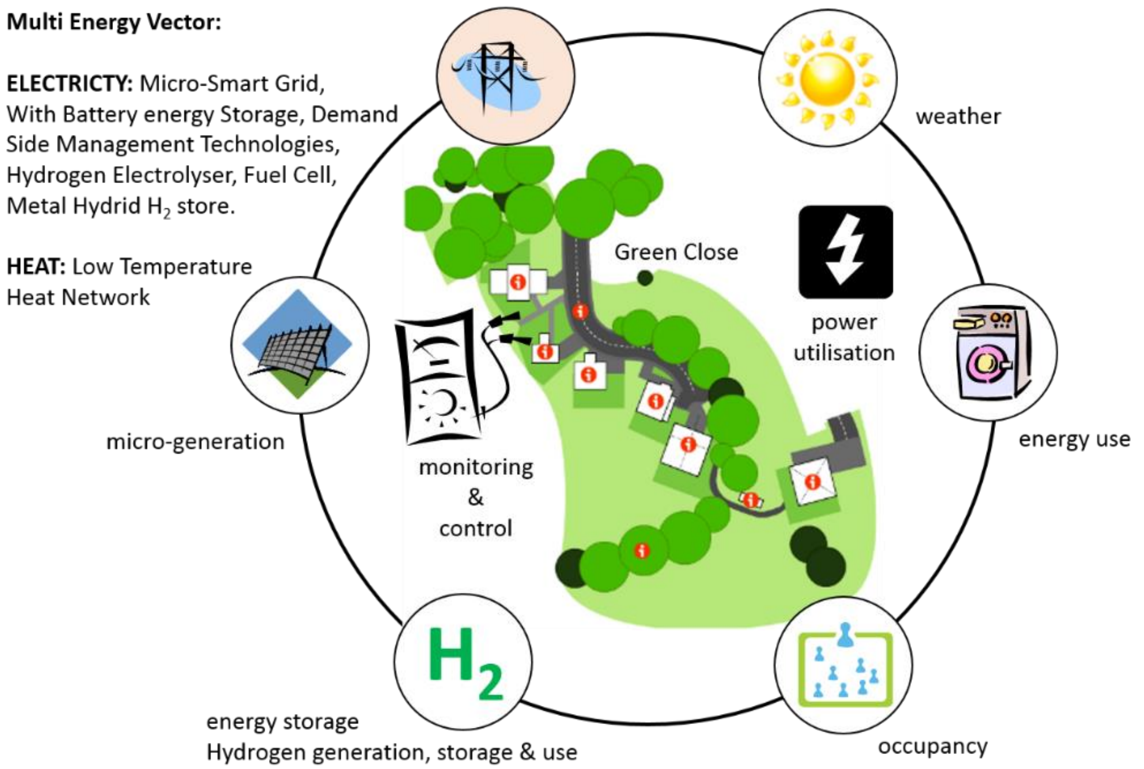
Project description

The image illustrates the multi-vector smart energy system at the Universities Creative energy Homes. The following Hydrogen infrastructure is Included in the facility – electricity grid linked Electrolyser, McPhy H2 Store and Fuel Cell. This research will build upon significant existing investment that created a unique research facility.



Deliverables

- A working demonstrator for hydrogen
- Novel Multi-Energy Vector control algorithms for Hydrogen Energy Generation-Storage-Use in the built environment

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Sustainable Electrocatalysts for H_2 Generation

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Project description

Polyoxometalates (POM) are molecular metal oxides constructed from early transition metals in their highest oxidation states. Their electrochemical properties (multiple accessible redox states, fast electrode kinetics, and cyclability), coupled with their capacity to stabilise highly oxidised heterometal ions, render them excellent water splitting catalysts capable of facilitating both oxygen and hydrogen evolution reactions. Here we will construct stable, electroactive POM-carbon nanotube composite materials for heterogenous water splitting under mild electrochemical conditions. The composite materials will exhibit significantly enhanced electrochemical stability and minimised leaching due to the nanoconfinement of the catalytic moieties.

Deliverables

- To synthesise nanocomposite of carbon nanotubes and earth-abundant polyoxometalates
- To electrochemically and spectroscopically characterise the composite materials
- To determine the electrocatalytic performance of the materials during electrolytic water splitting
- To incorporate the materials into a fully-functional electrolyser and determine their performance at the device level.

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To a 100% Hydrogen Domestic Boiler

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Project description

Hydrogen combustion produces approximately 142 MJ per kg, but its physical density is very low, at room conditions approximately 81 g/m^3. By comparison methane produces 50 MJ/kg with a density of 654 g/m^3. Currently, there are existing hydrogen infrastructure projects in progress in Europe (GRHYD in France) to use a mix of methane and hydrogen due to the safety issues and avoiding boiler burner redesign. Hydrogen burns quite differently to methane, with a faster flame speed, and a transparent flame, such that it is harder to control and maintain the flame in steady combustion, and the radiative transfer is weaker than for the visible methane flame. These characteristics require redesign of domestic boiler burners if hydrogen is to be used as a network fuel. A BEIS report by Frazer Nash in April 2018 described how industry has the opportunity to redesign for suitable domestic hydrogen burners. Worgas Ltd are a local company investigating the practical application.

