EPSRC Co-ordinator for Research Challenges in Hydrogen and Alternative Liquid Fuels (H&ALFs)

UK-HyRES

Report on Online Workshop: H&ALFs Research Challenges

November 2022

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1. Background and Objectives

On **Friday the 21 October 2022** UK-HyRES (https://ukhyres.co.uk) held an interactive and participatory online workshop focusing on co-creation and development of research project ideas. The **objective of the workshop was to present the structure of the proposed national Hub and co-develop the details of the projects within it**. There was an amazing response from across the hydrogen community with **over 90 participants**. Facilitated by *The Collective*, we first heard from Prof Tim Mays (UK-HyRES PI and Director), who welcomed all attendees, before Prof Rachael Rothman (Co-I and Co-Director) introduced our vision for the Hub. The agenda for the event is provided in Appendix A.

Dr Derek Craig delivered the opening address at the event. Derek is Deputy Director Cross-Council Programmes within the Engineering and Physical Sciences Research Council (EPSRC) as part of UK Research and Innovation (UKRI). He is responsible for strategic leadership and oversight of EPSRC's environmental sustainability and decarbonisation research and innovation agenda working closely with colleagues across UKRI and the external academic, business and policy communities. He set out EPSRC's vision and the funding landscape, as well as the objectives of EPSRC. This included the imperative to create added value to the UK industrial strategy, widely collaborate and to champion EPSRC's place-based agenda.

Through four themed breakout sessions, we collectively examined some of the research challenges identified through our previous workshops: Production, Storage & Distribution, Alternative Liquid Fuels, and End Use. Following these workshops, key research challenges were drawn out and listed, then circulated to 25 experts from the advisory board of UK-HyRES, and other respected members of the research/industrial communities. This enabled some prioritisation of challenge areas ahead of the showcase event. The experts were asked to assess whether a research area should be investigated by the Hub "now" (3 pts), "later" (1 pt) or "never" (0 pts). From the 12 responses, it was possible to identify consensus priority research areas and rank them. The advisors were also able to suggest priority areas that were not selected from the first four workshops. The resulting priority list is shown in Table 1.

2. Breakout Discussions

Unfortunately, due to the mourning period following the Queen's passing, UKRI postponed the in-person showcase event scheduled for mid-September. Instead, the showcase was run as an online event. This significantly delayed the final stages of the Theory of Change (ToC) process including the development of detailed projects. The showcase again followed ToC principles, this time focussing on the detail of the "what" and "why". The participants took part in four world cafes developing details of projects in 24 breakout groups. Scriberia were also present and recorded the workshop ideas through their illustrative graphic, shown in Appendix B. Primers were delivered, that discussed the technical theme challenges, from the UK-HyRES investigators, Prof Tim Mays (PI and Director), Prof Rachael Rothman (Co-I and Co-Director) and Prof Shanwen Tao (Co-I and Co-Director). These challenges were highlighted in the slide deck (available on the UK-HyRES website) and while they represented priorities, these lists were by no means exhaustive and represent live documents that will be updated throughout the life of the Hub.

In the first two sessions the participants joined breakouts to discuss topics from the first three rows in Table 1. In the third and fourth sessions, the topics in rows four to six of Table 1 were open for discussion. In each session participants discussed the highlighted research challenges and developed project outlines that could be undertaken in the first, second/third or later years of the hub. Breakouts were asked to justify why each project was important, i.e., what impact could be achieved by doing it. The projects highlighted have formed the basis of the initial projects outlined in the Hub proposal. Further projects will be developed over the coming five months (Phase 2) of the Co-ordinator extension to enable further engagement and co-creation.

Through the breakout discussion, participants were asked to record their responses on a collaborative cloud document. These outputs were then collated to facilitate both the initial projects, and the second tranche of projects, aligned to the identified research priorities. As these outcomes are not conclusive and will be updated through further community engagement, we have provided the full response to each question in Appendix C.

