Written Evidence Submitted by Newcastle University
(HNZ0089)

This evidence has been prepared by Newcastle University's Centre for Energy subgroup on green gas and carbon capture. The Centre for Energy – a Newcastle University Centre of Research Excellence – brings together a wealth of expertise across disciplines to unify efforts towards a new way of thinking about energy systems. The subgroup specifically brings together the University's expertise on green gas, including hydrogen, and carbon capture to inform policy development.

This submission sets out an overview of areas where our academics and policy experts can support the Committee's inquiry by providing research, insights, and analysis, as well as some initiatives we are working on that can support the inquiry's focus on the role of hydrogen in achieving net zero. The sections below provide detail on the University's hydrogen expertise, responses to the Committee's specific questions, and further detail of some specific work underway at the University.

---

1. Overview

From piloting technologies and ensuring success when they are deployed, to providing evidence to select committees and being seconded to government, Newcastle University's academics are a key part of the policy ecosystem and are at the forefront of the UK's energy policy development at a critical time in the country's efforts to decarbonise and tackle climate change. Our academics are undertaking world-leading research on hydrogen and how it fits into the wider energy system and can support the green recovery in the North East and beyond.

Taking a whole systems approach

- Newcastle hosts the National Centre for Energy Systems Integration (CESI) which brings together energy experts from around the world to help understand future supply and demand. CESI's work seeks to develop flexible, smart energy infrastructure that can give customers greater control of their energy use, help industry to meet tough new low carbon targets, and give government evidence about how best to optimise energy networks.
- Working with Northern Gas Networks and Northern Powergrid, we have established InTEGReL (Integrated Transport Electricity Gas Research Laboratory), a fully integrated whole energy systems development and demonstration facility, which has recently been awarded funding from the government's Getting Building Fund through the North East LEP.
- InTEGReL supports collaboration between industry and academia to break down traditional barriers between the gas, electricity, water and transport sectors, better utilising their assets to

deliver a more secure, affordable, low carbon energy system. A specific project will demonstrate technologies to enable housing decarbonisation.

Exploring the role of hydrogen

Newcastle University is a leader in hydrogen research, exploring the technical, economic, and societal opportunities and potential risks hydrogen brings. We are also exploring hydrogen's prospects for innovation, skills, and industry as well as the potential enablement for green growth and deliverable solutions for net zero.

- We are leading innovative research in hydrogen technology and, working with research partners, last year we developed the first thermodynamically-reversible chemical reactor capable of producing hydrogen as a pure product stream, removing the need for the costly separation of the final products. This represents a transformational step forward in the chemical industry and could kick start the green energy revolution, bringing hydrogen a step closer to being a viable fossil fuel alternative.
- Our research has also helped us understand how key barriers to customer uptake can be overcome and we are calling for greater public involvement in discussions about the benefits and costs of using blended hydrogen in order to build awareness and acceptance of it being used in homes. This was presented in a report funded through the Engineering and Physical Sciences Research Council (EPSRC) and based on a survey funded through Ofgem's Network Innovation Allowance as part of the HyDeploy project, which is being delivered by Cadent Gas and Northern Gas Networks.
- Established experts at Newcastle regularly contribute to Royal Society Policy Briefings in relevant areas, e.g. "Options for producing low-carbon hydrogen at scale" and "The potential and limitations of using carbon dioxide", whilst our emerging future leaders regularly contribute to the Science Media Centre, including in response to the 10-point plan, and are members of key forums, including the BEIS CCUS Young Professional's Forum.
- Newcastle University hosts a Royal Academy Chair of Emerging Technologies in solid looping and a Royal Academy of Engineering Research Fellow in gas separation membranes, technologies with the potential to revolutionise the production of 'blue' hydrogen at scale. Although in the long term, 'green' hydrogen should be the goal, initially most will be 'blue' hydrogen, i.e. made from natural gas. To reach net zero, there is therefore an immediate and inescapable link with carbon capture and storage (CCS). Although there are methods for CCS at TRL 8/9 (system complete and qualified/actual system proven in operational environment), there is significant scope to dramatically reduce costs and energy-intensity through innovation in new technologies, such as solid looping and membranes.

