HyTN
Development of Thermochemical Hydrogen Production from Nuclear
Final Feasibility Report

Keywords
HYDROGEN PRODUCTION; NUCLEAR ENERGY; THERMOCHEMICAL

Preface

The UK National Nuclear Laboratory has delivered Phase 1 of its HyTN project, which has been funded by BEIS as part of the UK Government's Low Carbon Hydrogen Supply 2 Competition.

To provide a wider context, the UK Government recognises that real challenges remain in delivering UK net zero by 2050. Great progress has been made towards decarbonising the UK electricity system, and the growing number of electric vehicles on our roads confirms the effectiveness of policies to begin decarbonising transport. But credible plans need to be developed to decarbonise the "hard-to-abate" sectors and remaining fossil fuel use across the UK. "Hard-to-abate" energy uses can be characterised as applications where it is impractical to connect to the UK's developing low carbon infrastructure, which may be due to reasons of geography, mobility or economics. Such "hard-to-abate" applications may include:

- Long-distance heavy haulage surface transport
- Long-haul aircraft
- Energy intensive high-temperature industries such as steel production and glass manufacture
- Industries with sites necessarily co-located with localised feedstock production such as cement works, where it is impractical/uneconomic to transport all the raw materials to the location of a carbon capture and storage (CCS) cluster.

Industry and associated investors need to be increasingly confident that technical solutions for "hard-to-abate" applications are in the pipeline over the next decade for cost-effective commercial deployment at scale in the 2040s. Without this, the commitment to UK 2050 net zero remains at risk.

The UK Government's Hydrogen Strategy, released in 2021, identifies the importance of hydrogen as one of a handful of new, low-carbon solutions that will be critical for the UK's transition to net zero. Since then, the Government has stepped up the ambition for UK hydrogen supply by 2030 from 5GW to 10GW. But to maximise the benefits of a UK hydrogen economy, hydrogen supply must continue to grow beyond this in order to:

- De-risk net zero
- Sustain energy intensive applications that require an alternative to fossil fuels
- Deliver vast quantities of low-cost hydrogen with no associated carbon emissions in order to fuel UK economic growth without compromising on the commitment to deliver net zero carbon emissions by 2050.

A number of sources internationally have articulated the long-term goal of producing hydrogen with a production cost of around $1/kg (at today's prices), which is the estimated target cost necessary to sustain a thriving and cost-effective hydrogen economy. There are no transition technologies available today that can deliver this target cost in the UK, so the chase is on to develop and commercialise low-cost hydrogen production technologies for deployment from the 2030s and at scale during the 2040s.

NNL's HyTN project explores thermochemical hydrogen production technologies that have been studied at laboratory and pilot plant scale. The conclusion from Phase 1 of the project is that there are a number of such technologies, but all are assessed as no higher than Technology Readiness Level (TRL) 4. For the more promising processes a range of technical issues has been identified for resolution. Phase 1 has also identified that until recently there was little investor interest in developing these processes because until recently fossil fuels were cheap and abundant when used to manufacture hydrogen and associated hydrogen products. Therefore, to date there has been relatively little R&D investment in thermochemical hydrogen production technologies compared with other product markets which could earn higher profit and investor return.

This presents an opportunity for the UK to rapidly catch up with recent international progress, and the UK is well resourced with the specialist knowledge necessary to apply to the technology development challenges.

NNL's approach, developed through Phase 1 of the HyTN project, is to take the integrated thermochemical hydrogen production processes offering most promise and to further develop and optimise the individual sub-processes through laboratory scale experimentation. The goal is to apply catalysis to industrial scale closed cycle chemical processes to improve reaction efficiencies and reduce the temperatures at which these reactions take place. This is an industrial approach that has been widely deployed and proven over the last 20 years and which now supports a range of chemical products produced more efficiently and cost-effectively than without catalysis. Thermochemical hydrogen production techniques have simply lacked the necessary investment to make progress and deliver the technical breakthroughs that can be expected. The proposed next steps for Phase 2 are to resolve unit process issues and lay out a plan for the development of an integrated demonstrator for a thermochemical hydrogen production plant.

The proposed Phase 2 for HyTN provides the opportunity to develop and improve the chemical processes, further develop the economic understanding and comparison with other hydrogen production technologies, and build a knowledge platform to attract and secure investment for further development by industry.