Table 1: *Research challenges identified as consensus priorities by expert advisors from a longer list output from the four themed Co-ordinator workshops.*

Theme	Research Challenge Area for Breakout Discussion
Production	Alt. Catalysts to iridium Anionic exchange membranes Solid oxide electrolyser dev. Seawater electrolysis research Bio-based routes Solar and nuclear hydrogen production
Storage & Distribution	Cryogenic material behaviour Permeation barrier development Thermal energy recovery Solid-state modelling scale-up
Cross-cutting	H_2 sensor development Storage vessel leakage and failure
Alt. Liq. Fuels	Catalysts for ammonia cracking Electrolysis of ammonia for hydrogen production Ammonia release safety Reducing NOx emissions from ammonia combustion Electrochemical synthesis of green ammonia and ALFs Catalysts for localised green ammonia synthesis
End use	Reduction of iron oxide to steel with H_2 Redesign of cement kilns Burner improvement to reduce NOx Catalysts for hydrogen and ammonia combustion to reduce NOx
Cross-cutting	H_2 as a GHG modelling Point-of-use purification

3. Concluding remarks

- Participant feedback showed that the community found this method of engagement both engaging and productive.
- Giving the participants a choice of which room to join meant that certain research challenges were discussed in increased detail.
- Several new lines of enquiry were discussed that will require further follow-up by the research team.

Appendix A: Research Challenges Online Showcase Agenda

UK-HYRES Showcase- Research Challenge and Prioritisation Workshop

Friday October 21 2022 0930-1400

Zoom link :
https://us06web.zoom.us/j/84215039396?pwd=NTlneFZQT0ZnNmY0bXJ5M1h0bk1Ydz09

Time	
0915	**Waiting Room opens**
0930	**Welcome from UK-HYRES** **Professor Tim Mays** **Followed by participant introductions**
	The UKHYRES journey so far **Professor Rachael Rothman**
	UKRI Context and ambition **Derek Craig UKRI Director of Cross Council Programmes**
	UKHYRES Vision for the Hub **Professor Rachael Rothman**

	Overview of the Challenges for Hydrogen Production and Storage **Professor Rachael Rothman and Professor Tim Mays** **Followed by breakout discussions focused on research opportunities and prioritisation and feedback**
1125	BREAK
	Overview of Hydrogen End use and Alternative Liquid Fuels **Professor Tim Mays and Professor Shanwen Tao** **Followed by breakout discussions focused on research opportunities and prioritisation and plenary feedback**
1300	BREAK
	Open floor - your chance to input Introduced by the UK-HYRES team
	Next Steps **Professor Tim Mays**
1400	CLOSE

Appendix B: An illustrative summary of the workshop produced by Scriberia.

Appendix C: Responses to identified research challenges and project ideas, grouped by theme.

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1. Production theme

Breakout Session 1 - Room 1

Production - Alternative oxygen evolution reaction catalysts to Iridium. Suggested title change: Minimising/eliminating Iridium in PEM electrolyser

	What Project	**Why?**
Now-Year 1	Hybrid with alternative/non-Ir materials to minimise Iridium in PEM electrolysers	Insufficient supply for TW-scale production (inefficient use of Ir in devices at present)
	Iridium-free acid-stable catalysts	Many base metals used in Alkaline systems, but few options in PEM that are sufficiently active and stable
	Understanding degradation and operation mechanisms using advanced diagnostics techniques	Advances need to be measured - thus need for characterisation and diagnostics
	Robust understanding of cell and stack operation on alternative catalysts - H2 crossover, high pressure operation, solid-liquid-gas interface during the operation	An experimental functional map is required to characterise new catalysts under a range of operating conditions - thus need for bespoke metrology
	Multi-scale porous materials characterisation - this is not just chemistry, electrode engineering is the route to successful operation	High performance comes from holistic approach to electrode development - this also calls for multi-scale structural characterisation
	Development of suitable ASTs to understand new catalysts under real operating conditions - start-stop / dynamic operation	Successful cats must operate in real conditions

Year 2-3	Optimising cell design to improve mass transport Considering beyond the catalyst (support + current collector etc.) Electrochemical engineering platform to look at technologically relevant cells and stacks to identify real-world operating issues	Extending operating envelope to higher current densities provides better dynamics and affords lower LCOH (Levelised cost of hydrogen) Most Ir used as current collector at present. Catalyst-support compatibility needs further work Innovations must translate to real systems and be scalable - thus need for an electrochemical engineering platform.
Year 3+	Single atom catalysts	100% metal usage, how stability could be an issue

Breakout Session 1 - Room 2

Production - Develop step-change anionic exchange membrane.

	What Project	**Why?**
Now-Year 1	Solar integrated AME electrolyser / reactor development. Development of low cost catalyst for low cost earth abundant materials through scale fabrication technologies. Improve efficiency by reducing over potential.	Reduce cost, Better performance Less electricity will be used to produce green hydrogen.