Scientific discovery, from molecules to systems, to enable the hydrogen economy

- Newcastle University are leaders in the fundamental science that underpins the technology for hydrogen generation, storage and use. Newcastle leads the North East Centre for Energy Materials (NECEM), which is a collaboration (funded by the Industrial Strategy Challenge Fund) between scientists and engineers at Newcastle, Durham and Northumbria Universities, together with SMEs, catapults and multinational companies Shell, Airbus and Siemens. Our research enables us to understand the behaviour of the interfaces of materials with their environment. This information enables us to improve the performance and stability of devices, e.g. fuel cells, electrolysers and solar reactors, which are critical to future green hydrogen generation and use.

- NECEM's sister centre, The EPSRC Doctoral Training in Renewable Energy at North East Universities (ReNU), is an added value doctoral training programme, which is creating a pipeline of highly skilled doctoral graduates equipped with the skills to drive forward innovation in small scale renewable and sustainable distributed energy, boosting 'green' skills in the North East workforce. In addition to the industrial partners, the portfolio includes further not-for-profit organisations such as the North East Automotive Alliance, local authorities and international universities. The research projects include modelling, developing and applying sustainable materials, feedstocks and systems for hydrogen and low carbon fuels.
- Through the UKRI National Interdisciplinary Centre for Circular Chemical Economy, Newcastle University's Chemistry and Computing Science experts are developing a circular resources flow of olefins and their complementary feedstocks (H_2, methanol, CO, hydrocarbons, etc.), which is essential for a fossil-independent UK chemical industry. Olefin production accounts for 25% of direct CO_2 emissions for the chemical sectors and downstream processes add 7% of the industrial emissions in the UK. This research aligns with the Net Zero Teesside CCUS project.
- Chemical separations account for 10 – 15% of global energy consumption and are inherent in many hydrogen production or carbon dioxide utilisation processes involving hydrogen. At Newcastle we lead the UK's first national 'virtual' membrane research centre "SynFabFun", which connects strengths nationally and internationally in this area. Moreover, we work on the integration of fundamental advances in chemical separations with electrochemical devices (batteries, fuel cells etc) in the H2FC SUPERGEN network, for example, which will be key in unlocking the flexibility, security and efficiency offered by hydrogen, as they enable the efficiency gains made possible through integration of different energy carriers (electricity, natural gas, hydrogen etc).

---

2. Committee's specific questions

The progress of recent and ongoing trials of hydrogen in the UK and abroad, and the next steps to most effectively build on this progress – Dr Sara Walker (Director of The Centre for Energy and Reader in Energy)

The University's National Centre for Energy Systems Integration (CESI) has recently completed a literature review for Northern Gas Networks, regarding the development of a Customer Energy Village at InTEGReL. This literature review clearly demonstrated a lack of real-world demonstration of hydrogen in domestic buildings. We are working closely with Northern Gas Networks on the development of hydrogen trials at InTEGReL, including proposed research to compare mathematical models/digital twins of hydrogen in domestic buildings with laboratory (such as Salford Energy House) and real-world (InTEGReL) results.

Many existing condensing gas boiler installations are sub-optimal in terms of installed capacity of boilers (typically oversized), operating temperatures (typically higher than necessary), and condensing and modulating (typically low effectiveness). As a next step, CESI strongly recommend that a hydrogen blend trial (such as that at Winlaton, Northern Gas Networks) be compared with improved operation settings for natural gas boilers. It is entirely probable that better operational settings of natural gas boilers offer the same carbon savings as a hydrogen-natural gas blend.

The engineering and commercial challenges associated with using hydrogen as a fuel, including production, storage, distribution and metrology, and how the Government could best address these – Dr Elizabeth Gibson (Reader in Energy Materials)

Electrolysis and fuel cell technology has been established for some time, but commercial technology employs platinum catalyst and expensive membranes, which leads to the high capital cost that has prevented widespread adoption of green hydrogen as a feedstock (raw material for industrial processes).