Deliverables

- Characterised hydrogen flames for several nozzles
- Characterised flames for various gas mixtures
- CFD model of small number of burner designs
- Optimisation of burner design from CFD results

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High Capacity Mixed Metal Borohydrides Ammoniates for Hydrogen Energy Storage Applications

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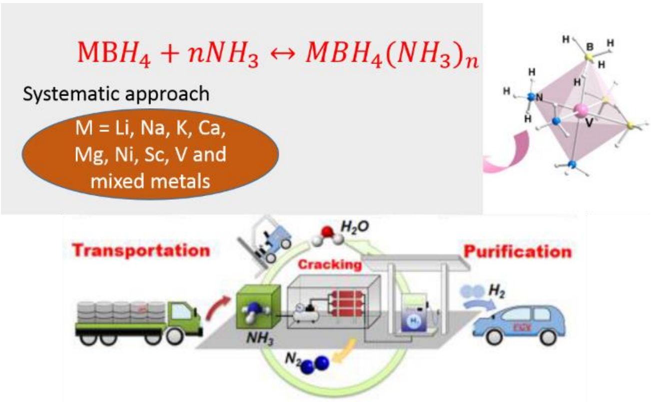
Project description

Hydrogen is a promising alternative energy carrier for the future due to its high specific energy and environmental friendliness. The development of hydrogen storage technologies to support renewable energy systems and low-carbon transportation is important. Currently, high pressure compressed hydrogen gas (700 bar) is used for vehicles, however they are very costly and achieve low energy densities. Many light weight hydrides, such as $LiBH_4$ and $LiAlH_4$, although having high storage capacities have major drawbacks of irreversibility and high working temperatures. Ammonia can be catalytically split in to N_2 and H_2 and its hydrogen content is about 17.3 wt.%, which can store 30 % more energy per volume than liquid H_2. Utilization of NH_3 for on-board storage system is hampered due to its toxicity. In recent years, a new class of materials called Metal Borohydride Ammoniates (MBAs) show improved hydrogen storage properties. MBAs tend to release hydrogen/ammonia gas at more practical temperatures and with greater purity. This research will focus on the development of novel Mixed Metal Borohydride Ammoniates (MMBAs) to achieve even higher hydrogen storage densities, elucidate the reaction mechanisms responsible for the decomposition process and investigate catalysts to accelerate the release of hydrogen from these materials. The project involves synthesis of various MMBAs, a variety of material characterisation techniques (e.g. XRD, TGA, DSC, FTIR, GC-MS) and hydrogen performance testing by the Sieverts' technique. There will also be opportunities to use large scale facilities such as neutron diffraction experiments at Institut Laue Langevin in France.



Deliverables

- Role of mixed metals on the hydrogen volumetric energy storage density
- Reaction mechanisms for H_2 and NH_3 release from different MBAs

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Materials Development and Characterisation of Novel Metal Hydride Slurries for Effective and Sustainable Air Conditioning

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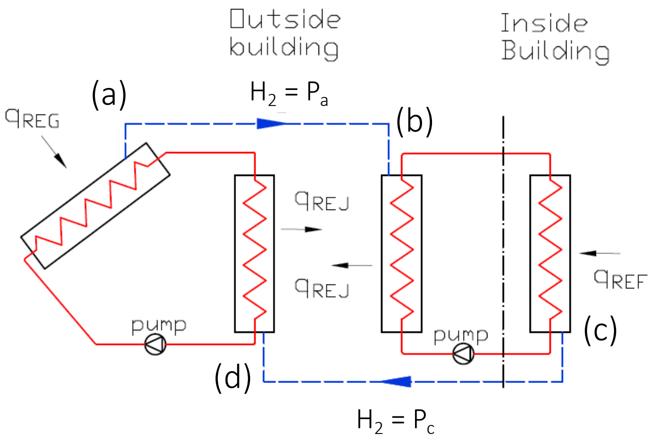
Project description

The group has developed thermal storage systems based on metal hydrides tuned to the operational temperature of heat sources. These use the high enthalpy of formation of the metal hydride to store and release large amounts of energy. Here we have an innovative concept based not of large dry powder beds with large heat exchangers but instead pumping significantly smaller amounts of metal hydride as a slurry around a heat exchanger system to provide cooling for air conditioning (A/C) system. Air conditioning can account for up to a third or more of electricity demand in warmer countries and this is rising year on year. For example in Saudi Arabia more than 50% of the electricity consumed during peak summer is now on A/C in Mumbai, India, A/C accounts for around 40% of power consumption and in Madrid, Spain, 30% of the energy consumed during peak electrical use is due to A/C. The advantage of the metal hydride in a slurry is that it has much improved thermal conductivity from a powder bed (that are typically as low as 0.1 $Wm^{-1}K^{-1}$). Also by pumping the hydride around the system much smaller amounts of hydride are required keeping costs lower. This innovative project requires a researcher with strong experimental interests to modify and characterise new materials, build test beds and analyse results. The researcher will be provided with a lot of support from the supervisors and surrounding research team to develop this innovative concept.



