

# Optimisation of hydrogen fuelling station operation and maintenance to maximise performance and resilience of key infrastructure

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# **Project description**

This project is in collaboration with ITM Power , who are leading the sector in the design and deployment of electrolyser based hydrogen solutions, including hydrogen refuelling stations (HRS). The deployment of early-to-the-market plants provides the opportunity to optimise not only the operation of the existing plants but to also improve the design of next generation fuelling stations. It is obviously desirable to maximise performance of the HRS not just for economic reasons, but in order to deliver the best customer experience. This project seeks to optimise the plant operation, where planning preventative maintenance can help reduce disruption to service and improve the commercial case of a plant. There are two approaches being proposed for the project:

#### 1. Component-based asset management

Investigation of the individual "components" (such as electrolyser, refrigerator system, compressor, etc.), analysing their operational, maintenance and fault data. Looking at the performance of a "component", we can identify how long it will be before a failure occurs and then recommend a preventative maintenance schedule. Operational parameters flow rates, temperature, (e.g. pressure, power demand, etc.) can provide early indications of a failure event in the near future when the component is no longer within normal operational parameters and identify any requirement for



unscheduled preventative maintenance. The project will analyse existing plant data using pattern recognition and machine learning methods to look for early signs of failure.

#### 2. System-based asset management

Taking a more system-wide or network-wide approach can help improve resilience. In a system we need to understand redundancies between components, as one component failure can be compensated by a redundant component. Where there is no or limited redundancy, a cost benefit analysis will be undertaken to guide future design principles for resilient HRS. In a network, there is a need to understand where the stations are located and what are the effects to reliable delivery if one













fails. This analysis will help guide strategic clustering of HRS defining the density and optimised geographic location.

To model a system or a network, a suitable alternative to a more traditional Fault Tree Analysis method would be a Petri net-based approach. It would be used to simulate system performance and evaluate its resilience when failures occur.

The approach taken (or a blend from the above) will be tailored to the successful candidate's expertise and interests. The project will involve periods of working at ITM Power, either at their new factory in Sheffield or at one of their HRS, to facilitate effective knowledge transfer between the University research group and the experts at ITM Power.



- 1. Component-based asset management
  - Schedule for optimised preventative maintenance
  - Methodology for detection and enacting unscheduled preventative maintenance
  - Design/operational recommendations to maximise reliability
- 2. System-based asset management
  - More resilient HFS through an optimised redundancy strategy
  - More resilient network of HFS, through strategic plan of clustering















# Modelling Hydrogen Storage in Quasi-Crystals

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### **Project description**

The aim of this project is to investigate computationally the main physical properties that nanometre size quasicrystals (QCs) inherit from the absence of periodicity and to investigate their potential in a few foreseen applications, notably in hydrogen storage and sustainable hydrogen production.

Amongst complex metallic alloys the atomic structure of a QC is without a doubt the most difficult to solve, however a number of stable QCs are now known (see an example of the ternary icosahedral Zn-Mg-Tm QC in figure 1). Of these new QCs, none were comprehensively studied from the standpoint of their potential applications, with the exception of some studies on the Ti–Zr-Ni system that shows potential for hydrogen storage (figure 2).

This project will assess computationally a wide range of QCs for their suitability as a novel hydrogen storage material and as a novel QC catalyst replacing current expensive Pt based catalysts in electrocatalytic water splitting. The project will re-launch the quest for inexpensive materials for energy applications with superior performance by utilising the computational methods, recently developed in the E. Besley's group, for understanding gas interactions, separation and diffusion in solid materials.



Figure 1: Atomic structure of the ternary icosahedral Zn-Mg-Tm quasicrystal (Acta Cryst 2020)



Figure 2: Mass change upon hydrogen loading of crystalline (front) and icosahedral quasicrystal (back) Ti-Zr-Ni alloys at constant Ni content and variable Ti/Zr ratio (ChemSocRev 2012)

This computational modelling will guide the synthesis of new QC formulations and their testing in hydrogen storage and electrocatalytic applications.