	More flexibility in use of water with better stability and life cycle	Achieve required durability. Understand degradation mechanisms
	Synthesis of new anion exchange membranes with high hydroxide conductivity, low water uptake, low gas crossover, and better chemical stability.	Solar integrated electrolysers will increase efficiency and can work independent of the grid.
	Ionomers are also important for improving the electrode reaction kinetics, better ionomers with solution processability, chemical stability, and high gas transport would be desirable.	
	Interface between ionomers/catalysts and local environment is very important and in situ study is required.	
	Molecular design and modelling to understand the fundamental structure-property relationship, e.g. macromolecular structure, water and OH- transport.	
	Mechanical properties of the membrane is very important to investigate.	Mechanical robust membrane is essential for prolong life of a reactor.
	Bipolar membranes with high conductivity/water dissociation activity, and better chemical stability.	
	Membrane development synergy with other membrane research programme (e.g. SynHiSel).	
	Operation on pure water (avoid circulation of KOH)	
	Diagnostics and characterisation of components, cells and stacks	
	Understand the challenges of dynamic operation - degradation	

	Have a suitable modelling platform for cell operation.	
Year 2-3	Fabrication of membrane electrode assembly from new ionomer, membrane, catalysts, and understanding the interfaces and performance stability, and degradation of components. Overcoming the bubble transport issue to overcome the current density issue. Address the interface and charge mobility issues. Overcoming the scale up issues. Durability and stability will be key elements. Need for an engineering (technology relevant) scale platform to observe and test operation in systems moving to a commercial scale. Development of Solar/ Renewable integrated rector and its evaluation and assessment. High pressure operation (achieve low H2 cross-over)	To address UK net zero target scale up is very important. To meet UK 10GW hydrogen by 2030. Get the technology ready for scale-up and commercialisation. Reactor assessment is essential to take technology forward.
Year 3+	Feasibility study and Engage with industrial partners Demonstration for community based grid independent energy supply by integrating with solar or wind.	Grid independence will provide more Renewable integration will make it viable for commercialisation also can make remote communities energy independent.

	Upscaling the membrane manufacturing and MEA fabrication (e.g. A4 sheet size), and demonstration in kW-scale stack Connection with renewable sources of electricity Solar and wind integrated AEM electrolyser	

Breakout Session 1 - Room 3

Production - Oxygen electrode spalling, hydrogen electrode Ni migration, improving durability and reducing manufacture cost of solid oxide electrolyser technology.

	What Project	**Why?**
Now-Year 1	hydrogen electrode Ni migration, new materials for H2 electrode integrating waste heat from different sources	Degradation with Ni migration. We need to improve durability, cut cost Some theoretical/modelling studies exist for integrating SOE with heat from nuclear reactors. Practical engineering investigations and solutions are needed for integrating waste heat with SOE.
Year 2-3	Large-scale manufacturing	

Year 3+		

Breakout Session 1 - Room 4

Production - Fundamental research on seawater electrolysis.

	What Project	**Why?**
Now-Year 1	(i). Develop Cl2 evolution resistant catalysts and understand the competitive kinetics. (ii). Techno Economic analysis and LCA. What are the UK constraints on freshwater w.r.t. The 10GW H2 production target (see Cranfield research). On site production from offshore wind is a potentially important area for the UK. (iii). Find sea water tolerant materials device level (iv). Dirty water more generally (especially for off-grid).	(i). Currently in high demand, but not available. (ii). Understand the cost element against the scale of production. There is currently some uncertainty on the cost of desalination, and how this approach would compete with direct electrolysis of saltwater. (iii). Often components like encapsulation materials are ignored and only considered active materials (eg. catalysts). But, we need to consider device level.
Year 2-3		

Year 3+		

Breakout Session 1 - Room 5

Production - Bio-based routes to hydrogen production.

	What Project	**Why?**
Now-Year 1	Thermal decomposition of biomass	Research to improve the efficiency of hydrogen production
Year 2-3	Electrochemical conversion of biomass to produce hydrogen	Biomass electrolysis is also possible.
Year 3+	Biological conversion of biomass	

Breakout Session 1 - Room 6

Production - Using solar energy as the energy source for hydrogen production.