Deliverables

- Selection of working pairs of metal hydrides
- Development of new alloys where necessary
- Selection of inert liquid and surfactant where necessary
- Modified Sieverts rig for slurries
- Data on hydride slurry kinetics and thermal properties
- Design and build of a prototype to test pairs
- Comparison of experimental data with numerical model

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Catalyst development for low-cost large-scale sustainable hydrogen production from seawater and renewable energy

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Project description

Hydrogen is considered one of the most promising clean energy carriers, thanks to its high gravimetric energy density (142 MJ/kg) and environmentally friendly use. It is a clean and desirable way to produce pure hydrogen at the cathode via electrolysis of water driven by renewable energy, however, the water splitting is highly dependent on having an efficient and stable oxygen evolution reaction (OER) at the anode, to counterbalance the hydrogen evolution reaction (HER) at the cathode. Furthermore, if water splitting is used to store a substantial portion of the world's energy, water distribution issues may arise if vast amounts of purified water are used for hydrogen fuel production. On the other hand, seawater is the most abundant aqueous electrolyte feedstock on Earth but its implementation in the water-splitting process presents many challenges, especially for the anodic reaction.

The most serious challenges in seawater splitting are posed by the chloride anions (around 0.5 M in seawater). Under acidic conditions, the OER equilibrium potential is only slightly higher than that of chlorine evolution, e.g., by 0.130 V, and in fact the OER is a four-electron oxidation requiring a high over potential while chlorine evolution is a facile two-electron oxidation with a kinetic advantage. While chlorine is a high value product, the amount of chlorine that would be generated to supply the world with hydrogen would quickly exceed demand.

Nevertheless, under alkaline conditions, the equilibrium potential of OER is significantly shifted to lower value but that of chorine evolution does not change so much, which facilitates OER over chorine evolution with 0.490 V difference in potential domain. Therefore, this project aims to develop highly efficient OER catalysts with over potential less than 0.480 V under alkaline conditions, as well as highly efficient and low cost HER catalysts such as transitional metal carbides and nitrogen doped carbon nanomaterials.

Deliverables

- A prototype electrolyser employing the catalysts and electrodes so developed and using seawater and renewable energy to produce sustainable hydrogen
- At least 3 high impact journal papers on catalyst materials and catalysis understanding.

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Understanding the Potential of Hydrogen Technology Adoption in a Complex Changing Energy System

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Project description

Energy is provided by multiple stakeholders who interact in complex systems in which past economic, engineering, technological, social, and regulatory decisions influence the relative potential of existing and new technologies to be adopted. Thus, yesterday's energy system influences the potential for new hydrogen technologies to be adopted, and decisions taken as we adopt new renewable technologies, will have long term consequences with regard to which new technologies will be adopted, as decision taken are likely to bias the energy systems development in favour of some technologies over others.

Given this context, this project would 1) characterise the existing energy system including the development of alternative non-hydrogen based renewable technologies 2) Categorise potential hydrogen technologies on economic, technological, and engineering grounds so as to evaluate their potential for successful adoption, 3) provided detailed analysis with regard to how the existing energy system supports and or hinders the development of the analysed technologies, and 4) provided understanding and strategic insights with regard to how engineering, managerial, regulatory, technological factors would need to change in order to foster stronger adoption of hydrogen technologies.

Deliverables

- The project would engage existing CDT stakeholders, in a collaborative process in which the PhD student would meet the 4 objectives detailed in the summary above
- The outcome would be academic and policy relevant publications, which would improve policy development in government, and regulatory bodies, but also inform strategic decisions taken by commercial stakeholders

Sustainable Hydrogen
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Neutron Spectroscopy of Surface Intermediates on Nanoporous Metal Catalysts for H_2 Storage Technologies

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Project description

In the future, the availability of abundant low carbon hydrogen is predicted to be a crucial factor for meeting the UK's growing energy needs while at the same time reducing carbon emissions. As direct storage of gaseous hydrogen is problematic, alternative hydrogen carriers are required, such as liquid fuels (ammonia, methanol or hydrocarbons) or high energy density hydrides (e.g. $LiAlH_4$ and $NaBH_4$). The formation of the storage compounds, their decomposition to generate hydrogen and recycling to the concomitant starting materials all require highly dispersed metal heterogenous catalysts. However, the fundamental mechanisms of relevant hydrogenation, chain growth or decomposition reactions are not fully understood meaning developing the next generation of catalysts with better performance is unfocussed, leading to incremental improvements rather than step changes.

The uniquely high incoherent neutron scattering of hydrogen provides excellent contrast between materials that contain hydrogen and those that do not. This can be a powerful tool to investigate the interaction between organic substrates and inorganic catalysts by 'seeing' only the minority adsorbed organic layer, where more traditional spectroscopies may be dominated by signals from the bulk of the catalyst or catalyst support. Unfortunately, due relatively small signal of surface species relative to the bulk material, high densities of hydrogen containing species are required for measurements, making the use of conventional supported metal catalysts challenging. Nanoporous metals, provide a potential solution to this issue, as their high active surface areas allow for greater concentration of adsorbed surface species to be interrogated using neutrons.