- Computational prediction of nanometer size quasi-crystal (QC) thin films and clusters with precisely controlled size and structure;
- Computational modelling of hydrogen uptake of the QCs
- Comparative computational study of the catalytic properties of QCs and Pt-based catalysts with a focus on water splitting.













# Machine-learning informed highly-selective metal organic framework membranes for hydrogen purification

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# **Project description**

Metal-organic frameworks (MOFs), a class of hybrid porous compounds composed of metal atoms or clusters, connected by organic linkers, are a promising alternative. MOFs have a higher synthetic flexibility in terms of morphology and chemical properties in comparison to the porous materials mentioned above. Consequently, numerous MOFs have been investigated in a wide range of applications including the selective adsorption of H<sub>2</sub>.

MOFs are in general first prepared as crystalline powders whilst the use of MOFs might be further expanded by the development of thin-films for the applications including membranes for continuous gas separation. However, the conversion of a powder synthesis to a thin-film synthesis is not a trivial task as a result of our limited understanding of MOF nucleation and crystal growth and various structures of MOFs have hindered development of a systematic approach for synthesis of MOF films.

Molecular simulation has become intensively used in the evaluation of a wide range of MOFs and MOF films for the various applications. However, molecular simulations can be considered as time-consuming and expensive. Thus, alternative methods such as machine learning (ML) techniques are considered. Although, recent publications have reported performance prediction of MOF powders, membranes or films, there has been no research on MOF thin-films yet.

In this study, we propose to develop an ML algorithm to provide optimum film synthesis conditions for MOF structures. We selected TIFSIX and SIFSIX series MOFs as they are ultramicroporous (< 0.5 nm), stable in water and H<sub>2</sub>S and CO<sub>2</sub> selective.



Selective MOF membrane separates gas molecules

- ML algorithm that can be modified for the development of other MOF structures H<sub>2</sub>-related separations.
- Composition database, which will yield to successful/unsuccessful TIFSIX/SIFSIX . membranes.
- H<sub>2</sub> purification performance of membranes manufactured via composition database.















# Designing efficient charge-transfer metal-semiconductors heterojunctions for hydrogen generation

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# **Project description**

M-SC heterojunctions can offer intriguing opportunities for solar photocatalysis. Using earth-abundant metals for these materials can not only reduce environmental impact but also place photochemical water splitting as a competitive hydrogen generation technology.

This project will assess a wide range of M-SC combinations for their suitability as photocatalysts for the generation of hydrogen from water, replacing current catalysts based on expensive precious metals. In particular, we will explore materials based on Nb semiconductors in conjunction with metals such as Co, Cu, Ni or Mo. Materials will be synthesised, fully characterized (by means of surface and optical techniques) and tested towards the photogeneration of hydrogen from water. First-principles computational methods will be used to determine the materials density of states (DOS), charge-density differences, and band offsets to provide an educated understanding of the materials efficiency trends.



- Design a new family of M-SC heterojunctions with great H<sub>2</sub> generation efficiency.
- Computational studies will help understanding the structure-activity relationship of these materials and allow for an educated design of the next materials' generation.
- Also, we expect the materials will attract industry attention towards the use of photochemical water splitting as a competitive strategy to current H<sub>2</sub> generation technologies.















# Nano-Quasicrystals for Hydrogen Storage

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# **Project description**

Producing only water as a waste product, sustainable hydrogen could offer credible decarbonisation solutions for energy supply, transport, commercial and domestic sectors. A major barrier to exploitation of hydrogen in energy applications especially vehicles is the lack of a safe, efficient and cost-effective storage system. Quasicrystal (QC) have potential to be a lightweight hydrogen storage material due to their unique multi-shell cluster structure, which provide a high density of interstitial sites to accommodate hydrogen. For example, the typical storage capacity is less than 2H/M (hydrogen atom per metal) in conventional metal/alloy hydrides, in comparison to 3.2 H/M of the theoretical capacity in QC hydrides. A wide range of advanced crystal materials have been investigated for hydrogen storage; yet little is known about QC with respect to energy storage, especially nano-sized QCs