The HyTN Phase 1 project has shown that thermochemical hydrogen production has the potential to deliver a step-change increase in UK hydrogen supply from 2040 onwards and a potential reduction in cost to supply a growing UK hydrogen market. Reducing the cost of hydrogen manufacture also makes more likely the use of this technology to provide feedstock to hydrocarbon production plants and reduce reliance on fossil-derived chemical feedstocks.

Potential entrants into the markets for both hydrogen use and hydrogen supply need to see projects like HyTN in the pipeline, with commercially deployable technology, from the 2030s, ready to deliver clean hydrogen at high volume and with low costs.

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Executive Summary

Nuclear power is already a high-capacity source of zero carbon electricity generation in the UK, making up approximately 40% of our existing clean electricity supply [1]. The next generation of nuclear reactors, Advanced Modular Reactors (AMRs), could play a similarly significant role in the world energy system, not just by producing electricity, but also through the generation of large quantities of hydrogen at a scale and cost that enable it to be used as a major energy vector. AMRs are the first nuclear technologies proven to operate at temperatures of up to 950°C and have the potential to unlock the operation of unique high-temperature processes for the production of hydrogen, which can be converted into other suitable energy vectors such as ammonia and synthetic hydrocarbons.

The HyTN (Hydrogen from Thermochemical and Nuclear) project aims to make use of the valuable properties of nuclear energy to realise a step change in the availability of hydrogen at large scale to a future energy system, not only displacing the use of fossil fuels but providing a feedstock replacement for the hydrocarbon and chemicals industry. Led by the UK's National Nuclear Laboratory (NNL), HyTN aims to develop thermochemical water-splitting technology which makes use of the heat from a nuclear reactor to generate hydrogen at low cost and zero carbon emissions.[1] Worldwide studies have already shown these thermochemical technologies for nuclear-enabled hydrogen production have significant potential to generate hydrogen at scale and low cost [2].

Evidence from this feasibility study has shown that the technology has the potential to achieve a marked increase in efficiency compared to existing hydrogen production technologies and unit hydrogen costs as low as £0.89/kg[2] [3]. Such price points are validated by publicly available reports which outline routes to deployment that achieve prices as low as $0.90/kg [2]. By utilising the heat from a nuclear reactor and a chemical catalyst driven process for generating hydrogen, thermochemical technologies are expected to be a more scalable solution than other zero carbon hydrogen production technologies.

HyTN has reviewed the global status of thermochemical hydrogen production and recommended that further development of the sulphur–iodine (S–I) and hybrid sulphur (HyS) processes could deliver the step change required based on unique UK Intellectual Property (IP). The review confirmed that global development of these technologies is at TRL 4, but the UK has, to date, played only a limited role in that development. Key challenges have been identified, as has an approach for engaging the UK's world-leading expertise in the identification of novel catalysts that would resolve the scale-up challenges faced to date. During the HyTN project, we have engaged with UK-based catalyst research networks and major industrial partners to identify the capabilities that could unlock this unique opportunity for the UK.

NNL is recommending a rapid programme of development for HyTN Phase 2 that would engage world-leading capabilities in the development of a potential step-change technology. An investment to deliver this programme is expected to raise interest among wider stakeholders and offer opportunities for private and academic research investments. This supports forward commercialisation of the technology in lock step with the commercialisation of advanced nuclear reactors to deliver a world-leading capability that helps to deliver net zero.

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[1] Thermochemical technologies are zero emission at the point of generation
[2] Price base date: 2016

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1. Introduction and HyTN Concept

HyTN is a concept for the development in the UK of hydrogen production technologies that could realise a step change in the availability of hydrogen at large scale to a future energy system, not only displacing the use of fossil fuels but also providing a feedstock replacement for the hydrocarbon and chemicals industry. Led by the UK's National Nuclear Laboratory (NNL), HyTN aims to develop thermochemical water splitting technology that makes use of the heat from a nuclear reactor to generate hydrogen at low cost with zero carbon emissions. Worldwide studies have already shown these thermochemical technologies for nuclear enabled hydrogen production have significant potential to generate hydrogen at scale and low cost [2].

Nuclear power is already a high-capacity source of zero carbon electricity generation in the UK, making up approximately 40% of our existing clean electricity supply. The next generation of nuclear reactors, Advanced Modular Reactors (AMRs), could play a similarly significant role in the world energy system, not just electricity, through the generation of large quantities of hydrogen at a scale and cost that enable it to be used as a major energy vector.