We will elucidate surface processes, using neutron methods, occurring on nanoporous Co and Cu catalysts for CO and CO_2 hydrogenation and chain growth reactions in alcohol synthesis and Fischer-Tropsch chemistry. This will require the development of new methods for in situ catalyst treatment in annular cell geometry at ISIS. Using a purpose-built flow cell to enable safe operation, we will also investigate the evolution of hydrogen from energy-dense materials such as sodium borohyride through catalytic activation. Inelastic neutron spectroscopy (INS) will be used to determine the nature of surface species after the reaction is quenched, while quasi elastic neutron scattering (QENS) will be used to determine surface diffusion rates of CH_x/ hydride species under reaction conditions. INS is necessary as the high light absorbance of the catalysts render them unsuitable for optical spectroscopy. QENS is the only technique suited to diffusion measurements on bulk metals under dynamic equilibrium conditions.

Deliverables

- Trained PhD student with skills in carrying out and disseminating research in world leading environments at ISIS, UK Catalysis Hub and the SuSHy CDT.
- Produce dedicated in situ flow QENS reactor.

- Research outputs in terms of publications and presentations at conferences on catalytic mechanisms of CO_2 hydrogenation and metal hydride decomposition.
- The work will provide proof of concept and evidence for collaborative larger UKRI proposals.

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Photocatalytic Covalent Organic Frameworks for Hydrogen Production and Storage

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Project description

COFs are among the most promising hydrogen storage materials, they are lightweight, robust and easily synthesised with high hydrogen storage capacity (>7 wt.%) and are much more stable than metal organic frameworks (MOFs) for long term use. However, like MOFs, these materials are network polymers, often with uniform pore sizes. While this allows gas molecules to enter easily there is little to stop them leaving just as readily, indeed at ambient temperatures the hydrogen storage capacity of both COFs and MOFs is typically around a third of that when measured at cryogenic temperatures.

In recent years, photocatalytic polymers and frameworks have also emerged as exciting new candidate in hydrogen evolution from water, the essentially infinite versatility and modular nature of organic molecules allows us to fine tune optical and electronic properties and thereby catalytic performance.

This project will produce photocatalytic molecular tectons based on dibenzothiophene-S,S-dioxide – one of the most promising organic fragments in hydrogen production from water – which will anchor over the pores in the surface of the COF through non-covalent interactions to create sites for hydrogen evolution from water and to reduce the size of the pores making them readily permeable to hydrogen but not oxygen to ensure that the COF becomes enriched in hydrogen exclusively, targeting a gravimetric capacity of 5 wt.% at 298K in the first instance. The US DOE has set a target gravimetric capacity of 4.5 wt % by 2020 and 5.5 wt % by 2025 for onboard hydrogen storage for light vehicles and the approach proposed here presents a genuine route to attaining this goal.

This approach will increase the thermal stability of the hydrogen enriched COFs at ambient temperatures and ultimately permit controlled generation, storage and release of hydrogen.

Deliverables

- Novel molecular/macromolecular photocatalysts for hydrogen evolution.
- Hybrid assemblies of photocatalysts on COFs surfaces which function to generate and store hydrogen from water.

Decarbonisation of UK Gas Network: Hydrogen Enrichment of Natural Gas by Methane Cracking

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Project description

Most of the UK's electricity is produced by burning fossil fuels, mainly natural gas (42% in 2016) and coal (9% in 2016). A very small amount is produced from other fuels (3.1% in 2016). Renewable technologies use natural energy to make electricity (eg; wind, wave, marine, hydro, biomass and solar) and it made up 24.5% of electricity generated in 2016. Despite promising advances made in the renewable energy sector, the UK is considerably lagging behind the carbon emission reduction targets.

Above data clearly show that decarbonisation of our gas network would lead to significant reduction of current carbon emission levels. Methane cracking allows enrichment of natural gas with hydrogen, a carbon free fuel. In this context, further development and early deployment of methane cracking technology has become an urgent priority.

This project would 1) study established catalysts and new catalysts formulations to enrich natural gas at a conversion rate of 50% and beyond, 2) develop methods to efficiently remove value added by-products at scale, 3) building on from current techno-economic analysis, develop further economic models and regulatory scenarios by integrating renewable electricity (in close collaboration with offshore renewable energy Catapult, economists and PhD students attached School of Business and Economics), 4) in collaboration of external stake-holders (such as offshore renewable energy Catapult and industry), opportunities for early deployment of the methane cracking technology will be investigated.

Deliverables

- The project would engage existing CDT stakeholders, in a collaborative process in which the PhD student would meet the 4 objectives detailed in the summary above.
- The outcome would be academic and policy relevant publications, which would improve policy development in government, and regulatory bodies, but also inform strategic decisions taken by commercial stakeholders

Algal Biomass to Hydrogen: A Circular Approach for Green Sustainable Processing with Enhanced Efficiency and Minimal Waste

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Project description

The project investigates hydrothermal conversion of algal biomass to H_2-rich gas in a sustainable circular approach. Figure 1 is a conceptual diagram of the technology pathway in general: Cultivated wet microalgae (MA) undergoes hydrothermal liquefaction (HTL) in subcritical water, and the products are separated into gases, oil phase (biocrude), and aqueous phase (organics-rich). The biocrude oil can be catalytically hydrotreated to hydrocarbon fuels, and the organics-rich aqueous phase undergoes gasification in supercritical water conditions to produce H_2-rich gas. The HTL process is the gateway to paths (1) and (2). HTL conditions (specifically reaction time, temperature) dictate the products' composition, and product separation technique influences the products' distribution between the aqueous and oil phases**.** Also, they influence the %H_2 in the gas exit stream. **This project investigates MA cultivation followed by the optimum conditions that favour an aqueous phase rich with organic matter -path (2)-, where organics undergo SCWG to produce H_2 gas.**