	What Project	**Why?**

Now-Year 1	Question around H2 or PV to heat - should we generate H2 locally in houses? TEA based on existing technology (solar PV + electrolyser at household level) - integration of technology in context of UK. May need small demonstrator or could use existing electrolyser data. Need accurate solar data. It would be good to form teams between material scientists and engineers to build prototypes for solar hydrogen production, generating real data that could be fed into TEA/LCA analyses. Modular/small scale electrolyser.	Understanding of where and when PV + electrolyser might make sense based on UK solar energy. Need for evidence of long-term stability (10000h) High temperature / pressure electrolysis + solar is relevant to established companies such as Ceres Power and SMEs like Supercritical Solutions
	Market analysis for nuclear and solar thermochemical H2 • Basic aims/targets for given reactor size? E.g. land costs, material costs, area needed • What are the next nuclear reactors in the UK going to look like and is it possible to directly interface with H2 production (thermochemically or high T electrolysis)	Need for evidence of long-term stability (10000h)
	Integration of solar/nuclear with H2	Understand how to make best use of High temperature heat
	Analysis of scaling of thermochemical/photochemical/electrolysis	

	Catalysts/materials in thermochemical. Materials stability. High T materials for use in 2 and 3 step thermochemical cycles -> material aims (E.g. Cerium Oxides, Copper Chloride hybrid cycles, operating temperature, durability, theoretical H2 production volume and rates, cost, manufacturability?)	Need evidence to drive forward to commercialisation Need evidence for possibility of retro-fitting to existing nuclear (and PV)
	Thermal management of electrolysers/ photoelectrolysers to enable coupling with potentially intermittent energy sources. Experimental work looking at how electrolyser performance is impacted by energy intermittency and the impact of thermal management on performance. Electrocatalysts (based on Earth abundant elements) that can operate under different temperature profiles	
	What about membranes? Have they reached saturation already or is there scope for further research and understanding?	
	Novel materials and architectures (including high pressure cells) for photoelectrocatalysis - fundamental analysis looking at how to improve efficiency of H2 production using direct reduction (i.e. all in one system, not generating electricity first then using that). Tandem semiconductor materials (earth abundant) incorporating Perovskite materials to increase yield of H2 production. Thermal management of photoelectrolysers.	Potential for orders of magnitude higher efficiency and unique selectivities. Opportunities to combine H2 production with valorisation reactions
Year 2-3		
Year 3+		

2. Storage theme

Breakout Session 1 - Room 7

Storage & Distribution - Material behaviour under cryogenic/ambient cycling. Including material embrittlement models and experiments.

	What Project	**Why?**
Now-Year 1	Support extending existing testing capability and capacity for materials testing in hydrogen at cryogenic temperatures, including under cycling Formation of Technical Working Groups to determine: • industry best-practice for performing these tests • Authoring of Standards • Establish suitable 'proxy testing' • Material Databases Investigate options for tankage materials that could be used at scale (e.g. from LNG and LN2 sectors) and screen for LH2 temperature effects Work with ATI, aerospace sector International collaboration e.g. Australia	Capacity doesn't exist to perform the number and range of experiments required for us to fully understand the material behaviour under these conditions. Standard testing definition required linked to international community Proxy testing: testing that does not use liquid hydrogen but another cryogen such as liquid nitrogen or helium that might be easier to handle, Alternatively 'pre-charged' samples. However, proxy testing will need to be established as conservative. Ultimately testing in liquid hydrogen will be required in order to assure safety.

Year 2-3	Formation of Liquid Hydrogen dedicated facilities in the UK with established supply of LH2. Separate out engineering test facility and need for small-scale test facilities close to appropriate test e.g. Ring test exposure under stress. Extending materials degradation test methods to liquid hydrogen temperatures Developing cold chain to materials examination e.g. transfer under LN2 to minimise hydrogen movement after exposure Exposure to temperatures below 20K. Materials understanding to underpin accelerated development/innovation NB are we also including the high-temperature side?	Dedicated hubs/facilities will consolidate UK capability and accelerate. Connect to cold-chain being developed for high-temperature exposure/degradation Underpinning research programme to support ATI, RR, Airbus, GKN, etc
Year 3+		

Breakout Session 1 - Room 8

Storage & Distribution - Develop novel non-metallic barriers to hydrogen permeation.

	What Project	Why?
Now-Year 1	Gaseous H2: Integration of permeation barrier materials into high pressure hydrogen storage safety strategies (various materials vs tank rupture protection) Liquid H2: R&D of crack resistant non-metallic barriers for liquid hydrogen carbon fibre composite tanks	Gaseous: linerless tanks may not be appropriate for all applications. Liquid H2: : Cracking in composite hydrogen tanks is a potential issue. Metallic liners as a solution have problems with differential thermal expansion coefficients. Non-metallic lining materials with a matched TEC are of interest. They need a high resistance to cracking during cycling from ambient in different temperature regimes.
Year 2-3	Full scale testing of carbon fibre tanks with liquid nitrogen.	
Year 3+	Full scale scale testing of carbon fibre tanks with liquid hydrogen requiring dedicated facilities,	To understand the interaction of the systems

Breakout Session 1 - Room

Storage & Distribution - Thermal energy recovery from compression and liquefaction and improvement of compressor technology.

