Sustainable Hydrogen

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2023 – SusHy Projects Booklet

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Enhancing the understanding of ammonia/hydrogen combustion via engine testing and analysis

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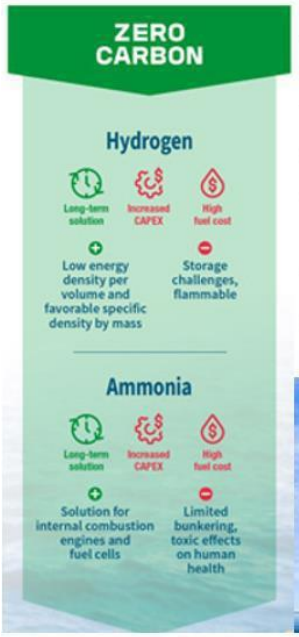
Project description

The overall goal is to improve understanding of the fundamental of ammonia/hydrogen combustion in internal combustion engines. The interactions fuel injection system (i.e. CMB.TECH mixing ring), engine operating conditions and combustion characteristics, with particular focus on emissions and performance are of interest. The ultimate goal is to anticipate how CMB.TECH can successfully enable marine vessels to employ ammonia as a propulsion fuel source.



Ammonia combustion expected to be suitable for maritime sector; but several challenges to be overcome in ammonia combustion, such as low flammability, high NOx emissions.

Deliverables

- Novel enzymatic Full test and emissions characterisation data
- Database relating operating conditions to combustion characteristic and emissions

Stakeholder collaboration: CMB-TECH

CMB.TECH

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Bioinspired catalysts for green hydrogen production technologies: natural and artificial metalloenzymes

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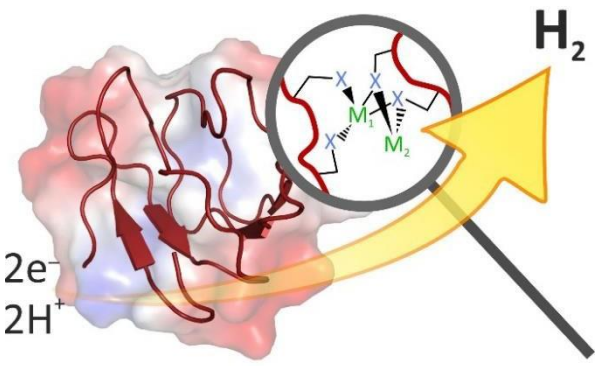
Project description

Nature is highly efficient at producing and utilizing hydrogen. In this project we will learn from the natural catalysts for hydrogen reactions, the hydrogenase enzymes, in order to design robust and sustainable bioelectrocatalysts for green hydrogen production. While hydrogen technologies are fast-approaching everyday life, it becomes crucially important to ensure that these are fully sustainable. Full implementation of "green hydrogen" (*i.e.* H_2 generated from renewable resources rather than fossil fuels) requires the availability of clean catalysts that can easily reduce protons from water into molecular hydrogen. Water electrolysers rely on rare noble metals, such as platinum and palladium, that are unsuitable for large scale operations for both economic and sustainability reasons. In nature, hydrogenase enzymes rely exclusively on cheap and abundant metals (iron and nickel) to produce hydrogen at high efficiency and extremely fast turnover rates. Unlike synthetic chemo-catalysts, enzymes can be produced entirely from renewable feedstocks and have a very low metal requirement. Previous studies have shown that hydrogenases can be embedded in artificial devices and can effectively produce hydrogen. However, the performance over time is low, due to inherent protein instability. This project will develop novel artificial metalloenzymes (ArM) with improved stability, to be integrated into hydrogen evolution devices. In the first phase of the project, small and robust proteins will be used as scaffolds to build bimetallic clusters (either FeFe or NiFe) that mimic those found in natural enzymes. The electrocatalytic features of these artificial enzymes will be tuned by modifying the local environment hosting the metal cluster by either protein engineering (first and second coordination sphere) and organometallic synthetic methods (non-protein ligands). In the second phase of the project, the artificial metalloenzymes will be tested for electrocatalytic H_2 production and compared with existing oxygen-tolerant natural hydrogenases available in our laboratory. Both natural and artificial enzymes will be immobilised on electrodes and the hydrogen evolution reaction (HER) will be characterised under standard conditions. In collaboration with our partners at QUB, the electrodes will be modified by applying bespoke conductive gels that will protect the enzymes and further improve stability. This will enable thin layers of bioelectrocatalyst to be coated on electrodes, whilst providing an engineered environment to protect the protein. Ionic liquids will be studied as electrically conducting co-dopants that have a proven track-record of protein stabilisation.



Deliverables

- Novel enzymatic catalysts for hydrogen generation based on earth abundant (Fe Ni) centres.
- Fabrication and validation of gel-protected electrodes for bioelectrochemical exploitation of hydrogenases

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Water splitting beyond the volcano plot

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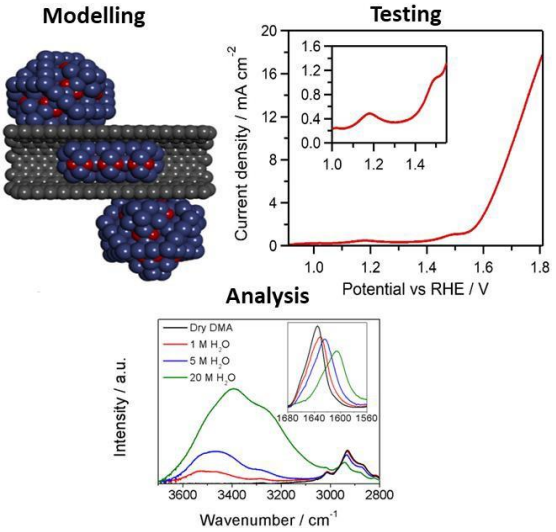
Project description