Why SCWG? a) SCWG is the only advanced hydrothermal technology known to convert the entirety of organic matter to H_2-rich gas *without the concurrent generation of chars and tars*. b) SCW indiscriminately dissolves all organics which makes SCWG a one-phase reaction with minimal diffusion limitations and very high rate, c) the aqueous phase after SCWG would be rich with nutrients that can be recycled for algal growth, c) SCWG is ideal for wet biomass thus no drying is required, d) the hot exit gas from SCWG contains high-grade heat, which can be integrated to enhance the process exergy efficiency.

Figure 1 offers flexibility to reach the desired product(s) based on the microalgae (feedstock) composition and process conditions. The criteria would be product purity, quantity, waste minimisation (towards circular economy), energy integration and economic feasibility. After investigation of HTL parameters the project workers will establish the best route to achieve the above-mentioned criteria. The project involves a focused experimental programme, feedstock and products analysis, theoretical investigations and simulation for best energy integration scenario, and of economic feasibility. We plan to focus on the existing technology barriers namely (i) efficient oil/water separation seeking organics-rich aqueous phase, (ii) optimum SCW gasifier design, (iii) maximum energy recovery and integration (via simulation), and (iv) maximum H_2 production. This programme is a start of more detailed and rigorous programme for an efficient & economically feasible H_2 production plant with zero waste.

Why microalgae? Use of microalgae offers significant advantages such as: sustainable supply (can be cultivated throughout the year and in most climates), fast growth rate, maximum biomass production, relatively high photosynthetic efficiency, minimum pre-treatment (maceration), no use of arable land and CO_2 capture & storage-a carbon neutral process for energy from sunlight. In general, algae biomass contains 20-30% carbohydrate, 10-20% lipid, and 40-60% protein. The ratio of the algae's composition fractions influences the effect of catalysts (K_2CO_3 or NaOH) and gasification products; of particular interest for this project is the protein fraction in microalgae, as it known to have adverse effects on gasification efficiencies, hydrogen generation and catalyst performance. Hence a key work package will be to study and understand these interactions. In the cultivation process; researchers have been able to manipulate microalgae growth conditions to favour a particular fraction (For example, under nitrogen limitation, microalgae tend to produce more lipid than carbohydrate and protein).The challenge of minimising protein fraction is another key goal of the project.

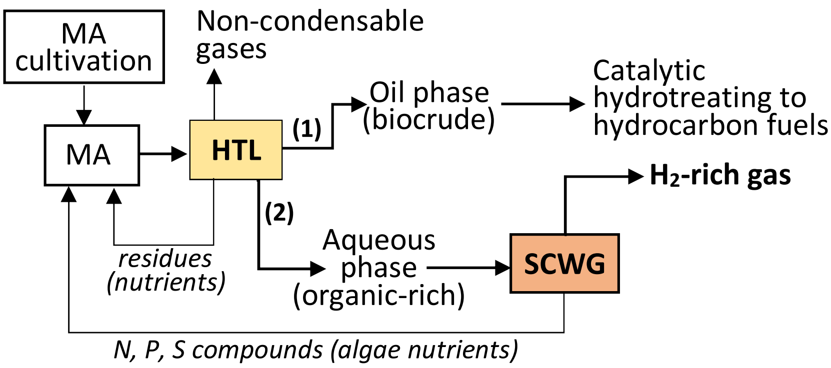

Figure 1. Conceptual diagram of the Process

Deliverables

- Designed HTL unit with flexibility of path towards desired final product(s).
- Designed SCWG unit to maximise H_2 production and recovery.
- Fully designed, energy integrated continuous process to convert feedstock microalgal biomass to H_2-rich gas, with maximum efficiency and minimal waste.
- At least 2 scientific publications and presentation of work in at least 2 relevant international conferences.

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Metal membranes for separating pure hydrogen from gas grids

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Project description

Hydrogen is widely regarded as a promising alternative to carbon-based fuels. However, developing hydrogen as a major energy carrier, will require solutions to many technological challenges, such as how to economically provide ultra-pure hydrogen for use with PEM-FC applications.

Hydrogen produced from natural gas reformers and from biomass sources, usually contains small amount of impurity gases, such as carbon monoxide, methane, and sulphur. Also, if hydrogen is distributed via pipelines, it tends to pick up various impurities. A PEM Fuel Cell (PEM-FC) converts hydrogen and oxygen gases into electricity; however, even very small amounts of impurities in the hydrogen can reduce the operating life of the PEM-FC.

Metallic diffusion membranes can be used to purify hydrogen. When certain Pd-based alloy foils are heated to about 300 °C, they will only allow hydrogen gas to pass through, resulting in parts-per-billion level pure hydrogen. However, the conventional Pd-Ag membrane alloy used is extremely expensive, and there are not able to tolerate certain impurities (i.e. they can be poisoned).