This project aims to develop high-performance nano QC materials for on-board vehicle hydrogen

storage. The student will synthesize nano QC via various synthetic methods, such as chemical vapour deposition and physical vapour deposition. The characterisation via XRD, SEM, TEM will reveal the structure of nano QCs. Hydrogen storage properties including capacity, kinetics, thermodynamics and reversibility will be evaluated by differential scanning calorimetry, thermogravimetric analysis, and pressurecomposition-isotherm techniques. Working alongside a computational project led by Prof E. Besley, this project will also study the interaction between hydrogen atom and host QC lattice via in-situ powder neutron diffraction to understand the relationship between structure and storage performance, therefore set the design protocol for nano QCs for hydrogen storage.



(a) It is proposed to use quasicrystals for on-board hydrogen storage, which is safer with higher volumetric efficiency compared to compressed gas. (b) Quasicrystal have potential to be a lightweight hydrogen storage material due to their unique multi-shell cluster structure which contains enormous hydrogen-favoured interstitial sites (represented by dark dots).
(c) SEM image of Mg-based quasicrystals.

- Synthesize nano-sized quasicrystals suitable for hydrogen storage with focus on Mg-based, Ti-based QC and Test the hydrogen storage properties
- Conduct in-situ experiments including neutron diffraction to investigate the interaction between hydrogen atom and host QC lattice
- Set the design protocol for using nano QCs for hydrogen storage













# Advanced Hydrogen Sensing Platform Based on Functionalized Metal-Organic Frameworks

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### **Project description**

Developing efficient sensor materials with superior performance for selective, fast, and sensitive detection of hydrogen is essential for environmental protection and human health. Metal–organic frameworks (MOFs), which are crystalline and porous solid materials constructed from metal nodes (metal ions or clusters) and functional organic ligands, have received attention for gas sensing due to their large surface area, adjustable pore size, tunable functional sites and intriguing properties, such as electrical conductivity, magnetism, ferroelectricity, luminescence and chromism. However, selectivity, sensitivity and stability are still the major challenges for MOFs–based sensors used in hydrogen detection. Accordingly, this project aims to fabricate novel multifunctional MOFs with improved sensitivity and stability for hydrogen detection. The rational design of these robust, multifunctional MOFs will be guided by computational predictions in after integrating metal nodes, functional ligands, and guest molecules with different properties to achieve selective sensing of hydrogen over multiple cycles. Computational modelling will be delivered in collaboration with the Computational Materials Group at Nottingham.



**Metal-organic Framework** 

- A library of novel, multifunctional MOFs with complete characterization data.
- Robust MOF-based hydrogen sensors capable of retaining high performance over multiple cycles.













# Quantifying environmental and resource impacts of the future UK hydrogen fuelled vehicle fleet

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# **Project description**

This PhD project will develop novel LCA models to assess the resource and environmental implications of deploying hydrogen fuelled vehicles in the UK's light duty and heavy duty road fleets. The comprehensive approach will consider current and future mix of hydrogen production routes; vehicle manufacture; use; and end-of-life vehicle management (e.g., recycling). Beyond more common LCA studies comparing technologies on vehicle level, this project will consider the turnover of UK vehicle fleet and uptake of hydrogen technologies to quantify cumulative resource and environmental implications.



Stakeholder collaboration : Saudi Aramco

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- Life cycle assessment model of hydrogen production routes in UK to 2050
- Co-delivery of UK light duty vehicle fleet model
- Full LCA models comprising hydrogen production, vehicle manufacture, use, and end-of-life vehicle management













# Insights on metal nanoclusters (MNCs) (de)hydrogenation for on-board hydrogen storage application using electron microscopy and spectroscopy techniques