Advances and understand of electrocatalysis have reaped significant improvement in the performance of fuel cell catalysts. While similar improvements in understanding have been achieved in water splitting, this has not translated to enhancement in electrocatalysis of these reactions. Primarily, this is due to the instability of bulk oxygen evolution catalysts at higher anodic potentials, under which metal leaching and performance fading is common, and common volcano relationship due to intermediated binding. However, they these limitations are NOT inevitable. Here we propose to build on our expertise in non-aqueous oxygen electrochemistry to develop new theory and catalysts for water splitting. Leaching of active metal sites occurs because multivalent metal oxides are partially soluble (and thus corrode) in aqueous environments, but a transition to non-aqueous/water mixtures would drastically alter the solvation chemistry and thus the performance and stability of the catalyst. Our recent work has revealed the principles that control protic aqueous reactions in water water/organic mixtures, and this will provide the foundation from which we will optimise catalytic performance. Unlike catalysis in aqueous environments, which rely solely on surface adsorption at active sites, we will tune reaction profiles by solvation (due to the rich solution chemistry available in water/organic mixtures). Working with two activity descriptors will allow us to overcome the hard thermodynamic limits (volcano relationships) found in conventional water splitting. Concurrently, these systems will be designed to reject multivalent ion solvation which will enhance catalyst stability and lifetime.



Deliverables

- New models that extend electrocatalytic theory to aprotic liquids.
- Electrolyte/catalysis combinations that offer improved stability and long-term performance for H_2O electrolysis compared to conventional aqueous based systems.
- First prototype demonstration.

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Machine Learning Discovery of Electrocatalysts for Sustainable Hydrogen Production

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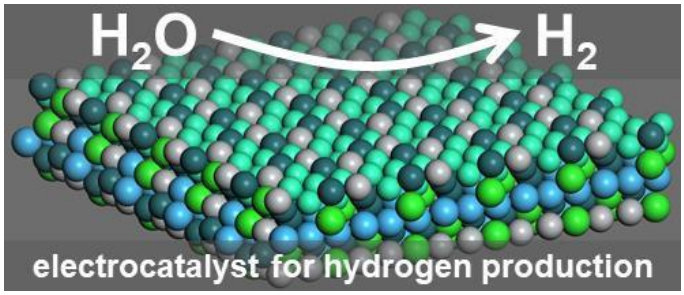
Project description

Sustainable production of green hydrogen from water splitting using renewable energy sources such as wind and solar is a very promising approach for both short-term balancing and long-term inter-seasonal energy storage. Development of efficient, stable and cheap electrocatalysts is of paramount importance to large scale green hydrogen production. The chemical compositional space of electrocatalysts is too large to be explored efficiently using pure experimental approaches. Discovery of new electrocatalysts for hydrogen production can be significantly accelerated by a combination of density functional theory (DFT), machine learning (ML), and experimental approaches. It has been demonstrated that the free energy of hydrogen adsorption can be used to quantify the activities of different electrocatalysts in the hydrogen evolution reaction. In this project, we plan to perform high-throughput DFT calculations of hydrogen adsorption on carefully selected high-entropy alloys (HEAs), and we will use these data to train an accurate ML model. Our ambition is to screen the HEA compositional space *exhaustively* using the ML model, in order to identify efficient and cheap HEA electrocatalysts for green hydrogen production. Working alongside our local and international experimental collaborators, the most promising candidate HEA electrocatalysts discovered from the ML screening will be synthesised and characterised, and their activities for electrocatalytic hydrogen production will be validated by experiments.



Deliverables

- Database of high entropy alloys with DFT predicted structural and thermodynamic properties on hydrogen adsorption
- Machine learning model for predicting the free energy of hydrogen adsorption on any given HEA surface

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Sustainable catalysts for low temperature and pressure ammonia synthesis

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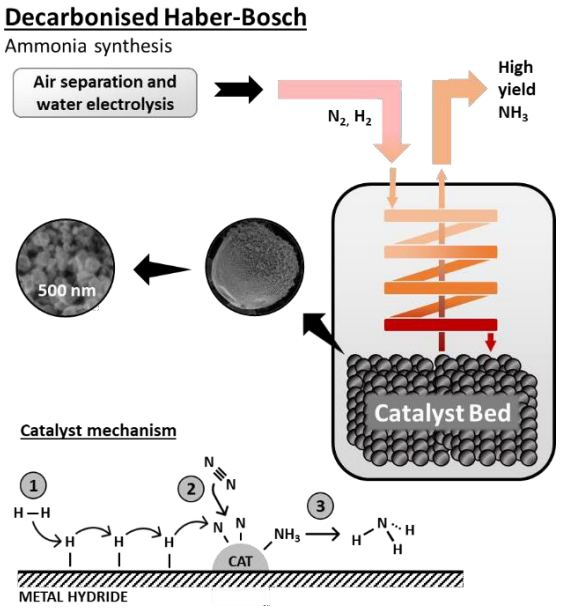
Project description

There is a lot of interest in using ammonia as a hydrogen rich energy vector, not just for the more efficient moving of energy to different markets, but also direct combustion of ammonia as a fuel to help decarbonise heavy vehicles such as for road freight, rail and marine sectors. Ammonia is produced industrially through the Haber Bosch process, but needs high temperatures (300 - 450°C) and high pressures (150 – 200 bar). Unfortunately, this makes the process unsuitable for smaller scale intermittent generation of ammonia for example distributed generation coupled with either wind or solar renewable energy. A more agile ammonia synthesis requires a catalyst that can operate at lower temperatures and lower pressures.