This project will investigate Pd-based alloys, which contain: (1) much lower amounts of Pd, which theoretical studies have suggested should have good hydrogen permeability values; and (2) additions that change the surface chemistry of the alloys (i.e. could make them more resistant to poisoning).

Deliverables

- Pd alloy foils and/or supported films with improved resilience to: (i) natural gas; and (ii) impurities and odorants likely to be found in converted hydrogen gas pipelines
- Lower cost Pd alloy membranes, via changes in composition and processing
- Design of system for Metal Membrane gas separation for integration with gas pipelines (CH_4/H_2 and H_2 grids)

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Modified transition metal catalysts for hydrogen and oxygen evolution

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Project description

Transition metal dichalcogenides (TMDs, eg MoS_2, WS_2) have been the subject of intense research in recent years as low-cost catalysts for H_2/O_2 evolution. The chemistry of the catalytically active sites is currently becoming more understood, and this project seeks to build on these recent advances through: (i) maximising edge sites through controlled TMD electrodeposition forming porous structures, (ii) modifying the catalytic sites through metal doping, (iii) optimising the stability of active sites.

Deliverables

- High impact publication

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Zero net-carbon fuels based on renewable hydrogen and bio-carbon

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Project description

Large scale hydrogen production currently lacks the infrastructure to be widely distributed. Projects today aim at converting whole sections of the natural gas grid to 100% hydrogen, a process that will take several decades and will not contribute to the GHG abatement goals set by the government.

Instead, synthetic methane could be injected into the natural gas grid with no changes to the infrastructure, transporting green hydrogen energy. If the carbon used in the synthesis is sourced from biological origins, the net carbon balance will be zero or even negative, depending on application and source.

A number of methane synthesis processes are known today. Nevertheless, depending on the use of carbon monoxide or dioxide in the synthesis, different catalysts and process parameters (pressure and temperature) are required.

The project will seek to identify optimised catalyst and operating parameter combinations, especially with a view on integrating the methanation process with a reversible high temperature fuel cell in co-electrolysis mode.

Deliverables

- Month12: literature review for publication.
- Month 18: systematic analysis of catalysts and processes.
- Month 24: test reactor built, ready for testing.
- Month 36: variety of catalysts integrated and tested.
- Month 48: systematic testing of catalysts and operating conditions concluded, operating conditions described and optimised.
- This PhD will produce a number of papers that will be targeted at high-impact journals.

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Inherently Safer Fuelling of Hydrogen Storage Tanks

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Project description

The inherently safer fuelling of a hydrogen storage container is a challenging problem. Independent on a container design, materials used, its volume, initial and nominal working pressure (NWP), temperature of delivering hydrogen, the regulation and standards require that the temperature inside the tank doesn't exceed 85°C, the pressure does not exceed 1.25×NWP, i.e. 87.5 MPa for 70 MPa onboard storage tanks, and the State of Charge (SOC) does not exceed 100%. The consumer expectations include the fuelling time of onboard storage of passenger car within 3 min. Longer fuelling time is acceptable for busses. The problem of fuelling control is complicated by changing pressure and temperature inside the tank and at inlet, changing diameter of fuelling nozzle to keep a required pressure ramp profile, requirements to the fuelling time, conjugate heat transfer from/to hydrogen through a piping system and a tank wall to/from the ambience, use of wall and liner materials of different thermal conductivity, thermal capacity, etc. The aim of this doctoral study is development and validation of CFD (Computational Fluid Dynamics) and reduced models for better understanding and reproduction of underlying physical phenomena of hydrogen tank fuelling (both onboard and stationary). The models should be used for prediction of thermal behaviour of different systems "hydrogen storage at refuelling site – piping system – dispenser – hydrogen storage tank – atmosphere" during fuelling. The research results will be used for the establishment of inherently safer and automated hydrogen fuelling protocol.

Deliverables

- Critical literature review
- Reduced model formulation
- CFD model formulation
- Validated reduced model
- Validated CFD model
- Recommendations for the update of regulations, codes and standards

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Explosion-Free in a Fire Composite Storage Cylinder for Compressed Hydrogen

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Project description

The main unresolved issue associated with onboard compressed hydrogen storage is a catastrophic rupture of lightweight composite pressure vessel (CPV) in a fire. Fire resistance rating (FRR) of today's CPV, i.e. time in a fire before rupture, is only 3-12 min. This is comparable with time of self-evacuation from a car at an accident scene and arrival of first responders. There were 23,100 road vehicle fires in Great Britain in 2013-14. Catastrophic rupture of CPV in a fire is a serious threat to life and property as reported elsewhere. Such accidents are not acceptable and should be excluded through the innovative engineering of CPV. The proposed project seeks to resolve this key safety issue through the further development and validation of the breakthrough leak-no-burst (LNB) safety technology for prevention of CPV catastrophic rupture in a fire, and thus eliminating hazards and associated risks from disastrous blast wave, fireball, and projectiles. Inherently safer compressed hydrogen storage systems will support the deployment of greener, secure and affordable energy supplies, particularly in low carbon transport sector, helping UK to meet its ambitious carbon emissions targets. The safety goal for hydrogen fuelled transport is to provide at least the same level of hazards and risk as for gasoline vehicles, which is not yet the case due to catastrophic failure of onboard storage in a fire. This academic research is strongly linked from the beginning with industry, both directly and through standard development organisations (SDOs) and regulators (UN GTR#13 IWG SGS). The project results will be used for the update of Regulations, Codes and Standards (RCS). The three main working directions are based on the LNB safety technology following Ulster University's Intellectual Property (PCT International Application P119851PC00 "Composite Pressure Vessel for Hydrogen Storage", filing date 14 February 2017). The project aims to develop a breakthrough explosion-free in a fire leak-no-burst (LNB) safety technology for CPV for hydrogen storage. The technology excludes catastrophic rupture of CPV in fire conditions and does not require the use of thermally activated pressure relief devices (TPRD).