Research at Newcastle University is developing new earth abundant electrocatalysts to replace platinum and is achieving promising results. One of the advantages of moving away from platinum is that more selective materials can be used, potentially avoiding the need for expensive membranes. However, larger amounts of earth abundant catalysts are needed compared to platinum to attain the same performance. More research is needed to improve the catalysts to reduce the amount of material required, but this is not the main contributor to the cost of the system. Funding is required for pilot scale testing of these new electrolysers, which is necessary to evaluate the performance when coupled to variable electricity supply, such as from wind or solar. Currently there are few funding opportunities available to academic researchers which provide the scale of resources needed (>£10m) for pilot testing on this scale and they are perceived as high risk (at this low technology readiness level, known as the 'valley of death', there is a requirement for large capital investment but little or no return).

One of the greatest challenges to green hydrogen is the capital investment required for electrolysis and the supply of renewable electricity. While the cost of PV has decreased rapidly over the last decade, and the solar to fuel efficiencies exceed 20%, the systems costs associated with coupling to electrolysis mean that green hydrogen ($3-7.5 kg–1 H_2 (IEA, 2019)) is not competitive with steam methane reforming. One way to address this is via direct solar to hydrogen generation and this is both a major stream of work at the Energy Materials Laboratory at Newcastle University and a vibrant research field in the UK (see www.solarfuelsnetwork.com). We have recently demonstrated on a lab scale a printable technology for direct solar to hydrogen generation using only water at neutral pH and further development of this approach is underway in our laboratory.

N. Põldme, L. O'Reilly, I. Fletcher, J. Portoles, I. V. Sazanovich, M. Towrie, C. Long, J. G. Vos, M. T. Pryce and E. A. Gibson, *Chem. Sci.*, , DOI:10.1039/C8SC02575D.

The engineering and commercial challenges associated with using hydrogen as a fuel, including production, storage, distribution and metrology, and how the Government could best address these – Dr Sara Walker

96% of hydrogen is derived from fossil fuel-based feedstock, with natural gas being the largest source. Hydrogen can be derived either via electrolysis or several thermo-chemical and material looping processes from solar, wind and biomass energy. Hydrogen production is a very well established and widespread industrial exercise and the main research challenge – and indeed the prerequisite for a clean hydrogen economy is a low or zero carbon production of hydrogen at scale and in an economically viable manner.

On its own, hydrogen is challenging to store and transport. This has led to a wide range of research that investigates multiple organic compounds, among which commercially available ammonia (NH_3) as an intermediary for storing and transporting H_2. Ammonia's density (674 g/l) offers advantages over storing H_2 (71 g/l). Although ammonia is currently produced under 200 bar at 400˚C and requires a catalyst, it may be renewably manufactured in future, the details of which (comparison between catalyst types / production environment and manufacturing energy) remain an active area of research. Without a medium to act as a hydrogen carrier, hydrogen will have to be stored at either high pressures (700 bar and above) or be liquified to enable storage with reasonable facilities. However, liquification of hydrogen requires substantial amounts of energy, due to the very low temperatures that are required to enable H_2 liquification (about -253℃).

There are a multitude of potential uses for hydrogen within the energy and transport sector. A Whole Energy Systems Integration approach, as taken by CESI, will enable evaluation of hydrogen for different end use sectors through a multi-disciplinary lens of energy scenarios. We can consider how the use of hydrogen to decarbonise one sector may affect options within another end-use sector, both positively and negatively. Therefore, it is important to take a Whole Energy Systems Integration approach to inform viable sector-use options for hydrogen to help the UK reach net zero by 2050. We believe further funding for research is needed to undertake this research, and that CESI has the skills and expertise to develop this research.

For example, if scenarios identify hydrogen as a least cost primary fuel for transport, what does that mean for hydrogen supply to other sectors? A Whole Energy Systems Integration approach can better understand how hydrogen for aviation transport might reduce availability of hydrogen for marine transport, for example, or how hydrogen demand growth in aviation transport might financially stimulate production of hydrogen for other uses. The proposed approach will allow the best options or combination of options to be identified.

Cost-benefit analysis of using hydrogen to meet Net Zero as well as the potential environmental impact of technologies required for its widespread use – Dr Sara Walker

Development of hydrogen in the overall energy system may be geographically heterogenous. For example, coupling of offshore wind and electrolysers may result in greater production and use of hydrogen along the UK North Sea coast. Industrial demand for hydrogen in clusters such as Teesside, Aberdeen, Grangemouth and Hull might better enable hydrogen production for other uses at these locations. The Whole Energy Systems Integration approach can evaluate spatial issues for hydrogen economy development. As such, widespread use might not be the appropriate target, it may be more appropriate to consider Local Energy Systems and spatial variability in energy system needs, assets and sectors for hydrogen and other energy vectors.