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# **Project description**

The development of volumetric efficient solid-state hydrogen (H2) storage materials is crucial for decarbonisation in the transport sector. As one of the most promising H2 storage materials, the advantages of magnesium hydride nanoparticles includes their high H2 storage capacity (7.6 wt.%) and low cost (\$3/kg). However, slow kinetics and a high working temperature (ca. 250 °C) limit its commercial application for on-board H2 storage. In order to improve its properties (higher kinetics, lower temperature), this project will utilise metal nanoclusters (MNCs), which are fundamentally different compared to more widely used metal nanoparticles (diameters >2 nm), where the majority of metal atoms remain 'hidden' within the lattice and are excluded from participation in useful chemistry. In contrast, the majority of the atoms in MNCs are fully accessible for physicochemical processes, while new functional properties, inaccessible in bulk metals or in nanoparticles, can emerge as a result of confinement in MNCs. Theoretical calculations predict that nano-tuning could reduce the (de)hydrogenation reaction energy when NCs of Mg/MgH2 are used, therefore reducing the working temperature [JACS, 2005, 127, 16675-80]. This would substantially reduce the on-board H2 storage cost enabling their use in fuel cell vehicles for zero-emission transport.

The specific steps will involve: (i) synthesis of graphitic carbon nitride (*g*-C3N4), which is an ideal support for stabilisation of MNCs due to its nitrogen "cavity" (Nottingham), (ii) depositing a series of MNCs with different sizes and composition (i.e. Mg and Pd, and their nano-alloys) on *g*-C3N4 and their characterisation: AC-STEM including chemical mapping and depth profile, and XPS / NAP-XPS in Diamond, (iii) Investigating the electronic changes on MNCs under H2 environment at different temperatures (AC-STEM and NAP-XPS in Diamond), (iv) evaluation of H2 storage properties including capacity, kinetics, thermodynamics and cycling test (in Nottingham).















Stakeholder collaboration: Diamond



- Fabrication of MNCs with atomically precise size and composition (focus on Mg, Pd and • their nano-alloys).
- Analytical approaches delivering atomic-level dynamic information for MNCs in ex-situ, • in-situ and operando conditions (H2 atm with different temperatures up to 350 °C with focus on NAP-XPS and STEM).
- Design a protocol for metal clusters investigations under hydrogen for I09-XPS/NAP-• XPS and STEM.
- Provide new links between Sustainable Hydrogen CDT, 109, ePSIC, Ammonia • Demonstrator and Nottingham.















# Modular Additive Manufacturing for Next-generation

### Hydrogen Storage

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# **Project description**

Compact hydrogen storage is a major challenge for hydrogen powered vehicles, with current state-ofthe-art storage vessels being too large and operating at dangerously high pressures. Solid state metal hydrides (MH) can store large quantities of hydrogen in much smaller volumes and at lower pressure. However, MH stores have not made it to market because suitable vessels have not yet been developed. This project will investigate the design and manufacture of a new type of compact MH storage vessel – the *Type S* vessel. It will perform multiple functions, including heat management (due to exothermic and endothermic charging and discharging cycles), and MH bed breathing (due to MH expansion and contraction whilst cycling). To address these requirements, the project will use metal additive manufacturing (AM) in an entirely new way, using individual latticed sub-components, or modules, which are joined together to create the vessel interior. By the end of the project, the student will have successfully demonstrated this new design and manufacturing approach for MH storage applications.

The student will investigate this modular manufacturing approach with a combination of AM processing and metrology, numerical modelling (e.g., finite element analysis), and component-level testing (e.g., microstructure analysis, joint strength and leak testing). They will gain a broad set of skills and knowledge relevant to modern design and analysis techniques, as well as manufacturing and materials science.



- Through the investigation of the modular lattice design approach, the project will generate structure-performance relationships which will underpin a novel computational AM design toolkit. This will be configurable for a range of thermo-mechanical applications throughout the renewable energy, automotive and aerospace sectors.
- Reduced scale Type S vessel prototypes will prove the manufacturing concept, the effectiveness of the *in situ* joining methods, detect outstanding technical challenges and provide cost and performance data for the project partner and future stakeholders.