Deliverables

- Review of hazards and risk analysis
- Typical accident scenario
- Library of thermal properties of materials relevant to CPV design
- Validated model of CPV performance in a fire
- CPV fire tests to validate LNB technology
- Recommendations for the update of RCS

Sustainable Hydrogen

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Prevention and Mitigation of Accidents with Hydrogen-Powered Vehicles in Confined Spaces

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Project description

The specific hazards and associated risks of hydrogen vehicles use in tunnels are largely unknown and thus prevention and mitigation strategies are not developed or validated. Previous activities were mainly focussed on the fire scenarios with fossil fuels and did not address the hydrogen specific hazards, like pressure and thermal effects during accidents related with high pressure hydrogen storage. Therefore, Regulations, Codes and Standards (RCS) require a scientifically sound basis for the understanding of relevant safety aspects, validated engineering models and tools for reliable prediction of an accident dynamics in confined space, and development of innovative prevention and mitigation strategies and engineering solutions. The main unresolved safety concerns include but are not limited to: what are requirements to hydrogen-powered vehicles entering confined structures such as tunnels, what are appropriate venting strategies for confined and congested space, what are hydrogen specific prevention and mitigation concepts to efficiently tackle hydrogen dispersion and combustion, would hydrogen pressure and thermal effects impact the integrity of tunnel structures, e.g. concrete spalling, how may an initiating event lead to devastating consequences through the domino effect, and how to prevent catastrophic rupture of a high-pressure hydrogen tank in a fire to eradicate any possibility of devastating blast waves and fireballs in these confined traffic infrastructures, which are generally perceived as hazardous sceneries per se. These knowledge gaps and technological bottlenecks in hydrogen safety hamper the further inherently safer deployment of hydrogen-powered vehicles, and the public acceptance of the technology.

The scope of this doctoral study could include: identification and prioritisation of relevant knowledge gaps; performing analytical and numerical studies to close identified knowledge gaps; development of innovative safety strategies and engineering solutions to prevent and mitigate accidents with hydrogen powered vehicles in confined infrastructure, e.g. due to pressure peaking phenomenon in garage-like enclosures; determination of specific hazard and risk relevant parameters; development and validation of novel engineering tools, required for the hazard and associated risk assessment; evaluation of effectiveness of conventional and innovative prevention and mitigation techniques and accident management strategies with respect to the specific hazards implied with hydrogen use in the confined infrastructure, etc.

The expected impact of the study could include but is not limited to: validated contemporary models and tools for hydrogen safety engineering and use of hydrogen transport systems in confined environment; deeper knowledge of the underlying physical phenomena; innovative prevention and mitigation strategies; guidelines for inherently safer design and use of hydrogen systems in confined infrastructures; elimination of the possibility of a “spectacular”, high consequences tunnel catastrophic accident with serious impact on the public acceptance of hydrogen technologies (the “show stopper”).

The study will focus on computational fluid dynamics (CFD) modelling, use of the relevant software (FLUENT, OpenFOAM, etc.), multi-processor Linux-based hardware, etc. The results of this doctoral research will be used in HySAFER’s externally funded projects and should be reported at international conferences. Publication of results in peer reviewed journals is expected.

Deliverables

- Critical literature review of hydrogen vehicles hazards and accidents, accidents prevention and mitigation strategies in tunnels and similar confined structures
- Numerical model(s) formulation to predict pressure and thermal hazards from onboard hydrogen tank rupture in a tunnel
- Validation of the numerical model(s)
- Recommendations for the update of RCS

Sustainable Hydrogen
CENTRE FOR DOCTORAL TRAINING

Pressure and Thermal Effects of High-Pressure Hydrogen Jets

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Project description

High-pressure hydrogen jet releases, if ignited, can generate not only thermal effects on humans and structures in the form of high-temperature flows and thermal radiation but also hazardous pressure effects (overpressure and impulse). A hydrogen jet released into the air may be ignited immediately, resulting in a jet fire, i.e. non-premixed turbulent combustion, or after some time, resulting in delayed ignition, whereby the combustion of the turbulent premixed hydrogen-air cloud can lead to significant overpressures before a jet fire is formed. Contemporary tools such as Computational Fluid Dynamics (CFD) and reduced models are needed to predict pressure dynamics and loads which are dependent on the release parameters (pressure and release diameter), jet parameters (free or impinging jet), ignition location and delay in timing of ignition, etc. Within this study such tools will be developed and validated against available experimental data. Results of CFD simulations can be used to inform the development of predictive engineering correlations. The results of the studies on impinging jets will have a twofold application facilitating the understanding of the potential damage caused but also informing understanding of the mitigation potential of a structure, dependent on whether the jet impinges on a piece of equipment/infrastructure or a barrier. Scenarios involving delayed ignition of turbulent releases in enclosed or congested spaces may be added to the study. The Ulster multi-phenomena deflagration model with suitable modifications can be employed for the CFD modelling of combustion of the turbulent inhomogeneous hydrogen-air mixture in the jet. The candidate should undertake coupled CFD-Finite Element Method (FEM) study of hydrogen jet fire effects on structures stability and integrity, e.g. tunnel structures, residential buildings, etc. The outputs from this study will inform guidance for safety engineers, and advance understanding of delayed ignition of hydrogen jets.