Currently ruthenium is the only catalyst that has acceptable kinetics at low temperatures. This project will investigate more sustainable catalysts that avoids the use of resource limited platinum group metals. The novel catalyst design will utilise transition metal alloys, supported on metal hydrides. The metal hydride will act as a hydrogen pump, supplying hydrogen to the catalyst enabling rapid hydrogenation of the adsorbed nitrogen. Catalyst will be deposited onto metal hydride supports using magnetron sputtering to control the catalyst coverage, but also to investigate compositional change of the deposited catalyst through graded deposition.



To produce several test transition metal alloys that dissociate nitrogen effectively (i.e., substitute to Ruthenium) and successfully magnetron sputter (PVD) coat onto an effective hydride support, which dissociates the hydrogen efficiently. Catalyst activity will be compared with the material characteristics in order to optimise the design of the catalyst and hydride support.

Deliverables

- Identified transition metal catalysts with comparable activity to ruthenium.
- Optimised catalyst coating onto metal hydride particulates.
- Maximise the synergistic effect between the catalyst and metal hydride support.
- Experimentally validate the catalyst efficacy during intermittent operation.

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Advanced characterisation of hydrogen storage alloys by in-situ X-ray photoelectron spectroscopy

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Project description

Often, metal hydride systems that can be cycled under relatively mild temperatures and pressures, need quite extreme conditions in order to initially activate them. Understanding the barriers to activation will be a major step forward in the design of easy to activate metal hydride systems. XPS is the most powerful technique for exploring the chemical and electronic structure of surfaces. It can tell us exactly what atoms are present in the sample surface and in which chemical state. It is extremely surface sensitive, allowing us to explore the atoms and molecules at the very edge of a material – where all the interactions with a gas environment take place. This is particularly important for hydrogen storage materials since the surface atoms are the gateway to the rest of the material. Oxygen atoms at the surface, the oxidation states of the metal atoms, and the stoichiometry are all likely to play a role, especially in the initial activation step of the materials that currently imposes more extreme conditions than the storage and release processes. Combined with depth profiling via argon sputtering, XPS can also probe layer by layer into the material to follow the diffusion of the oxides and preferential segregation of different metal species.

This project will use two state-of-the-art XPS instruments at the University of Nottingham. The first is a near-ambient pressure XPS (NAP-XPS) that can operate at pressures from 10^{-10} mbar to 25 mbar of H_2 and other gases. This will be used to the interaction of H_2 with the surface and depth profiling of materials. It is also equipped with mass-spectrometry to measure any volatile components that leave the surface during heating in low pressures of H_2. The second is a unique, custom built instrument developed through SusHy CDT research that can rapidly take a material under vacuum from a reaction chamber replicating the activation process at high temperature and high pressure (10 bar H_2) into the XPS analysis chamber for characterisation in under 60 seconds.

Deliverables

- An in-situ XPS instrument for characterising hydrogen storage materials.
- Improved hydrogen storage alloys with lower activation conditions.

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Sustainable hydrogen production from wastewater with renewable energies

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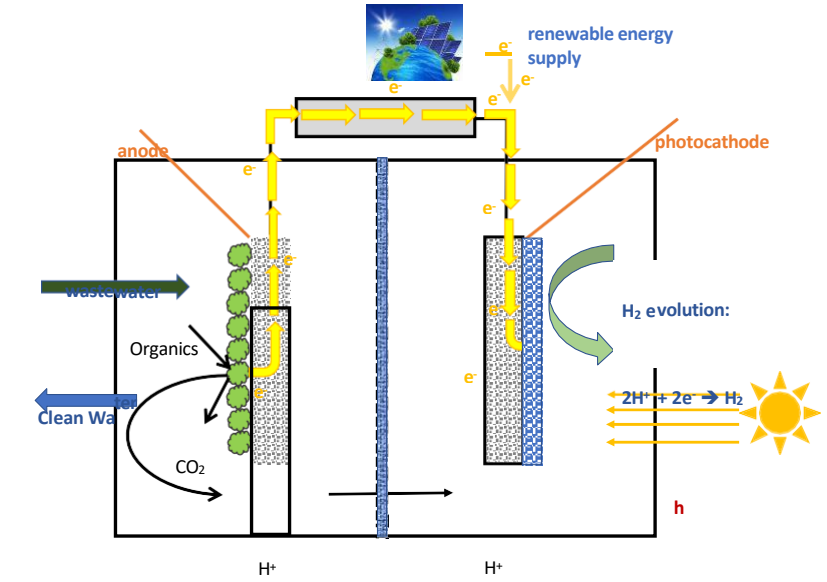
Project description

UK has a legal obligation to achieve net-zero greenhouse gas emissions by 2050. Hydrogen will an important component in our quest for transition to low-carbon or zero-carbon energy network. Currently hydrogen is mostly produced through petrochemical route with Steam Methane Reforming, which has high carbon footprint and not sustainable. Other technologies, such as Catalytic Methane Decomposition from biomass, electrolysis and Solar water splitting have demonstrated potentials utilising renewable resources. However, the cost for expensive catalysts and materials, as well as high energy demands are challenges to tackle. Currently Water industry is consuming 3% of UK's electricity for aerating, pumping and treatment of wastewater, the fourth most energy-intensive sector in the UK. It is responsible for 5% of the 200 million tonnes/year of greenhouse gas emission in the UK. On the other hand, the internal chemical energy of mixed wastewater is around 16.8 MJ/tonne, and domestic wastewater has 7.6 MJ/tonne. With 11 million tonnes of wastewater collected everyday in the UK, the energy in the total wastewater could be up to 51.3 GWh/day.