# Efficient Hydrogen Separation using Proton-Conducting Ceramic Membranes and Electrochemical Cells

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# **Project description**

To achieve energy-efficient and low-cost hydrogen separation using proton conducting ceramic membranes for hydrogen rich streams generated through reforming of natural gas as well as onsite purification of hydrogen close to the point of end use for dilute hydrogen streams distributed through natural gas pipelines using ceramic proton electrochemical cells (hydrogen pumps). Hydrogen plays a vital role in helping the UK meet its 2050 target of net-zero greenhouse gas emissions through decarbonisation of its energy system including electricity, transport and heating sectors. Most hydrogen used today is produced from fossil fuels (e.g., through steam reforming of natural gas, coal gasification). The product gases consist mainly of H<sub>2</sub> and CO<sub>2</sub>, as well as other impurity gases such as CH<sub>4</sub>, and CO. Therefore energy-efficient and low-cost hydrogen separation constitutes a crucial process to more toward to hydrogen economy.

Dense ceramic membranes made of mixed protonic-electronic conductors (MPECs) are capable of separating hydrogen from the gas mixtures with 100% selectivity, reduced energy penalty and cost compared to the well-established techniques such as the adsorption technique. pressure swing Ceramic proton conductors can also be used to fabricate electrochemical cells (hydrogen pumps) to obtain high purity hydrogen from dilute hydrogen streams when the existing hydrogen separation techniques become highly inefficient and costly. This is particularly important to facilitate distribution of hydrogen using existing natural gas pipelines. The ceramic proton electrochemical cells could enable extraction of high purity hydrogen from the natural gas blend with 10-20 vol% hydrogen close to the point of end use.



- New proton conductors with high proton conductivity and stability under operation conditions.
- New high performance and stable mixed protonic-electronic conductor ceramic membranes with H<sub>2</sub> permeability > 1.0 mL cm<sup>-2</sup> min<sup>-1</sup> at 700- 1000 °C with a 1 bar pressure gradient meeting commercial requirements.













 Ceramic proton electrochemical cells exhibiting high H<sub>2</sub> separation rate > 5.0 mL cm<sup>-2</sup> min<sup>-1</sup> under 1.0 V at 300–500 °C with the Faraday's efficiency above 98%.

















# Computational Modelling of Solid-State Hydrogen Storage Materials

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# **Project description**

Significant effort has been devoted to searching for alternative solid-state hydrogen storage materials over the last few decades. Many different types of solid-state materials have been studied, and among them, intermetallic hydrides and complex metal hydrides have received significant attention, because they can operate at moderate conditions and have relatively high gravimetric hydrogen densities. However, some of these materials suffer from poor thermodynamics, kinetics or reversibility. In collaboration with our experimental collaborators at Nottingham, this project aims to understand the composition-structure-property correlations of solid-state hydrogen storage materials through accurate density functional theory simulations of both existing and hypothetical materials. Fundamental understanding will be derived, and new materials design strategies will be informed from these atomistic simulations, with which we will design new solid-state hydrogen storage materials with improved kinetic and thermodynamic properties for hydrogen storage applications. Working alongside our Nottingham-based experimental collaborators, the most promising candidate materials discovered from the computational simulations will be synthesised and characterised, and their hydrogen storage properties will be validated by experiments. This project also forms part of our ongoing collaboration with Sandia National Laboratories in the US on joint experimental-computational studies of hydrogen storage materials. The successful candidate will have the opportunity to visit Sandia National Laboratories to carry out joint research activities during their PhD.



#### Deliverables

• Database of solid-state hydrogen storage materials with computationally predicted structural and thermodynamic properties relevant to hydrogen storage applications















# Evaluation of 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. 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, 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 Chivas Brothers and Shell Research will be actively involved in the project development and progress by providing wastewater samples, access to the manufacturing sites, providing data and access to Shell Biological lab. 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.















- 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.

















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).