The relative advantages and disadvantages of hydrogen compared to other low-carbon options (such as electrification or heat networks), the applications for which hydrogen should be prioritised and why, and how any uncertainty in the optimal technology should be managed – Dr Elizabeth Gibson

In the past, hydrogenation has not been considered as a mainstream route to methane and hydrocarbon fuels because hydrogen is largely derived from steam reforming of natural gas. However, the reverse reaction is performed efficiently over nickel catalysts and small-scale commercial methanisers, are commonplace. The opportunity for "green" methane using captured CO_2 and green hydrogen is missing from the Energy White Paper, despite the established science in this area and commercial expertise in the UK. New policy should consider the potential provided by green hydrogen as a feedstock as well as a fuel, and the capital costs of large-scale electrolysers coupled to methanisers should be considered against the cost of replacing networks and appliances to operate with pure hydrogen.

Much of the government's plans for net zero energy rely on carbon capture and storage (cost), but do not consider the opportunity of captured CO_2 as a feedstock (value). Having a secure supply of CO_2 and green hydrogen (from CCUS + electrolysis, or gasification of waste) enables a chemical economy decoupled from fossil resources and instead based on the Sabatier process and Fischer Tropsch synthesis. An example of Newcastle University research in this area has developed a plasma-promoted FT reactor (Akay/Zhang/Al Harrasi) and novel hydrogenation catalysts (Doherty/Knight). The UK is a global leader in catalysis and is well placed to drive this technology forward and to integrate it into the established refinery processes to produce transport fuels, solvents and olefins. Investment in research to establish pilot plants located in the UK is required to translate the technology from TRL5-6 to commercial scale. On this basis, the government should recognise that green hydrogen is a bridge between CCUS and "Jet Zero", and consider increasing resources for the Net Zero Hydrogen Fund.

3. Specific work ongoing at Newcastle University

a. Newcastle University work on fuels for hydrogen

- **Energy Materials Lab developing CO_2 and water conversion**
- **Energy from waste: Hydrogen production via thermochemical processes – Dr Anh Phan (Senior Lecturer of Chemical Engineering)**
- **Producing Green Hydrogen through water electrolysis – Dr Prodip Das (Lecturer and Assistant Professor in Mechanical Engineering), Professor Keith Scott (Professor of Electrical Engineering), Dr Mohamed Mamlouk (Senior Lecturer, School of Engineering)**

Energy Materials Lab developing CO_2 and water conversion

The Energy Materials Laboratory at Newcastle University is developing direct routes to convert CO_2 and water to syngas or hydrocarbons using sunlight. This technology would overcome the day/night and seasonal variation issue of solar irradiance, so that the energy from sunlight can be stored as an energy dense fuel which can be used with existing infrastructure. Currently, the conversion efficiencies for direct solar to fuel generation is low, but it is anticipated that commercially viable PV/electrolysis would be possibly by 2030, with direct solar to fuel approaches available by 2050.

While the impact will be long term, the approach would not rely on large-scale infrastructure and would instead enable distributed "solar refineries", with relatively low capital investment, throughout the UK. The potential is for "personalised" energy and new business models. Solar refineries avoid the technological challenges and cost of burying the captured CO_2. They also offer industries an opportunity to market "sustainable" products to consumers, who are becoming increasingly environmentally conscious, providing a high-margin entry point for hydrogen from artificial photosynthesis in the short term.

Energy from waste: hydrogen production via thermochemical processes – Dr Anh Phan

Hydrogen is commonly produced from steam reforming of natural gas , which contributes an enormous amount of greenhouse gas emissions (e.g. 9-12 tonnes of CO_2 per tonne of H_2 produced). Gasification, a partial oxidation process of carbonaceous substances at a temperature range of 900-1500ºC, is considered as the most cost-effective and efficient method to produce hydrogen that can replace steam reforming of fossil fuels[1, 2].