Bioelectrochemical systems (BES) are emerging technology use whole microorganisms as the biocatalysts to harness energy in wastewater by oxidising organic matter to generate electrons which flow between the anode and cathode. The electrons and protons produced are used on the cathode for reduction reactions, such as hydrogen evolution (HER) in microbial electrolysis cells (MECs), resulting in reduced overall energy demand for hydrogen production. From our previous research, while removing organic matters from wastewater, the bioanode is able to provide 1/3 of energy required, or reduce overpotential up to 200 mV for hydrogen production [1,2]. However, the current density of MECs is low and resulted in low hydrogen yield. The rapid development of photoelectrochemical systems (PEC) utilisation solar energy provides a possible solution with hybrid system combining MEC and PECs harnessing the synergy from both waste and solar energy. Recent study showed 23mA/cm2 was achieved with such hybrid system without additional electricity input [3], which makes this a promising technology with potential for large scale applications. In this project, technology development on novel materials and reactor designs to achieve high efficiency and yield in HER with wastewater and low cost materials will be investigated; evaluation of this technology in terms of life cycle assessment (LCA) and technology economic assessment (TEA) to compare the technology with other hydrogen production technologies will also be conducted using the data from technological study. Our industrial partners Argent Energy will be actively involved in the project development and progress by providing wastewater samples, access to the manufacturing sites, providing data and access to facilities. We envisage the project not only advancing technology for water industry with low cost, sustainable system simultaneously treating wastewater and efficiently generating hydrogen, but also providing reasoning and understanding of the influence of the novel technology, in terms of carbon budget and social economic impacts to change high energy demand and carbon emission industrial sectors towards Net zero and achieving clean growth.



Anode
$C_xH_yO_z + (2x-z)H_2O \rightarrow (y+4x-2z)H^+ + xCO_2 + (y+4x-2z)\ e^-$

membrane

Deliverables

- Providing multidisciplinary training to a PhD student with skills in Engineering, chemistry, biotechnology and social economics, problem solving and critical analysis at the SuSHy CDT.
- Design and prepare reactors for hydrogen production with BES and PEC.
- The work will provide feasibility and evidence for further collaborative with water industry and larger UKRI proposals.

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Machine-Learning-assisted multiscale modelling and optimisation of sustainable hydrogen production by electrolysis of biomass wastes and water

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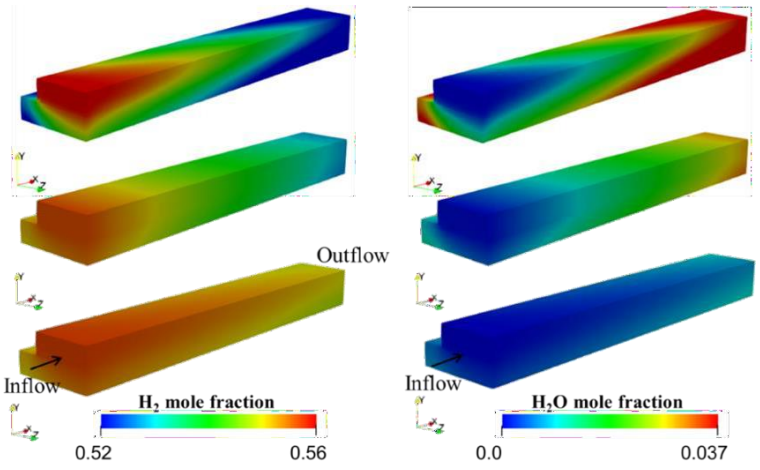
Project description

Delivering green hydrogen production at scale presents considerable challenges, but also offers enormous potential towards achieving net zero carbon targets. Using renewable energy sources to power the electrolysis of water provides a clean and green route to produce hydrogen that can act as a form of energy storage, and can subsequently be used in fuel cells for a convenient and mobile mode of clean electricity generation with only water as by-product. Recently, novel electrochemical methods have been proposed for co-production of both hydrogen and important chemicals using waste biomass and water as feedstocks. Despite these new opportunities, key challenges remain to deliver the potential contribution of electrochemical hydrogen production to a more sustainable future.

We propose to build multiscale simulations of electrolysis systems in order to achieve optimised engineering design and operation for hydrogen production using renewable power supplies and sustainable feedstocks. We will develop models to represent the complex physical and chemical phenomena taking place within electrolysers at multiple length- and time-scales, ranging from multi-catalyst composition and electronic synergies, electrode and membrane material microstructure, chemical reaction kinetics, multi-phase flow, flow of charge, heat transport, and interfacial effects (gas/liquid/solid boundaries). We will adopt multiple modelling techniques from the molecular scale (MD), through multi-dimensional microscopic models (FE, LBM) and reduced-dimension models up to whole-stack models; these will be integrated with machine learning techniques to deliver rapid, physically meaningful surrogate models that can deliver the multi-objective optimisation required for these complex systems.