AMRs are the first nuclear technologies proven to operate at temperatures of up to 950°C and have the potential to unlock the operation of unique high-temperature processes for the production of hydrogen at higher efficiencies than existing reactor technology. This can then be converted into other suitable energy vectors such as ammonia and synthetic hydrocarbons; these have the same chemical composition as hydrocarbons but are derived from non-fossil fuel sources. Ammonia and hydrocarbons are products with uses beyond simply as fuels, for example, in long-haul aviation, which allows AMRs to be positioned as significant enablers of economic activity. Moreover, in the modelling studies completed as part of this project and summarised in this report, it is shown that thermochemical methods have the potential to deliver thermodynamic efficiencies that greatly exceed those of electrochemical processes, leading to lower unit costs compared to electrochemical production.

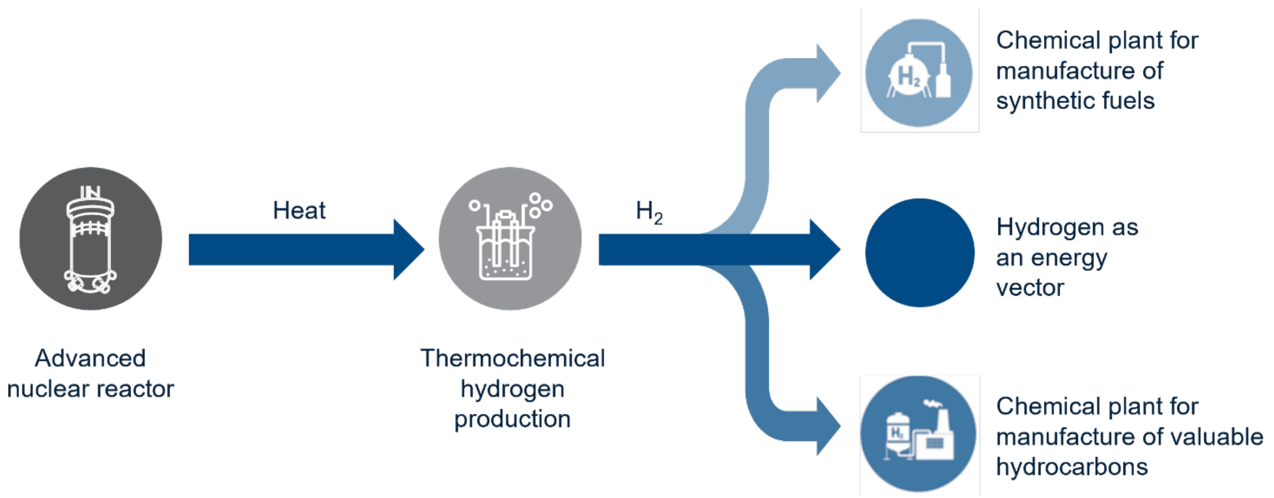

Figure 1: Diagram outlining how thermochemical hydrogen production can be used to feed multiple applications with large-scale, low-cost hydrogen.

Figure 1 outlines how thermochemical hydrogen production makes use of the heat from an AMR to generate hydrogen as a feedstock for multiple applications including manufacture of synthetic fuels, directly as an energy vector or for the manufacture of other hydrocarbon-based products such as plastics.

HyTN has reviewed the global status of thermochemical hydrogen production and recommended that further development of the sulphur–iodine process (S–I) and hybrid sulphur process (HyS) could deliver a step-change technology based on unique UK IP. The review confirmed that global development of these technologies is at Technology Readiness Level (TRL) 4, and the UK has, to date, played only a limited role in that development. Through this review, key challenges to technological maturity have been identified and an approach for engaging the UK's world-leading expertise in the identification of novel catalysts that would resolve the scale-up challenges faced to date has been presented. In the course of the HyTN project, we have engaged with UK-based catalyst research networks and major industrial partners to identify the capabilities that could unlock a unique opportunity for the UK.