At Newcastle University, we have developed a modulus gasifier that can be used for a wide range of feedstocks particularly low-valued feedstocks such as municipal solid waste with minimum pre-treatment and scale/load independent. The feedstock is decomposed into intermediates and subsequently gasified using CO_2 and steam as a gasifying medium. The process is tightly controlled and simple in operation and maintenance (TRL: 3-4). The advantages of our system are:

- Up to 78 mol% H_2 recovered at the moderate temperature ≤ 1000ºC.
- Less than 10 mol% CO2 content in the syngas.
- 97% process efficiency.
- 96% carbon conversion.
- Low unburnt carbon in ash residues (< 0.01 wt%).
- Flexible in operation.

The key features of this novel approach can provide:

- An alternative route to utilise of CO_2, in flue gas from, i.e. power plants and eliminating capturing and storage steps.
- Produce H_2 and synthetic gas (syngas), which are clean energy at the same time it can be used in a multiple downstream application such as:
  - Power and electricity generation.
  - Chemical synthesis: methanol, ethanol, alcohol, dimethyl ether and ammonia.
  - Fuel synthesis via Fischer-Tropsch synthesis

We also looked at integrated approach in waste management. From our techno-economic analysis, integrated hydrogen production via gasification and material recovery from waste is economically competitive compared to hydrogen from fossil fuels.

If the novel gasification design as developed at UNEW is applied into the integrated material recovery and waste-to-hydrogen, the cost for hydrogen production is significantly reduced due to several advantages as shown above, which can be up to 24%.

More than 50 million tonnes of hydrogen is produced every year, a figure expected to increase by 17% per year [3] due to its wide range applications such as chemical (57%), petroleum (37%) and agro-based (6%) industries. Hydrogen is considered as a clean fuel and as an energy carrier in fuel cells for generating electricity, powering electric vehicles including in aerospace applications. Thus, hydrogen will play an important role as an alternative energy vector and a bridge to a sustainable energy future. However, the major scientific challenge before the technology necessary for change from petroleum to hydrogen for transport applications can be implemented is the development of a suitable storage method that can be safely stored in a vehicle and delivered as required under operational conditions. The goal for 2030 is a hydrogen powered vehicle with > 400 miles (644 km) range and storage of ~ 13 kg of hydrogen [4].

[1] Ptasinski Krzysztof, J., Thermodynamic efficiency of biomass gasification and biofuels conversion. Biofuels, Bioproducts and Biorefining, 2008. 2(3): p. 239-253.; [2] Acharya, B., A. Dutta, and P. Basu, An investigation into steam gasification of biomass for hydrogen enriched gas production in presence of CaO. International Journal of Hydrogen Energy, 2010. 35(4): p. 1582-1589.; [3] Kalamaras, C.M. and A.M. Efstathiou, Hydrogen Production Technologies: Current State and Future Developments. Conference Papers in Energy, 2013. 1(1): p. 1-9.; [4] Energy, U.D.o., Hydrogen Storage Tech Team Roadmap. 2017.

Producing Green Hydrogen through water electrolysis – Prof. Keith Scott, Dr Mohammed Mamlouk, Dr Prodip Das

Electrolysis is a promising option for green and renewable hydrogen production, using solar or wind energy. Electrolysis uses an electric current to split water into hydrogen and oxygen in an electrolyser. Like fuel cells, electrolysers consist of an anode and a cathode separated by an electrolyte. Several teams at Newcastle are working on renewable H_2 production using water electrolysis to then generate electricity via input to a fuel cell when desired. This research offers an innovative avenue to address the challenges of intermittent generation from renewables, such as long-term storage and long-range transport of renewable energy. However, designing an efficient and portable system for solar-to-H_2 or wind-to-H_2 is challenging.

To overcome the challenge, Dr Das and his team are working on the design of a regenerative fuel cell via a multiphysics model to convert renewable electricity into H_2 (during intense sunlight or high wind) and then utilise the same unit to generate electricity from renewable H_2 (during the night or low wind). However, a regenerative fuel cell system requires a fuel cell that is efficient in both generation and regeneration modes for converting hydrogen to electricity and vice versa. Additionally, such a fuel cell needs an efficient and cost-effective catalyst to drive the chemical reaction, a durable hydrophobic porous transport layer, and a high-temperature electrolyte membrane. Dr Das and his team are working with universities and industry partners to overcome these challenges.