- 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<sub>4</sub>/H<sub>2</sub> and H<sub>2</sub> grids)















# Prevention and mitigation of incidents involving hydrogen use in a domestic setting

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# **Project description**

With a growing interest in the introduction of hydrogen to the natural gas grid, and its resultant use, including pure hydrogen, in homes for heating, cooking and power supply it is important to understand the specific hazards and associated risks pertinent to the use of hydrogen in a domestic setting. Appliances such as fuel cells, boilers, and burners, are being developed specifically for use with hydrogen and hydrogen blends. Validated contemporary CFD models and reduced engineering tools for reliable prediction of an incident dynamics in a residential setting are needed for reliable hydrogen safety engineering. Safety challenges include understanding the behaviour of a leak of hydrogen or hydrogen blends, including harmful impurities, validation of the similarity law for concentration decay in momentum-dominated jets for blends, application of the under-expanded jet theory to blends, assessment of leak and dispersion of flammable gas from flanges and joints, safety strategies to exclude accumulation of flammable mixtures, and appropriate venting strategies. The effect of buoyancy on the release of hydrogen blends could also be investigated. Hydrogen specific prevention and mitigation concepts are needed to efficiently tackle hydrogen dispersion and combustion in residential environments. There is a need to understand and exclude the potential thermal and pressure effects of an incident on the integrity of the property.

The expected impact of the study could include: validated contemporary CFD models and engineering tools for hydrogen safety engineering; deeper knowledge of the underlying physical phenomena; innovative prevention and mitigation strategies; guidelines for inherently safer design and use of hydrogen in a domestic setting, etc.

The study will focus on a combination of theoretical and numerical (CFD) studies, the use of ANSYS Fluent as a computational engine, multi-processor Linux-based hardware of HPC suite, etc. The results of this doctoral research will be aligned to HySAFER's externally funded projects and reported at international conferences as relevant. Publication of results in peerreviewed journals is expected.



- Identification and prioritisation of relevant knowledge gaps.
- Theoretical and numerical studies to close knowledge gaps and address technological bottlenecks.
- Development of innovative safety strategies and engineering solutions to prevent and mitigate incidents with hydrogen and its blends in domestic settings.













- Determination and characterisation of specific hazard and associated risks.
- Development and validation of novel engineering tools required for hazards and risk assessment.
- Evaluation of the effectiveness of conventional and innovative prevention and mitigation techniques and incident management strategies concerning specific hazards implied with the use of hydrogen or its blends in domestic settings, etc













Safety of using ammonia in for the hydrogen economy

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### **Project description**

There is a growing focus on hydrogen technologies and the role they likely to have in the development of the future low-carbon economy. The experience accumulated with use of ammonia in industries and its transportation around the globe offers practical, cost-effective means for storage and transport of large quantities of hydrogen compared to compressed gaseous or liquid forms. Ammonia is characterised by its liquid state at ambient conditions, high volumetric and gravimetric energy density. There is a substantial track record and experience on the inherently safer use of ammonia in the industrial environment as it is widely utilised in chemical processing, food production, as an agricultural fertiliser, etc. Emerging of ammonia in a different capacity, i.e. as hydrogen carrier, calls for a reassessment of hazards and associated risks it presents to life, property and environment. This PhD project aims to develop scientifically underpinned safety strategies and engineering solutions for handling large quantities of ammonia used as hydrogen carrier during transport and storage onboard and using relevant infrastructure. The project will review hazards, including toxicity effects, existing prevention and mitigation safety strategies when dealing safely with ammonia. New practices associated with extended use of ammonia for hydrogen economy will be investigated, scenarios of unscheduled ammonia release in enclosures and the open atmosphere will be identified and prioritised. The research outcomes are expected in the form of recommendations for inherently safer use of ammonia for hydrogen applications and may include, e.g. requirements to ventilation in enclosures where ammonia is handled, strategy for the choice of ammonia piping and pumping pressures, a methodology to define hazard distances for different release scenarios in the open atmosphere, others. It is envisaged that the research will rely on the use of Computational Fluid Dynamics (CFD) to study the propagation of ammonia cloud following its accidental discharge and evaporation, the build-up of ammonia concentration and its effect on exposed people. The successful candidate is expected to have a strong background in one of the following disciplines: mathematics, physics, chemistry, fluid dynamics, heat and mass transfer, combustion. Any previous experience of theoretical analysis and/or numerical studies is welcome. The research will be conducted at the HySAFER Centre. The candidate

will focus on CFD modelling and numerical simulations, use relevant software (ANSYS Fluent, FieldView, etc.) and the state-of-the-art computational resources – multi-processor

workstations available at HySAFER Centre and HPC facility available within EPSRC KELVIN-2 project. This research will be aligned to HySAFER's















externally funded projects and reported at international conferences. Publication of results in peerreviewed journals is expected.