Deliverables

- A toolkit for integration of models across length scales for multi-scale optimisation
- Machine learning surrogate models to implement within optimisation
- Multi-objective optimisation toolbox for design and operation
- An optimised design for co-production of hydrogen and chemicals

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Understanding the lifecycle carbon footprint and costs of sustainable hydrogen energy systems

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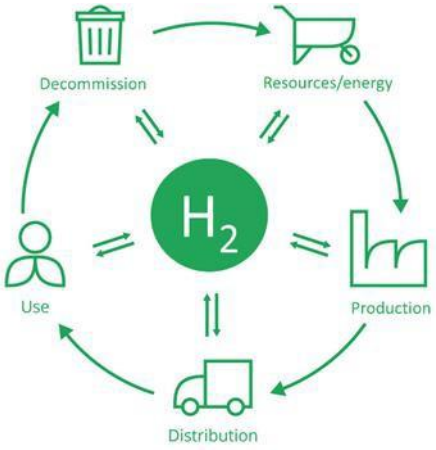
Project description

Hydrogen is considered as a clean fuel for the future. Yet it is important to recognize that its production, distribution, and usage may have negative impacts on the environment, society, and the affordability. Examining the carbon footprint, energy requirements, costs and social impacts from a life cycle viewpoint of different hydrogen technology routes (e.g., green turquoise or blue hydrogen) will form a complete picture of the sustainability of the future hydrogen technology options.

Here the research challenge is to gain insights into the whole energy and industrial system around the new hydrogen production and application routes over the entire lifecycle, instead of just looking at single point. Sustainability may only be assessed by means of a systems-wide approach, which combines economic, environmental, and social impact indicators. This project will combine system integration (SI), technoeconomic and lifecycle assessments (TEA & LCA) and multi-criteria decision making (MCDA) framework as essential tools, to enable such industrial symbiosis innovation, by systemic assessing hot spots of carbon footprint and their associated economic, environmental, and social impacts, and identifying opportunities for improvement at the whole industrial system level. We will integrate the aforementioned suite of whole system tools, and link them with a process digital twins to create a real-time assessment platform for the wider hydrogen systems. The innovative aspect is the proposed digital-twin informed MCDA framework embracing the SI, TEA, LCA and social impact data, allowing real time reflection of impacts with changing processes and technologies, and thus, enabling advisory features for sustainability-aware decision making during the early stage of sustainable hydrogen technology development.



Deliverables

- A novel methodology and framework that can systemically assess the life cycle carbon footprint, and their associated life cycle cost and environmental impact for novel hydrogen systems, infrastructures, and integrations; compared to the state-of-the art technology evaluations in the UK, Asia and global context.

Stakeholder Collaboration: Guangdong Longhu Sci & Tech company Lt

LONGHU 龙湖科技 Longhu Scl. & Tech.

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Social Hydrogen: H_S

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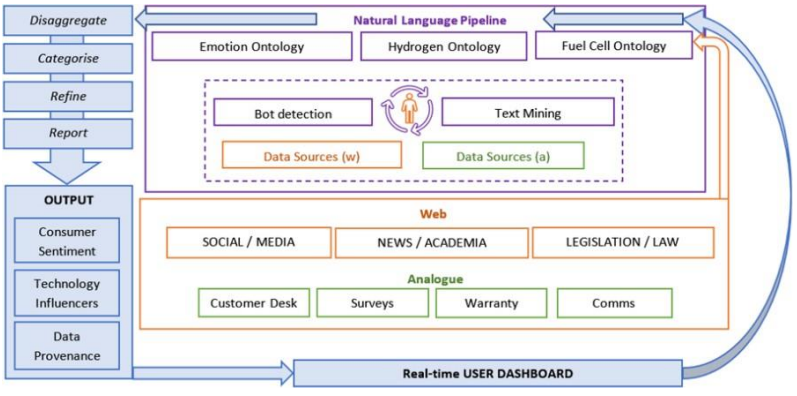
Project description

To move to the next generation of fuel cells not only requires the science but also the acceptance and demand from customers, which is influenced by the messaging, promotion, and support of critical public and private stakeholders. To fully understand the complex landscape (political, commercial and consumer) the project will develop a system of systems of ontologies that can mine information from social media platforms, publicly available commercial documents and government web sites and policy documents to build a real-time map of the drivers, inhibitors, perceptions and consumer influencers. The real-time analysis will provide semantic models of the landscape and have various lenses that will highlight the socio-technological change required e.g. the degree of uncertainty towards technologies and their use in everyday items like vehicles. In turn, this will direct how future messaging, policy, and advertising needs to be engineered to respond to the existing 'social' landscape.

The generic system of system ontology and real-time mapping capability will be trialled using an automotive case study, evaluating the use of hydrogen for the case study's transportation fleet. Current awareness and perceptions of hydrogen fuel cells suggest that demand for vehicles is extremely low due to many misconceptions and better publicity and support of alternatives e.g. battery. Specifically, this research will aid automotive companies in developing their next generation powertrain vehicle offerings (core and augmented), which will inform and aid the supply chain. It will also provide government with insights into the blockers and how they can enable a quicker route to net zero across the population. This project will take elements of an existing digital tool, EMOTIVE (developed and owned by the research team). However, a new architecture will need to be researched and developed for this proposed work including the system of systems ontologies. A new Hydrogen Natural Language Pipeline with semantic technologies will be developed within the system of systems framework.

The Team are well placed to deliver this project as they hold extensive experience in EMOTIVE technologies and years of experience in the hydrogen domain, as evidenced by the latest funded project *Robust Lifecycle Design and Health Monitoring for Fuel-Cell Extended Performance (RESILIENCE)* – (Supergen EPSRC EP/K02101X/1).