Prof Scott and Dr Mamlouk are developing and scaling up polymer membrane electrolysers using proton exchange and alkaline membranes and ionic liquids. Their work focuses on lowering the cost, increasing the sustainability and increasing the durability of the technology. They have shown that their non-precious metal catalyst can achieve similar performance to that of precious metal Platinum and Iridium dioxide, so unlike established technology, their system is not limited by the earth abundance of the materials and offers significant cost reduction by 60%.

Prof Scott and Dr Mamlouk also built a large testing bed with kWs capacity for electrolysers systems to optimise emerging systems and evaluate new electrolyser technologies. They have worked with EDF Energy to demonstrate intermittent storage of renewable electricity into pressurised hydrogen that can be injected directly to gas grid. They used electricity generation data from a 177 MW EDF wind farm in Dorenell into proton exchange membrane water electrolyte capable of producing pressurised hydrogen electrochemically resulting in higher efficiency, improved durability, and safety by eliminating the need to use mechanical compressors. The data generated was used to build mathematical models of the system to allow correct sizing for electrolyser, economic assessment, and establishing payback time for storage of excess electricity from Dorenell wind farm.

The team have also developed a hydrogen generation system which requires no electrical energy input and convert direct energy from mechanical energy to hydrogen. This can be interesting to convert direct offshore wind power into hydrogen. Their novel electrolyser, generates hydrogen at a significantly lower cost than commercial systems by eliminating need for power converters, and the ability to use earth abundant materials such as stainless steel.

b. Newcastle University's work on hydrogen conversion and storage

- **Overcoming barriers to developing efficient hydrogen fuel cells for heating and transport – Dr Prodip Das, Professor Keith Scott and Dr Mohammed Mamlouk**
- **Hydrogen to liquid fuels and chemicals – Professor Keith Scott and Dr Mohammed Mamlouk**
- **Carbon-based materials for hydrogen storage – Dr Anh Phan**

Overcoming barriers to developing efficient hydrogen fuel cells for heating and transport – Dr Prodip Das, Professor Keith Scott and Dr Mohammed Mamlouk

Hydrogen fuel cells have emerged as promising candidates for power generation because of their potential high-energy efficiency, environmental friendliness, and compatibility with sustainable fuels and renewable energy sources. They can be used in a wide range of applications, including transportation, combined heat and power, material handling, stationary, portable, and emergency backup power applications.

Hydrogen fuel cells work like Lithium-ion batteries, but they do not run down or need recharging and emit only water, so there are no greenhouse gas emissions and no air pollutants that create smog and cause health problems at the point of operation. Also, fuel cells are quiet during operation as they have fewer moving parts.

However, key challenges remain in the fuel cell industry. At Newcastle University, Dr Das is working closely with the US national laboratories, universities, and industry partners to overcome cost, performance, and durability barriers. Dr Das and his team are using an innovative and synergistic combination of experiment and physics-based modelling to understand physicochemical processes inside the fuel cells, find trade-offs and operation of the various interactions, and overcome current critical barriers for fuel cells, including cost, performance, durability, and water and thermal management issues.

Prof Scott and Dr Mamlouk have developed a super lightweight reversible fuel cell for the world's first variable buoyancy unmanned aerial vehicle in all-weather real-time surveillance system for atmospheric satellite applications, funded through the Innovate UK Phoenix project. The reversible fuel cell is able to store solar power in the form of hydrogen during the daylight and provide power for continuous operation of aircraft at high altitudes. The innovation won several awards including best collaborative project award.

They also have a range of large test beds for testing of kWs size fuel cell systems and have developed low-cost non-fluorinated membranes that do not require platinum or precious metal catalyst allowing significant cost reduction of fuel cell systems, achieving highest reported power density for alkaline anion exchange membrane fuel cells. They are using 3D modelling to optimise performance & improve understanding.