Figure 2 shows how thermochemical hydrogen production (specifically, the S–I process in this instance) makes use of the heat from an advanced nuclear reactor to drive a number of unit processes that split the water feed into hydrogen and oxygen. HyTN has identified that a method for accelerating development of the technology will be to focus on resolving issues within each of these unit processes prior to integrating them into future demonstration systems. This project proposes the use of a digital twin to understand the impact of developments in the unit processes on performance of the whole system prior to the development and deployment of a complete integrated demonstrator. The digital twin will integrate unit operations tested and proven on a laboratory scale. Using this approach has the added benefit that resolution of issues within the unit processes will also resolve outstanding issues in the HyS process, which could serve as a stepping stone to future deployment.

Thermochemical processes are, in concept, closed-loop processes, meaning that additional feedstocks other than water should not be required to manufacture hydrogen. Whilst further work is required on the development of long lifetime reaction vessels and catalysts to control the reaction, the lifetime waste generated by the process could be minimised through careful development.

NNL has identified a significant potential market for hydrogen from thermochemical technologies, with an addressable value of up to £34.2 bn per year (see Table 3). By developing thermochemical hydrogen production in lock step with AMR development, something the UK is pursuing under the AMR Research Development and Demonstration Programme, the technology could be realised for commercial deployment by the late 2030s, with a rapid expansion through the 2040s to help deliver net zero and replace transition technologies. HyTN estimates that this could avoid 132 Mt/CO_2 per annum and create 265,000 jobs.

This report summarises the findings and recommendations of the HyTN feasibility study. It brings together the outputs of five separate reports, produced as part of this study, that further detail how thermochemical hydrogen production could be developed in the UK and support a future hydrogen economy [4] [5] [6] [3] [7]. The project presents a technology that, through revolutionising scale up of zero carbon hydrogen generation and reducing the unit cost of hydrogen compared to other technologies, would allow hydrogen to play a role beyond that which is currently predicted for a net zero energy system and place the UK as a world leader in the deployment of nuclear-enabled hydrogen generation.

2. Background

The UK Hydrogen Strategy [8], published in 2021, highlights the potential for thermochemical water splitting to play a role in hydrogen production from the mid to late 2030s whilst noting the need for further work to develop to a commercial technology. HyTN identified how global investment in R&D related to thermochemical technology is substantially less than investment in electrolysers [4].

This, however, presents an opportunity for rapid progress in the development of the technology, where research can be targeted at the main barriers to development and deployment. The HyTN project feasibility study has reviewed these barriers to deployment and outlines an approach for focusing future investment to enable the development of the technology in line with the forecasts for deployment in the late 2030s, as outlined by the UK Hydrogen Strategy.

A variety of thermochemical hydrogen production processes have been proposed by global research groups. These include both pure thermochemical processes and hybrid processes, which incorporate both thermochemical (heat powered) and electrochemical (electricity powered) steps. The most developed of these are variations on three processes – the sulphur–iodine (S–I) process, the hybrid sulphur (HyS) process, which is also known as the Westinghouse process, and the copper–chlorine (Cu–Cl) process [4]. Further discussion of the processes and recommendations for development in the UK are provided in Section 3 – Demonstration Design.

All of the processes require some level of high-temperature heat input to drive the reaction and a range of catalysts to control the reactions. Selection of suitable catalysts can reduce the heat (and energy) input required, ultimately enabling commercial deployment of the technology. Catalysis is utilised by more than 80% of industrially manufactured products and underpins more than 30% of European GDP [9]. For example, 40% of petroleum manufactured today uses a process called fluid catalytic cracking. Catalysis improves the economic performance of manufacturing processes by improving the reaction selectivity for a specific product and by lowering the operating temperature, which reduces the production energy costs and increases the operating lifetime of the plant. A second example of this process of development away from the industrial chemicals sector is the manufacture of margarine. In the 1990s, evidence of the health impacts of trans-unsaturated fatty acids became clearer and global margarine manufacturers moved to reduce trans-fats in their products. One of the methods for doing this is through the introduction of novel catalysts in the production process that reduce the production of trans-fats [10]. The selection and use of catalysts is a proven and widely adopted approach to optimise modern industrial chemical processes, with world-leading expertise based in the UK.

Following BEIS guidelines, HyTN has assessed the technology readiness level of thermochemical hydrogen production to be at level 4. The challenges of moving to higher TRLs are far from unique and are typical of most industrial chemical processes. In fact, many of the most widely used and largest-scale industrial processes (ammonia manufacture) have the same (or similar) issues requiring optimisation so they can operate efficiently when driven by renewable energy sources. What has changed because of the climate emergency is the willingness to focus on optimising these processes, whereas previously these inefficiencies were largely ignored in the drive to maintain small margins on low-value end products.