	What Project	**Why?**
Now-Year 1	System level energy analysis for hybrid and/or liquefaction, exergy balance Quality heat capture from compression process and how this can improve performance	Understanding the system level energy balance and control of boil off or a circular system Level and quality of heat and how it can be utilised, rather than waste, towards zero waste
Year 2-3	Heat exchangers for liquid hydrogen Alternative compressor technology	Fundamental understanding of heat exchanger behaviour in cryogenic applications, particularly for mobile/transport scenarios Compressor technology for gaseous systems are relatively well defined but cryogenic compressed requires novel approaches.
Year 3+	Hybrid systems for gaseous and liquid hydrogen	Refuelling stations design of the future

Breakout Session 1 - Room 10

Storage & Distribution - New solid state materials and scale-up of existing solid state storage.

	What Project	**Why?**
Now-Year 1	Materials modelling and discovery incl. AI and machine learning	Can speed up identification of materials with the right characteristics for applications as opposed to laborious experimental work
Year 2-3	Technology coupling of solid state stores with	
Year 3+		

Breakout Session 1 - Room 11

Cross-cutting - Development of novel H_2 sensors, e.g. low-cost, in-line, real time & cryo-compatible.

	What Project	**Why?**
Now-Year 1		Range of materials What sort of concentrations in various leaks - can we sense at these levels What application, where, and what function

		Can we integrate sensors in multifunctional composites, ‘on all the time’ live sensing, 1. Determine concentration of h2 - what level an we tolerate 2. Material degradation, integrate sensor into material and sense material props with time. Can we use visual indicators and proxies, can we develop coatings Leakages Hydrogen detection (alarms) Hydrogen quantification (reports) Gas composition Hydrogen composition in gas blends Gas purity Impurities in hydrogen (impact material degradation and end-use-appliances like fuel cells) H2 gas flow Flow measurement for fiscal metering Materials degradation

		Sensors build into materials to understand material degradation Simulations to assist Hydrogen sensor development
Year 2-3	Sensors for Methane/Hydrogen mixtures	Hydrogen injection into the gas grid will have different mixture concentrations. Safety considerations in domestic and industrial situations will require accurate sensing. Simulations will help to identify mixture compositions to assist sensor development.
Year 3+		Sensors for combustion situations where there is no visible flame (hydrogen flames can be non-visible).

Breakout Session 1 - Room 12

Cross-cutting - Modelling leakage and failure mechanics of storage vessels, including O_2/N_2 condensation.

	What Project	**Why?**
Now-Year 1	In LH2 - condensation of O2, secondary ignition, fast evaporation and flame acceleration. Explosion overpressure, LH2 expands 800x on release, generates turbulence, accelerate flame size. Boiling liq. evaporation violent explosion - big issue Distribution of lh2, safety in fuelling, static ignition on planes.	SH2IFT project showed LH2 spills on water ignite themselves

Year 2-3		
Year 3+		

3. ALF theme

Breakout Session 2 - Room 1

Ammonia & Alt Liquid Fuels - Catalyst development for NH_3 -> H_2 cracking.

	What Project	**Why?**
Now-Year 1	Reduced energy input for efficient cracking - at lower temperatures	Better match to available heat from end-application Reduced energy input
	Reducing reliance on scare materials resources without sacrificing lifetime	
	Development of catalyst supports and porous media (flow)	Catalysts need to be supported to the effective and work in a device
	Reactor design and control (minimise corrosion from ammonia up to the point of the catalyst)	Effective device development critical for realising impact
	Lower operating temperature ammonia decomposition catalysts	Meet requirements of industrial processes. Match with waste heat streams
	Recognising requirements for point-of use conversion for (low-temperature) applications	Potential earth-abundant catalyst and operating regime - mapping onto system requirements
	Materials discovery	

	Membrane reactors - design to include catalyst support in multi-scale model	
Year 2-3	Scale-up/representative cell test facilities, including cycling and ageing Direct use of ammonia in cells (SOCs) vs use of produced H2 Improved understanding of reaction kinetics	Accelerate innovation and adoption - open to SME sector collaboration
Year 3+		

Breakout Session 2 - Room 2

Ammonia & Alt Liquid Fuels - Electro-catalysts for electrolysis of ammonia for hydrogen production

	What Project	**Why?**
Now-Year 1	Development of low cost electrodes with Pt and Ir free catalyst. Scale up of fabrication technologies to large scale reactor development.	Reduction of cost of process This technology will help to produce demand based hydrogen.