- Prioritised list of accident scenarios,
- Engineering model and/or CFD simulation problem formulation(s) for assessment of hazards in identified accident scenarios,
- Model implementation and completing simulations,
- Validation of the model(s) against available experimental data (or highly accurate solutions),
- Development of safety recommendations for handling ammonia as hydrogen carrier.













# Modelling and simulation of premixed combustion in large-scale confined geometries

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# **Project description**

Pressure and thermal effects from large-scale deflagrations in large-scale confined geometries like a tunnel can be extremely hazardous due to the transition of initially laminar premixed combustion to the fast deflagration and potentially through the deflagration-to-detonation transition (DDT) to detonation. The role of various flame front instabilities and combustion acceleration mechanisms, especially in a confined and congested environment, is still not fully understood especially at large scales. Moreover, the interaction and thus the development of different instabilities and mechanisms on deflagration dynamics is not yet clarified. The Ulster's multi-phenomena deflagration model is under continuous development during last two decades in different parts of the globe. The model currently accounts for the dependence of burning velocity on changing during combustion pressure and temperature of the unburnt mixture, turbulence generated by flame front itself, turbulence in unburnt mixture, increase of burning rate due to preferential diffusion in stretched curved flamelets in the turbulent flame brush, fractal structure of turbulent flame front, etc. The model has been under continuous validation against a growing number of large-scale experiments, primarily hydrogen-air deflagrations, DDT and even detonations. It is expected that a candidate will develop the model further using the state-of-the-art in the field and expand the validation domain to the problems of practical importance including deflagrations of non-uniform hydrogen-air mixtures in tunnels or similar confined geometries. Experimental data on large-scale deflagrations are available for use as validation tests from ongoing projects, e.g. experiments on hydrogen release and deflagration in a large-scale tunnel at Health and Safety Executive test grounds within the H2020 HyTunnel-CS project, as well as previous projects in which Ulster University participated, partners in various European projects, and from literature. The successful candidate is expected to have a strong background in one of the following disciplines: physics, fluid dynamics, heat and mass transfer, combustion, computational fluid dynamics, safety engineering, etc. Any previous experience of analytical analysis and/or numerical modelling is welcome. The research will be conducted at the HySAFER Centre. The candidate will focus on CFD modelling and numerical simulations, use relevant software (ANSYS Fluent, FieldView, etc.) and the

state-of-the-art computational resources multi-processor workstations available at HySAFER Centre and HPC facility available within EPSRC KELVIN-2 project. This research will be aligned to HySAFER's externally funded projects reported and at international conferences. Publication of results in peerreviewed journals is expected.



Explosion experiment



**Explosion CFD simulation** 















- Analytical and/or CFD model formulation and development
- Model(s) validation















# Safety assessment and mitigation of hazards from TPRD in-situ of hydrogen vehicle

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# **Project description**

High-pressure hydrogen releases from thermally activated pressure relief device (TPRD), if ignited, can generate significant thermal and pressure loads on humans and structures. TPRD is required by regulation to exclude onboard hydrogen tank rupture in a fire by the release of hydrogen. The design and position of TPRD should be optimised to provide the shortest time of reaction to the fire and to allow passengers' rescue and self-evacuation in the case of accident without being compromised by hydrogen jet fire resulting from TPRD release.

This study aims to develop a comprehensive computational fluid dynamic (CFD) model for highpressure hydrogen release and combustion from a realistic TPRD nozzle to aid safer design of TPRD for high-pressure hydrogen storage onboard vehicles. The research project will address the following design challenges:

- TPRD nozzle and pipeline design should provide for minimal possible flame length and associated hazard distances not to impede on passengers' self-evacuation and operation of rescue services.
- In the same time the TPRD design should exclude flame blow-off during tank blowdown to avoid accumulation of hydrogen and formation of explosible hydrogen-air mixture.
- Ignited or unignited hydrogen release from TPRD should exclude potential for development of the pressure peaking phenomenon (PPP) if initiated in a domestic garage or maintenance workshop.