Deliverables

- Critical literature review
- CFD and/or CFD-FEM model formulation and development
- Validation of CFD and/or CFD-FEM model
- Engineering correlation(s) to predict hydrogen jet fire hazards
- Recommendations for the update of RCS

Sustainable Hydrogen
CENTRE FOR DOCTORAL TRAINING

Safety of Liquified Hydrogen in Energy Applications

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Project description

Liquified hydrogen (LH2) is the most efficient way to transport hydrogen over large distances at emerging state of hydrogen infrastructure when pipelines are not yet available to deliver hydrogen to refuelling stations and homes. This is the inherently safer way to store and distribute large amount of hydrogen at refuelling stations. The development of innovative safety strategies and engineering solutions for LH2 systems and infrastructure requires fundamental understanding of underlying physical phenomena and validated engineering models and tools for safety design. The models and safety measures to prevent and mitigate accidents involving LH2 systems and infrastructure have to be developed. The following phenomena have to be studied yet to underpin the development of the technology: multiphase release and dispersion of LH2 in the open atmosphere and confined spaces; release and dispersion of cryogenic hydrogen; thermal hazards from low temperatures; ignition parameters and flammability limits of cryogenic hydrogen; explosion of LH2 tank in BLEVE (Boiling Liquide Expanding Vapour Explosion) regime; pressure and thermal loads from LH2 and cryogenic hydrogen combustion in confined and congested areas; etc. The suitability of available tools for gaseous hydrogen to releases of LH2 and cryogenic hydrogen should be critically analysed. Novel analytical and numerical tools for calculation of hazard distance for LH2 and cryogenic hydrogen should be developed based on an improved understanding of the underlying physics. The developed models must be validated against experimental data that is obtained in collaboration with H2020 project PRESLHY.

Deliverables

- Critical literature review
- Analytical and/or numerical models for assessment of hazards associated with the selected LH2 accident scenarios
- Validation of analytical and/or numerical tools
- Peer-reviewed publication(s)

University of Nottingham UK | CHINA | MALAYSIA
Loughborough University
UNIVERSITY OF BIRMINGHAM
Ulster University
EPSRC Engineering and Physical Sciences Research Council

Sustainable Hydrogen
CENTRE FOR DOCTORAL TRAINING

Assessment of Hazards of High-Pressure Hydrogen Tank Rupture Using Coupled CFD-FEM Modelling

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Project description

Hydrogen fuelled vehicles are being deployed as a part of the deep decarbonisation strategy. Hydrogen fuelled cars are expected to provide the same level of experience and comfort as fossil fuel vehicles including driving range of at least 400-500 km, which requires 4-5 kg of hydrogen onboard of a car. Use of gaseous hydrogen stored in composite pressure vessels at pressures 700 bar and higher is the main-stream solution for onboard hydrogen storage including light-, medium and heavy-duty transport applications. Fire resistance of modern composite tanks is about 3-12 minutes, which makes rupture of such tanks a major safety challenge in case of pressure relief device failure. Blast wave and fire ball following the high-pressure tank rupture in a fire represent its major pressure and thermal hazards threatening life and property losses. Analysis of experimental data proves that the car deformation and displacement (1) expends significant amount of mechanical energy of compressed hydrogen, (2) affects hydrogen combustion and fireball dynamics. Thus, hazards analysis methods for open atmosphere tank rupture, including Computational Fluid Dynamics (CFD), are not applicable to real onboard storage (often mounted under a vehicle). Analysis of car deformation and displacement is essential to predict pressure and thermal loads on humans and structures, which is typically accounted using Finite Element Methods (FEM). The project aims to develop a coupled CFD-FEM model applicable to analysis of onboard tank rupture in a wide range of conditions – tank volume, pressure, mounting position on a vehicle; vehicle location (open atmosphere, workshop, tunnel etc.). ANSYS family of Fluid and Structure computational tools will be used as a platform for model development. Experimental data available in the literature and to be obtained in ongoing FCH-JU HyTunnel-CS project will be used for the model validation. Outcomes of this project will inform car OEMs, health and safety authorities, fire and rescue services about hazards of potential hydrogen-fuelled vehicle fire accidents. The research results will feed development of engineering methodology to assess blast wave overpressure and fireball size in the event of catastrophic tank rupture and development of appropriate prevention and mitigation strategies.

Deliverables

- Critical literature review
- Problem formulation for the coupled CFD-FEM model
- Coupled CFD-FEM model implementation
- Validation of the coupled CFD-FEM model
- Formulation of recommendations for mitigation of the onboard tank rupture accidents
- Peer-reviewed publication(s)