	Catalyst challenge while working in aqueous and non-aqueous condition. The aqueous condition is very complex, as the condition will be acidic or basic. High efficient catalysts need high energy and while low energy catalysts have low efficiency so energy balance is required.	Creating energy balance
Year 2-3	Electrode and cell design to maximise the electrocatalyst efficiency Energy balance in breaking N-H bond, Detail investigation of Durability and stability assessment during the operation conditions. Controlling the rate of reaction on each electrode and understanding the separation process. Development of electrodes for electrolysis. Improving understanding of reaction mechanisms & degradation mechanisms of different electrocatalysts via development of novel in-situ and in-operando diagnostic techniques.	Cell design and assessment is essential for commercialisation Reaction mechanisms will help to understand which step is energy intensive and how to overcome the issue. Reaction mechanisms and degradation mechanisms are currently poorly understood. New techniques will offer insights into routes for improving activity and durability.
Year 3+	Integration of renewable electricity with the electrolyser. System level consideration to practical application instead of simply discussing about catalyst.	For commercial aspects.

Breakout Session 2 - Room 3

Ammonia & Alt Liquid Fuels - Ammonia release safety modelling, including cryogenic ammonia release on water.

	What Project	**Why?**
Now-Year 1	Model development and validation of liquefied ammonia hazard assessment • Multiphase flow • dispersion • Vaporisation modelling • Will need fuelling protocol Need experimental data for large ammonia releases and for vaporisation of ammonia.	To understand the implications of using ammonia in situations it is not used in
Year 2-3	Model development of ammonia release on water and in particular sea water • Further develop above to take into account potential 3 phase flow (liquid H_2O, liquid NH_3, air/NH_3 mix) Safety aspects of release • Reactivity of ammonia/water? Ecotoxicity and impacts on marine life	Development of liquid NH_3 for shipping.

Year 3+		

Breakout Session 2 - Room 4

Ammonia & Alt Liquid Fuels - Modelling the combustion conditions for reduced NOx emissions.

	What Project	**Why?**
Now-Year 1	Ammonia combustion practical challenges - advanced strategies for ignition, fuel mixing, unknown kinetics/combustion characteristics	Large number of fundamental unknowns around combustion behaviour, difficult to start/sustain combustion and for that reason mixtures are used but the exact blend (and its characteristics are unknown). Modelling and experiments needed in both IC and gas turbines.
Year 2-3	After treatment - post combustion reduction of NOx where ammonia is fuel Combustion chamber design - design for ammonia combustion	Fixed and transport, current post treatment won't work How do we design for the ignition, standoff and temperature regions in combustion chambers.
Year 3+	Combustion Simulation studies to help industrial designs.	Ammonia "slip" from combustion, post combustion catalytic treatment and recovery of H_2 feeding back to combustion. Simulation work to optimise such processes.

	May be back-to-drawing-board and redesign of equipment assisted by simulation techniques to reduce NOx emissions from ammonia combustion	

Breakout Session 2 - Room 5

Ammonia & Alt Liquid Fuels - Efficient catalysts for electrochemical synthesis of ammonia and other ALFs.

	What Project	**Why?**
Now-Year 1	Direct N2 electrolysis to ammonia compared to two steps of water to H2 them H2 and N2 to ammonia, production rate as well as efficiency	
	Demonstration devices - scale up from single cell (there is some promising work in US where reasonable rates recorded, how can we take this forward)	Needed to enable optimisation.
	Online monitoring	Need for quantification/benchmarking of systems
	Mechanistic understanding - Why Li?	Only Li mediated system works. Controversy in the literature and a requirement to understand why on this works exists
	Alternative approaches (nitrate)	

	Improving control strategies to increase the efficiency and dynamic response capability of electrochemical ammonia synthesis. CO2 electrolysis to MeOH / EtOH / DME (direct vs. indirect syngas?). LCA/TEA in addition to technology development research	Demand exists for carbon fuels from end-users (shipping etc)
Year 2-3	Solar routes to ammonia and ALFs	To leverage the progress in PV, PEC/PC occurring more widely. Photodriven systems may provide specific advantages vs electrochemical
Year 3+		

Breakout Session 2 - Room 6

Ammonia & Alt Liquid Fuels - Catalysts for green ammonia synthesis by conventional Haber-Bosch process.