Hydrogen to liquid fuels and chemicals – Professor Keith Scott and Dr Mohammed Mamlouk

Prof Scott and Dr Mamlouk are part of a consortium to determine the energy and air quality impacts and potential future applications of a novel ammonia-fuelled heavy duty internal combustion engine. Their work is evaluating potential reductions in energy demand in the 'green' ammonia production process, making use of the new green ammonia pilot plant at the Rutherford Appleton Laboratories. It assesses the relative advantages and challenges of the approach using evidence-based life cycle analysis across a spectrum of competing decarbonised powertrain technologies for long-range heavy-duty transport (ground, freight rail and marine).

Carbon-based materials for hydrogen storage – Dr Anh Phan

Common hydrogen storage methods are high pressure gas, liquid hydrogen, adsorption on porous materials, complex hydrides and hydrogen intercalation in metals [1] in which only compression and liquefaction methods are commercialised. To store 13 kg of hydrogen in compressed gas storage requires high pressures, up to 700 bar, while liquid H_2 storage requires temperature below 20 K to achieve desired storage capacities (~ 0.2 m^3) in a vehicle.

However, both storage technologies have major drawbacks for mobile applications in terms of economical and safety aspects. The solid-state hydrogen storage has been considered a safe and affordable method for H_2 storage in vehicles as it can operate at or near ambient temperatures and low pressures (< 100 bar) to achieve practical storage densities [2]. However, more research needs to be done on solid materials for sufficiently on-board hydrogen storage capacities for vehicles.

[1] Schlapbach, L. and A. Züttel, Hydrogen-storage materials for mobile applications. Nature, 2001. 414(6861): p. 353-358; [2] Broom, D.P., C.J. Webb, K.E. Hurst, P.A. Parilla, T. Gennett, C.M. Brown, R. Zacharia, E. Tylianakis, E. Klontzas, G.E. Froudakis, T.A. Steriotis, P.N. Trikalitis, D.L. Anton, B. Hardy, D. Tamburello, C. Corgnale, B.A. van Hassel, D. Cossement, R. Chahine, and M. Hirscher, Outlook and challenges for hydrogen storage in nanoporous materials. Applied Physics A, 2016. 122(3): p. 151.

c. Newcastle University's work on hydrogen use

- **Developing models to design innovative fuel cells for electric vehicles at lower cost – Dr Prodip Das**
- **Using hydrogen for carbon capture in heavy industry – Dr Prodip Das**
- **Hydrogen combustion modelling for power generation and propulsion – Professor Nilanjan Chakraborty (Professor of Fluid Dynamics) and Dr. Umair Ahmed (Lecturer in Computational Fluid Dynamics and Thermofluids)**

Developing models to design innovative fuel cells for electric vehicles at lower cost – Dr Prodip Das

Hydrogen is an option for zero-emission e-transport as it's a much quicker source for refuelling vehicles than recharging a battery, with longer range. Hydrogen fuel cell electric vehicles (FCEVs) have several benefits over hydrogen in combustion-based technologies, as fuel cells can operate at higher efficiencies than combustion engines and can convert the chemical energy in the fuel to electrical energy with efficiencies of up to 60%. Hydrogen in fuel cells does not produce any greenhouse gases, while hydrogen in combustion engine produces greenhouse gases, such as NO and NO_2.

Newcastle University is working on developing a scientifically rigorous multi-scale computational model that can enable FCEV manufacturers to design next-generation FCEVs without the cost of creating numerous prototypes to test every new material or new type and configuration of the cells. The multi-scale model will enable us to establish a linkage between the transport properties of porous materials and explain material-transport interactions and structure-property relationships, which will lead us to tune and optimise diffusion-media and electrodes for fuel cells and clean energy applications.

Using hydrogen for carbon capture in heavy industry – Dr Prodip Das

While hydrogen is considered as the fuel of the future, it also has a huge potential for application in carbon capture and storage (CCS). Molten-carbonate fuel cells (MCFCs) are high-temperature fuel cells that operate at temperatures of 600 °C and have the ability to utilise hydrogen and CO_2 to generate heat and power while providing a provision to capture excess CO_2. MCFCs can efficiently capture and concentrate carbon dioxide streams from large industrial sources. Combustion exhausts from heavy industry processes can be directed to an MCFC, which produces power while capturing and concentrating carbon dioxide for permanent storage.