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Deliverables

- Sematic ontology of the hydrogen fuel domain
- Interrogatable semantic system to determine enablers, inhibitors/blockers, and key influencers
- Commercial facing dashboard for data segmentation and analysis
- Foundation for an automated digital text-mining interface.
- Interface for collaborators to interrogate the social map to aid decision making

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Reliability modelling of equipment engaged in the production (electrolysers) and usage of hydrogen

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Project description

This project aims to improve reliability and reduce degradation in equipment engaged in the production (electrolysers) and usage of hydrogen. Highly reliable and long-lasting systems are essential for the successful uptake and deployment of novel technologies. The release of an unreliable product can undermine the success of an otherwise promising technology. Despite electrolysers and users of hydrogen forming a technology cornerstone of a green hydrogen economy, there is very little research on their reliability at both the cell and system level.

This project will use advanced reliability techniques to establish reliability and degradation models equipment engaged in the production (electrolysers) and usage of hydrogen. These models will be used to examine the reliability of these systems, establishing key routes to failure and preventative action required to mitigate risk and reduce downtime.

The research will also establish new methodologies for assessing reliability, utilising the hybridisation of deterministic physics-based models with stochastic coloured petri nets. These will be augmented with machine learning methods to give capability for predicting lifetime in different applications. Models will be validated at the cell level through experiments and at the system level through data sharing and literature data. Novel experimental strategies for degrading cell/system performance to enable accurate reliability prediction will be investigated. This experimental framework will be transferable across applications yielding a ‘system level’ capability across platforms.

Deliverables

• Production of open-source experimental degradation dataset of equipment, engaged in the production (electrolysers) and usage of hydrogen at lab scale.
• Open-source reliability model equipment engaged in the production (electrolysers) and usage of hydrogen

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Low cost sustainable battolyser technology

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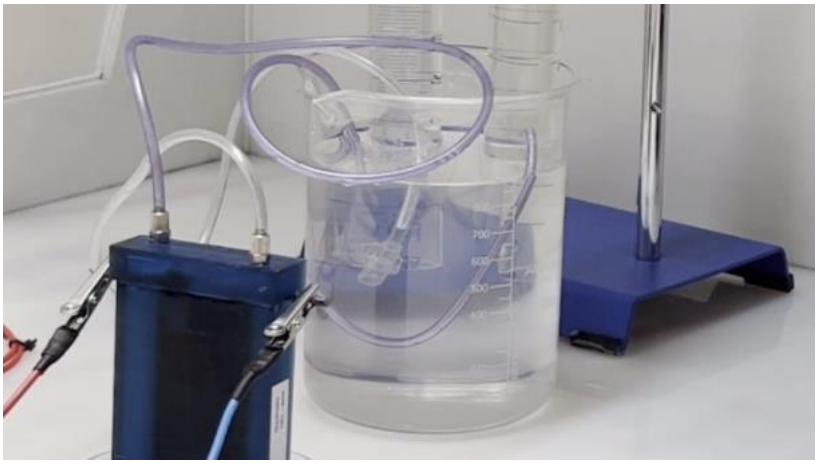
Project description

A battolyser is a battery/electrolyser combined in the physical form of a flow battery. It has the advantages that it can work with poor utilisation (e.g. from renewables) and flexible seamless switching. It also has the potential to be manufactured at lower cost than an electrolyser because it doesn't use rare earth catalysts. An additional advantage is that it can provide battery functionality.

This project will look at identifying, manufacture and testing of different battolyser chemistries to achieve minimum key performance targets on durability.



Deliverables

- Understanding the fundamental science questions responsible for degradation under battolyser operation
- Designing a battolyser using sustainability principles
- Small scale test rig and instrumentation produced for validating battolyser technology
- Test results analysed to check durability

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Smart Operation Management for Hydrogen Fuel Cell Vehicle Fleet

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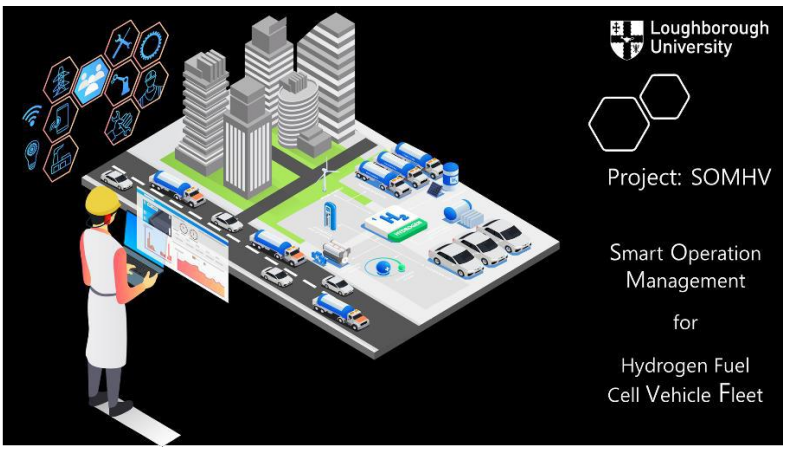
Project description

Hydrogen fuel cell demonstrates huge potential in deep decarbonisation of the energy system, which has been applied in many fields. Hydrogen fuel cell vehicles have been promoted to the core place in future product map in UK. The superior zero emission potential of hydrogen fuel cell vehicles will benefit to the acceleration of transition to net-zero emission stage. The popularization of hydrogen fuel cell vehicles comes across some barrier. Stubbornly high using cost, including expenditure in purchase, operation, maintenance and performance degradation, all discounts the uptake from consumer. Public transportation is one ideal platform to demonstrate the promising capacity of novel energy techniques. Hydrogen fuel cell buses have been put into operation in London, Belfast, Birmingham, and some other cities in UK. A lower operating cost will help to increase the competitiveness and prompt market acceptance of hydrogen fuel cell bus fleet. Therefore, it is quite necessary to conduct proper management on the operation of hydrogen fuel cell bus fleet. The fleet management including fleet time-table design, fleet operation speed coordinate, fleet operation cost optimization, etc.