	What Project	**Why?**
Now-Year 1	Development of new promoters and co catalysts for current catalysts	Reduce operating temperature, Links in with established catalysts in mature industry, Lower catalyst cost as industrial process will use tons, Increase sensitivity to oxygenates lower operating cost

	Improving control strategies to increase the efficiency and dynamic response capability of electrochemical ammonia synthesis. Improving the consistency and lifetime of the electrolytic cells through better water and thermal management.	
Year 2-3	Exsolution and support materials to control particle size	Smaller particle size can increase activity
Year 3+		

4. End use theme

Breakout Session 2 - Room 7

End Use - Direct reduction of iron oxide to steel with H_2.

	What Project	**Why?**
Now- Year 1	Understand the reaction kinetics of hydrogen reduction reaction for iron oxide (iron ore). How will the contaminants in the iron ore such as silicates affect the process? How is the hydrogen produced iron (DRI) (which is different from pig iron) going to be used in steelmaking? Making the high temperature burner rigs and reduction rigs to expose the materials and then the materials development programmes for building H-DRI plant.	Do we have enough large-scale electrolysis to produce enough hydrogen for steel plants? (85Mt/y required globally, as rough order magnitude; ~0.5Mt/year for the UK [using 3.5MWh/tFe and 3MtFe/yr, need about 10TWh/y electricity vs 312 TWh production).. Or, will we do this in countries where electricity is cheaper, ie good solar PV provinces? *NB H-DRI can also offer demand flexibility, don't have to run at 100% - H as a store isn't so vital.* H-DRI plant has been operated at 0.5 Mt/y scale already - Cleveland Cliffs in Trinidad in early 2000s. INSEAD/Wharton Case INS891, Weber and Eichberger, Stahl und Eisen 122(2):59-64, 2002. Eg balance sheet plant and co-location - is the product metal the energy store, or hydrogen? Eg co-locate solar PV or wind, hydrogen production and metal production? What is the traded commodity - iron ore or iron, alumina or Al metal? Eg ship HBI or zinc or Al from Mexico or Algeria to the EAF plant in

		Europe. What is the regulatory environment going to be , eg an embedded carbon tax on imported iron - eg to avoid diversion? (eg breakpoint is €50/tCO2 carbon price and €40/MWh electricity price, 3.5 MWh/tFe using green (electrolyser) H2 - Vogl et al) Engineering large scale refining plant involves dealing with impure feedstock (currently a big concern in the industry for H-DRI) - eg how to refine the Si and S in the iron ore in a H-DRI plant or the subsequent EAF steelmaking steps. High temperature degradation issues and integrity of the ironmaking plant in H/H2O environment at 1000C (also in Aerospace) - i.e. how to engineer the plant, at scale. Also H-DRI isn't as exothermic, so in general there may be a question for ironmaking that we may need to heat - is this direct electric heating or burning hydrogen / synfuel? Then, as with other industrial and aerospace high temperature heat questions, there's all the questions about burner materials and degradation.
Year 2-3	Developing the high temperature H tolerant materials for H-DRI and burners etc.	
Year 3+		

Breakout Session 2 - Room 8

End Use - Redesign of cement kilns to reduce CO_2 emissions.

	What Project	**Why?**
Now-Year 1	Techno-economic analysis of using CO2 from the kilns directly for combining with hydrogen to produce fuels/chemicals on site, then use that for heating up the kilns. Techno-economic analysis of using different heat resources and energy resources (e.g. from nuclear)	Other countries such as USA are working on the decarbonization of cement production Hydrogen to provide heat for the kilns and energy for grounding
Year 2-3		
Year 3+		

Breakout Session 2 - Room 9

End Use - Improve H_2 and NH_3 burners to reduce NOx emissions.

	What Project	**Why?**
Now-Year 1	Combustion strategy to reduce NOx emissions - depending on combustion environment Fundamental combustion strategies	Reduce NOx emissions - particularly from shipping Optimise combustion efficiency

	Understand fuel-air mixing and ignition, flame propagation inside the burner Widen scope to consider degradation and safe operation of burner, injector components in the combustion environment Partial cracking approaches: optimise hydrogen/ammonia ratio, considering the effect of pressure Role for catalyst in pre-cracking/combustion - relationship with parallel work packages	Ensure safe operation and consider the fuel mixture ratios
Year 2-3	Consider hybrid burner technologies Consider changes to combustion products /flue gas - may contain unburnt hydrogen, for example	Operation across range of fuel mixtures (and reduce NOx emissions) Avoid unwanted release of hydrogen Safety and environmental considerations Potential effect on materials used in combustion chamber and exhaust
Year 3+	New burner design - to accelerate adoption	Lowest NOx and higher performance