TPRD assembly performance should exclude its false initiation during fast hydrogen fueling

Research outcomes of this study are expected in the form of recommendations for safe design of TPRD for onboard hydrogen storage. The candidate will work alongside HySAFER team members contributing to development of regulations, codes and standards in the area of hydrogen fuelled vehicles safety. Strong background in one or more of the following disciplines is expected: mathematics, physics, chemistry, fluid dynamics, heat and mass transfer, combustion, computational fluid dynamics. Any previous experience of theoretical analysis and/or numerical studies is welcome. The PhD researcher will focus on CFD modelling and numerical simulations, use relevant software

(ANSYS Fluent, FieldView, etc.) and the state-of-the-art computational resources – multi-processor workstations available at HySAFER Centre and HPC facility available within EPSRC KELVIN-2 project. This research will be aligned to HySAFER's externally funded projects and reported at international conferences. Publication of results in peer-reviewed journals is expected.















#### Deliverables

- Collection of information about TPRD and automobile fires
- CFD and/or CFD-FEM model formulation and development
- Validation of CFD and/or CFD-FEM model
- Parametric studies using CFD and/or CFD-FEM model
- Formulation of recommendations for TPRD design











Engineering and Physical Sciences Research Council



# Using coupled CFD-FEM modelling for the safety assessment of hydrogen-powered vehicles

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# **Project description**

Hydrogen-power vehicles are being parked in garages, maintenance shops, underground parking, tunnels and other confined spaces. Blast wave and fireball following the high-pressure tank rupture in a fire represent a major hazard threatening life and incurring property losses. Vehicle deformation and displacement after onboard hydrogen storage tank rupture consumes a part of mechanical energy of compressed hydrogen, affects hydrogen combustion and thus the contribution of chemical energy to the blast wave strength. The fireball dynamics is also affected by the presence of the vehicle. Hazards of under-vehicle tank rupture in the open atmosphere do not apply to confined scenarios, e.g. tunnels where the blast wave propagates with little decay compared to the open space and fireball propagates with large velocity for long distances compared to the open space. Assessment of energy to deform and displace vehicles is essential to develop engineering tools with a realistic prediction of pressure and thermal loads that would not be over-conservative. This energy can be assessed using the Finite Element Method (FEM) modelling and simulations. The project aims to develop a coupled CFD-FEM model applicable to the analysis of consequences of onboard hydrogen storage tank rupture in a range of conditions - tank volume, pressure, mounting position on a vehicle, vehicle location, etc. Computational tools for fluid flow simulations and structural analysis will be used as a platform for model development. Experimental data available in the literature and from HyTunnel-CS project will

be used for the model validation. This doctoral study includes identification and prioritisation of knowledge gaps and technological bottlenecks; performing theoretical and numerical studies to close knowledge identified gaps; numerical analysis of structural response to thermal and pressure loads; quantitative assessment of pressure and thermal hazards and associated risks; development and validation of innovative engineering solutions and tools for hydrogen safety engineering, etc. The following aspects and phenomena will be considered: contribution of chemical energy of hydrogen combustion into the strength of the blast wave; blast wave and fireball effect on the structural elements of confined spaces; mitigation of the blast wave e.g. by projectiles. tunnel splits. laybys, etc.; including vehicle, and hazard distance assessment; reduction of projectiles hazards based on the tank location, etc. The expected















outcomes of the study include: validated contemporary models; a deeper knowledge of the underlying physical phenomena; innovative prevention and mitigation strategies; etc. The successful candidate will work at HySAFER Centre and will focus on CFD-FEM modelling with use of relevant ANSYS software and Northern Ireland High Performance Computing (NI-HPC) Kelvin-2 cluster. The results of this doctoral research will be used in HySAFER's externally funder projects and will be reported at international conferences. Publication of results in peer-reviewed journals is expected.

- 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