The planned research will focus on operation cost optimization for hydrogen fuel cell bus fleet. The operation cost is the combination of expenditure in purchase, operation, maintenance, performance degradation and recycle for reutilization, which is the whole lifetime target. In the planned target, 3D virtual driving scenarios of the fleet and high-accurate fuel cell bus models will be constructed to underpin the management strategy design. Then, a smart fleet operation management strategy, which will manage energy flow within hydrogen fuel cell powertrain in each bus in the fleet, will be developed based on AI and advanced control theories with target to minimize total operation cost of the fleet. Corresponding test and validation will be conducted in a newly built hardware-in-the-loop simulator to justify capacity of the raised solution in practical application.



Deliverables

- 3D virtual scenarios of fuel cell bus fleet operation.
- Multi-scale fuel cell bus models (single-vehicle and vehicle-fleet level).
- Management strategies for fuel cell bus fleet operation

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High-order Large Eddy Simulation of hydrogen combustion under gas turbine conditions

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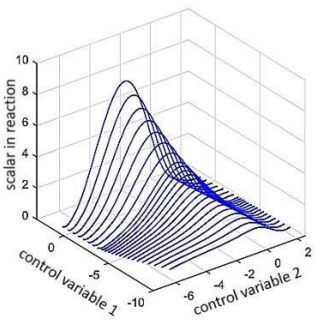
Project description

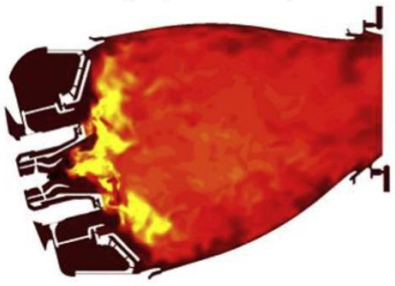
Lean hydrogen combustion for gas turbines is one of the main research topics in the nationwide effort to meet UK's net-zero target by 2050. With the development of high-performance computing facilities, Computational Fluid Dynamics (CFD) using Large Eddy Simulation (LES) has become an important numerical tool for the research of combustion. It can produce accurate data and physical details which are required in combustor design but difficult to be obtained reliably by lower-cost CFD methods such as Reynolds-averaged Navier-Stokes (RANS) simulation. Currently LES for combustion is predominantly based on the finite-volume (FV) formulation. Its computational cost is still rather high when used on industrial gas turbine geometries.

A recent study by Loughborough University compared the high-order spectral/hp element solver Nektar++ and the widely used FV solver OpenFOAM. It was shown that, at the same level of accuracy, the high-order solver is computationally 3-8 times cheaper than the FV solver for the LES simulation of non-reacting flows in representative industrial gas turbine geometries. To leverage the numerical efficiency of this spectral/hp element formulation, a high-order combustion solver is currently being developed by the principal investigator of this project within the high-order CFD platform Nektar++. The solver uses the Flamelet Generated Manifolds (FGM) method to model the chemistry in combustion. The FGM method typically adopts the approximation of equal diffusivity for different species and reduces the complex reaction chemistry to a precalculated table against several control variables which are solved for with the corresponding transport equations in the CFD solver. It provides a cost-efficient way to incorporate chemistry in combustion CFD and has been shown to produce accurate results for different hydrocarbon fuels. The applicability of the conventional FGM methods to hydrogen combustion is compromised due to the preferential diffusion of hydrogen. In this project a modified FGM scheme needs to be developed for the above high-order combustion solver. The problem will be addressed both at the stage of FGM table generation and when solving the control variables. At the same time, compared to the FV method, the spectral/hp element formulation offers new flexibilities in modelling turbulence. This will be utilised in the current project to derive more accurate models to account for the interactions between the FGM control variables and the turbulence not resolved by the CFD mesh.

FGM table [van Oijen et al. 2016]



LES of gas turbine combustion
[Gicquel et al. 2012]



Supported by the modern means of data collection, the rapidly progressing machine learning techniques open a new avenue to the research in fluid

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mechanics. In this project, machine learning will be embedded in the physical modelling for the high-order LES simulations of hydrogen combustion. The proposed research will take full advantage of the database to be produced at Loughborough University under a recent EPSRC grant (EP/W014815/1).

Deliverables

- Mathematical formulation of the new FGM control variables and their transport equations in the flow
- Mathematical formulation of the sub-element turbulence models for high-order CFD
- A validated reliable and efficient high-order combustion CFD solver for LES of hydrogen combustion
- Validated LES simulations of hydrogen combustion under practical gas turbine conditions

Sustainable Hydrogen
CENTRE FOR DOCTORAL TRAINING

Thermoacoustic characteristics of micro-mix hydrogen flames

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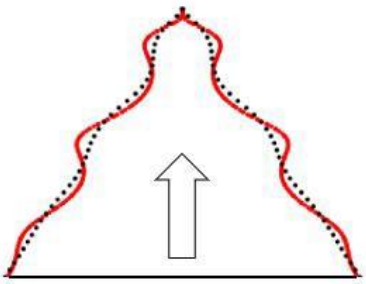
Project description

Lean hydrogen combustion for gas turbines has been subject to extensive research as a potential solution to achieve future emission targets in the aviation and energy sectors. Micro-mixing devices are proposed as an effective design to produce stable hydrogen flames. Meanwhile, lean combustion is typically susceptible to thermoacoustic instability. Such instability is due to the coupling between the unsteady heat release from the flame and the acoustic waves produced by the unsteady heat release. When uncontrolled, the thermos-acoustic instability can undermine the performance of the gas turbine and cause significant damage in a serious case. The flame response to acoustic disturbances is, therefore, important to the safe operation of the combustor.