Breakout Session 2 - Room 10

End Use - Develop suitable catalysts which can improve combustion of hydrogen and ammonia with reduced NOx emission

	What Project	**Why?**
Now-Year 1	In-situ and on-board ammonia cracking using catalyst and waste heat: -Identifying the cost-effective and efficient catalyst -Thermal integration with the engine waste heat -Identifying the optimal percentage of cracking that reduces the cost and NOx	Cost of catalyst is always a big issue Blends of hydrogen and ammonia can result in manageable NOx levels while reducing the load on catalysts and thus reducing the cots.
Year 2-3	How can the use of catalysts be minimised? -Improved design of catalytic reactors for combustion of hydrogen and ammonia.	Cost of catalyst added to the cost of hydrogen makes combustion of hydrogen/ammonia infeasible.
Year 3+	Prototyping and testing of onboard ammonia catalytic cracking reactor	

Breakout Session 2 - Room 11

Cross-cutting - Modelling to understand the effects of H_2 as a greenhouse gas.

Useful information:

https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachment_data/file/1067137/fugitive-hydrogen-emissions-future-hydrogen-economy.pdf

https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachment_data/file/1092809/low-carbon-hydrogen-standard-guidance-v2.1.pdf

https://www.aerosociety.com/get-involved/specialist-groups/air-transport/greener-by-design/

https://www.ati.org.uk/wp-content/uploads/2022/07/insight-aviation-emissions-modelling.pdf

From Robin Morris to Everyone 01:36 PM

NB H2 GHG: NERC grant supporting work in this area https://www.ukri.org/opportunity/environmental-response-to-hydrogen-emissions/

	What Project	**Why?**
Now-Year 1	Leakage and permeation Work with ATI to define what is needed in this space.	Need policy and standards

	Does environmental assessment (including LCA) take into account H2 in global warming potential. How do we make sure that potential H2 release is taken into account for environmental assessment?	
Year 2-3		
Year 3+		

Breakout Session 2 - Room 12

Cross-cutting - Develop point-of-use purification.

	What Project	**Why?**
Now-Year 1	Process integration of H2 purification technologies and processes, such as pressure swing adsorption with membrane separation. Suitable for H2 blending and extraction.	Fuel cells require high purity, although some inert gases such as N2 will have little negative effects on fuel cell performance.

	Hybrid PSA-Membrane is proven very effective. Fundamental research in new-generation membrane materials with high permeability and selectivity, and manufacturing of membranes that give high gas performance and high selectivity. Development of scalable technology, electrochemical purification technology, impurity tolerant, high temperature proton conductive membranes. Mapping the chemical composition of hydrogen streams derived from different feedstock & production techniques to understand impurity content.	Purification of H2 from syngas and steam methane reforming Pressure swing absorption - eff around 90% - they don't absorb inert gases like argon. Challenges with stability to moisture and steam. Can we develop hydrophobic versions that don't absorb steam/moisture? Membrane technology (porous polymers and metal based) (robustness of membrane limited and low permeability limited) There are opportunities for purification at a range of scales to enable various use cases. E.g. domestic scale de-blending of hydrogen, so a scalable purification technology is attractive. PSA difficult to downscale. Membrane & electrochemical technologies more promising for scaling-down. Important to understand impurity characteristics, as well as a view on how they are likely to evolve as production shifts away from predominantly grey hydrogen to a wide variety in future. Electrochemical pumping promising can operate at high temperatures, can work with solid oxide fuel cells NPL partnered consortia lead by Cadent, repurposing networks to transport h2 - line packing - can it be purified for vehicles. Detailed projects (check) some low TRL options that should be developed. Linde looking at de-blending combined PSA and membrane technology, large scale. Improve energy efficiency

		Membrane balance selectivity and permeability translation on scale up - works in academic environment due to performance tail off on ageing Metal membranes good selectivity but tolerance to impurities an issue - materials challenge to improve tolerance while scale up and reduce PGMs Background research into levels of contamination from source or storage Can we make purification tech cheaper than electrolysers, for medium scale de-blending ie. petrol stations
Year 2	In-depth study of mechanism, sensitivity towards impurities and performance in relevant environment.	Can we clean up h2 in a first stage of fuel cells,
Year 3+	Demonstration of separation process in collaboration with industrial partners.	