This process can capture about 90% of CO_2 from industrial exhaust streams, while generating additional power, unlike traditional carbon capture technologies which consume significant power. This is also useful for the heavy industry, where hydrogen could be an option to replace natural gas, such as in creating heat for glass manufacturing or as a feedstock in other processes while generating electricity. Dr Das and his team are looking into the techno-economic analysis of MCFCs for combined heat and power and CCS, which would support an affordable transition of UK industry towards net zero carbon emissions.

Hydrogen combustion modelling for power generation and propulsion – Professor Nilanjan Chakraborty and Dr. Umair Ahmed

New generation combustion devices must be simultaneously energy-efficient and environmentally friendly due to limited fossil fuel reserves, posing scientific challenges. This has also led to the increased usage of alternative fuels that are less dependent on crude oil, such as biomass-driven syngas and solar fuels (e.g. hydrogen, methanol). Generally referred to as High Hydrogen Content (HHC) fuels, these alternative fuels find their applications in the automotive as well as stationary power sectors. The usage of HHC fuels poses significant challenges in achieving stable and clean operation due to their unusual combustion characteristics (due to the very low mass of hydrogen), such as fast flame speed and high diffusivity associated with H_2 [1]. The presence of the light hydrogen means that characteristics of HHC fuel combustion are very different from traditional fuels and the effects need to be considered for its combustion in gas turbine applications [2-4]. Therefore, an improved understanding of combustion of HHC fuels at elevated pressures and its implications in modelling are urgently needed to implement this promising technology in the existing infrastructure and reduce reliance on conventional fossil fuels and the environmental impact of combustion (e.g. greenhouse gas emission).

A research programme at Newcastle University is focusing on the development of high-fidelity combustion models for HHC based on Computational Fluid Dynamics (CFD). As most existing combustion devices are designed to operate based on hydrocarbon fuels, the switch from hydrocarbon to HHC fuels will happen gradually. In the interim period, hydrogen is expected to be blended in different proportions with hydrocarbon fuel to effect a gradual reduction in greenhouse gas emission in order to meet environmental regulations. It is now common for syngas or shale gas fuels to be widely available for power generation in the form of Synthetic Natural Gases (SNG) and Compressed Natural Gases (CNGs) in an effort to reduce CO_2 emission, and these fuels contain variable amounts of different gaseous fuels in the blends, including hydrogen. These alternative fuels will play increasingly important roles in reducing harmful environmental impacts. Further development of advanced modelling techniques is required to account for the presence of light species such as hydrogen in mixtures of air or natural gas, and to enable the analysis of the combustion of alternative fuels. The simulations by the Newcastle team can accurately predict combustion behaviour of HHC fuels so that challenges of pollutant emission, flashback, and thermo-acoustic stability can be appropriately addressed. The information will be important for the utilisation and incorporation of HHC fuels into the current infrastructure for power generation and transport/propulsion sectors and to develop future generation combustors for sustainable fuels.

The incorporation of hydrogen in the infrastructure of power generation also needs to address the cost of generation of hydrogen and its transportation. In this respect, ammonia (NH_3) is often used as a hydrogen carrier [5]. As NH_3 is already used in chemical, refrigeration and fertilizer industries, there is no major obstacle in using it for combustion purposes. There have already been some attempts to use NH_3 for power generation purpose for land-based stationary gas turbine and marine propulsion sectors [5]. However, the heating value of NH_3 is low in comparison to conventional hydrocarbon fuels and there can also potentially be a possibility of increased NO_x emission as a result of NH_3 combustion [5]. Thus, it is necessary to optimise NH_3 combustion in terms of heat release and pollutant emission. However, numerical simulations and modelling of ammonia combustion are in infancy. There is a necessity to assess if the existing modelling methodologies for hydrocarbon and hydrogen combustion remain valid for NH_3 combustion. However, not much information is available on this and more research is necessary.

[1.] Dixon-Lewis (1979) Phil. Trans. Roy. Soc., Lond, 292, 45; [2.] Ern, Giovangigli (1997) Comb. Theor. Mod., 2, 349.; [3.] Ern,Giovangigli, (1999) Comb. Sci. Tech., 149,157.; [4.] Grcar et al. (2009) Proc. Comb. Inst., 32, 1173.; [5.] Kobayashi et al. (2018) Proc. Comb. Inst., 37, 109.

(January 2021)