The direct effect of acoustic disturbance on the combustor flow is to cause the fluctuation in the inflow to the combustor. In this project the flame response of the micro-mixing hydrogen combustor to the inflow fluctuation will be analysed by Computational Fluid Dynamics (CFD) using Large Eddy Simulations (LES). The open-source CFD package OpenFOAM will be used to perform these simulations with the inflow fluctuation prescribed at the frequencies and amplitudes of relevance to the thermoacoustic instability in gas turbines. From the CFD results the unsteady heat release of the combustion process will be examined for different forcing frequencies and amplitudes of the inflow fluctuation. This will be followed by further interrogation of the flow field details to identify the physical mechanisms underlying the unsteady heat release. Subsequently, perturbation theories will be implemented in the open-source computing platform FEniCS to reconstruct both the linear and nonlinear responses of the flame to the inflow disturbance. This CFD and theoretical research will make use of the experimental work on micro-mixing hydrogen combustion currently ongoing at Loughborough University under a recent EPSRC grant (EP/W014815/1). The results from this project can be used in a low-order thermoacoustic analysis tool to assess the susceptibility of the whole combustion system towards thermoacoustic instability.



Flame front under acoustic perturbation [Lim et al 2021]

Micro-mix hydrogen flame [FH Aachen]

Deliverables

- LES simulation of micro-mixing hydrogen flame validated by experiments
- LES simulations of micro-mixing hydrogen flame under inflow forcing at 100Hz – 600Hz, which is of relevance to thermoacoustic instability, and the Flame Describing Function for this frequency range

- Numerical solvers developed in the FEniCS framework for the perturbation analysis of the micro-mixing hydrogen flame
- Reconstruction of the fundamental mode and harmonics of the micro-mixing hydrogen flame under periodic inflow forcing based on perturbation theories

Sustainable Hydrogen
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Metal membranes for separating pure hydrogen from gas grids

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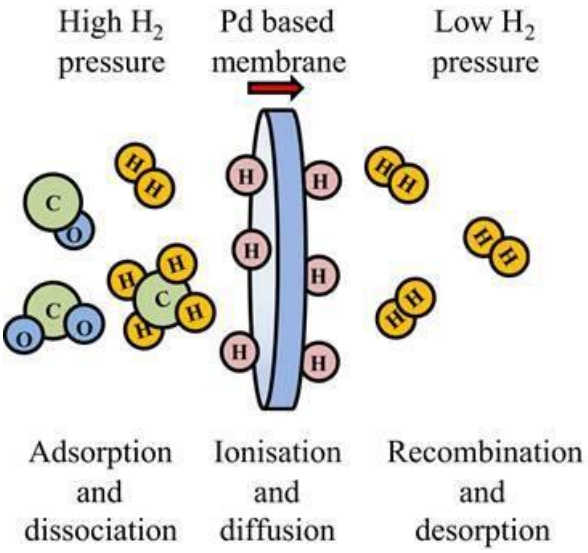
Project description

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)

Porous Transport Layer Development for Proton Exchange Membrane Water Electrolysers

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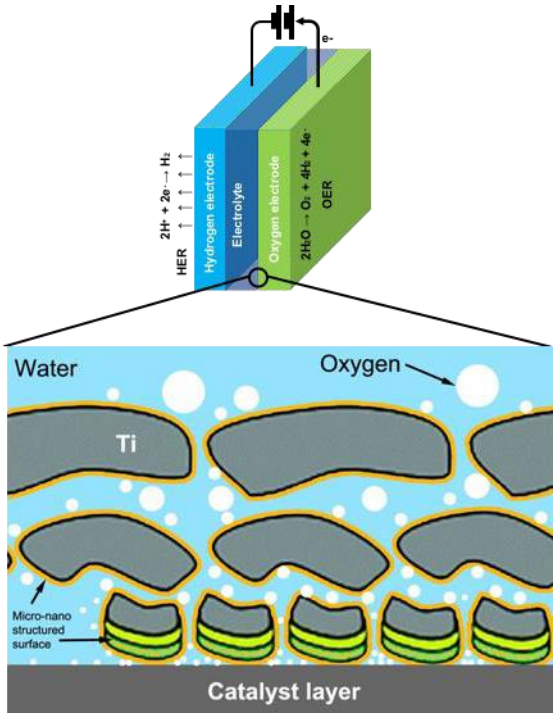
Project description

The biggest challenge with current proton exchange membrane water electrolysers (PEMWE) is their poor power performance. The poor transport behaviour of oxygen bubbles within the porous transport layer (PTL) at the anode has been a major factor limiting the high current density operation in practical applications. In this PhD project, we'll develop a new generation of Ti-based PTLs with controlled pore distribution using additive manufacturing techniques based on the 3D printing. Micro-nano structures will be created on the pore surface in PTLs through post surface modification to facilitate the water contacting and desorption of bubbles formed during the operation.



Deliverables

- 3D printing approach to fabricate PTLs with controlled pore distribution.
- Knowledge on the PTLs with gradient distribution of the pore size and porosity.
- Surface Pt modification techniques of the Ti-PTLs with micro-nano structured surface.
- PTL evaluation in the single cell test.