These historical and present-day inefficiencies have now started to be addressed as a result of the drive to reduce not just Scope 1 and Scope 2 greenhouse gas emissions (those associated directly with an entity and the energy it purchases), but also Scope 3 emissions (of the products companies sell and other supply chain emissions). Reducing Scope 3 emissions can be achieved either by removing carbon from products being sold (such as the replacement of methane with hydrogen generated through steam methane reformation with carbon capture and storage) or by identifying large-scale, low-cost technologies to replace the feedstock directly with a carbon-neutral alternative.

HyTN is targeted at the development of technologies that can, in the long term, reduce the cost of carbon-neutral feedstocks to a level at which they can compete with fossil-based incumbents. Previous studies have shown that, when combined with advanced nuclear technology and a revolutionary approach to deployment of the technology, the cost of hydrogen production can achieve parity with that of fossil fuels [2]. In 2021, NNL published a report, co-authored with the Energy Systems Catapult and Lucid Catalyst, that incorporated similar concepts into a UK whole system energy model for the first time [11]. Incorporating the most ambitious cost of synthetic fuels (those derived from advanced nuclear with thermochemical hydrogen production, direct air capture and Fischer–Tropsch synthesis) into the Energy System Modelling Environment (ESME) resulted in 148 TWh of energy being drawn through this vector in a net zero compliant energy system.

This modelling effect is further compounded by two realities. First, that the cost of asset replacement within the global energy transition greatly distorts the optionality for deploying entirely new energy distribution mechanisms. For example, whilst developing synthetic fuel plants may be capital-intensive, it is likely to be far less capital-intensive than wholesale replacement of the global aviation fleet. Second, that flexibility is key to developing technology solutions that will thrive in a global marketplace. This is exemplified by the experience of refineries during the COVID-19 pandemic, where process flexibility allowed a rapid switchover from the production of gasoline and jet fuel to fuel distillate, which can be used in other applications [12]. The reality is that oil refineries operate flexibly on a daily and even hourly basis and such flexibility, in terms of the quantities of products that are derived from the primary source, would be required to integrate low-carbon technologies into our existing economic system. Figure 1 outlines how HyTN sits at the centre of providing a flexible future energy and materials vector in a similar way to current generation refineries and chemical production facilities.

HyTN further explored this concept in Section 2 of the report "Review of future market demand, applications and technology options for large scale hydrogen production from nuclear energy" [4]. The report highlighted that over 1000 TWh of energy is consumed per year within the UK energy system in forms other than electricity. By focusing on a technology that could offer a step change in the delivery of low-cost hydrogen, HyTN could provide a useful low-carbon energy vector that enables the manufacture of high-value derivative products that de-risk achieving net zero in multiple sectors. Should the technology reach full commercial readiness, it could be at price points that make it an economically attractive energy vector, something reinforced by further analysis within the HyTN feasibility study, even before considering the additional costs of asset replacement that will be incurred by other decarbonisation vectors. The report laid out the initial steps for how this technology could be used to enable refinery-scale multi-product sites, in the same way the oil and gas sector already operates facilities designed to flex their production capacity to maximise the value of the products being generated.

3. Demonstration Design

3.1. Route to Demonstration

HyTN recommended two priority thermochemical hydrogen production processes for development, the sulphur–iodine (S–I) process and Hybrid Sulphur (HyS) process [4]. Whilst the copper–chlorine (Cu–Cl) process was reviewed, this project viewed the viability of the process as low, with significant barriers to development. Furthermore, modelling of the process indicated lower than expected forecast performance efficiencies.

The S–I process is a three-step autocatalytic cyclic process, outlined in Figure 2, for the synthesis of hydrogen from water, driven by heat from a nuclear reactor. Japan Atomic Energy Agency (JAEA) has demonstrated a pilot-scale facility to understand the feasibility of thermochemical hydrogen production coupled to an AMR, and which produced 30 L/h of hydrogen for 150 hours [13]. Despite this successful feasibility project, several technical challenges emerged from these tests and the TRL for this technology continues to be assessed as 4, as only basic technological components have been tested and integrated. Further work is required to improve the basic technological components so the system as a whole can operate at the levels of efficiency required to be competitive with alternative hydrogen production technologies.

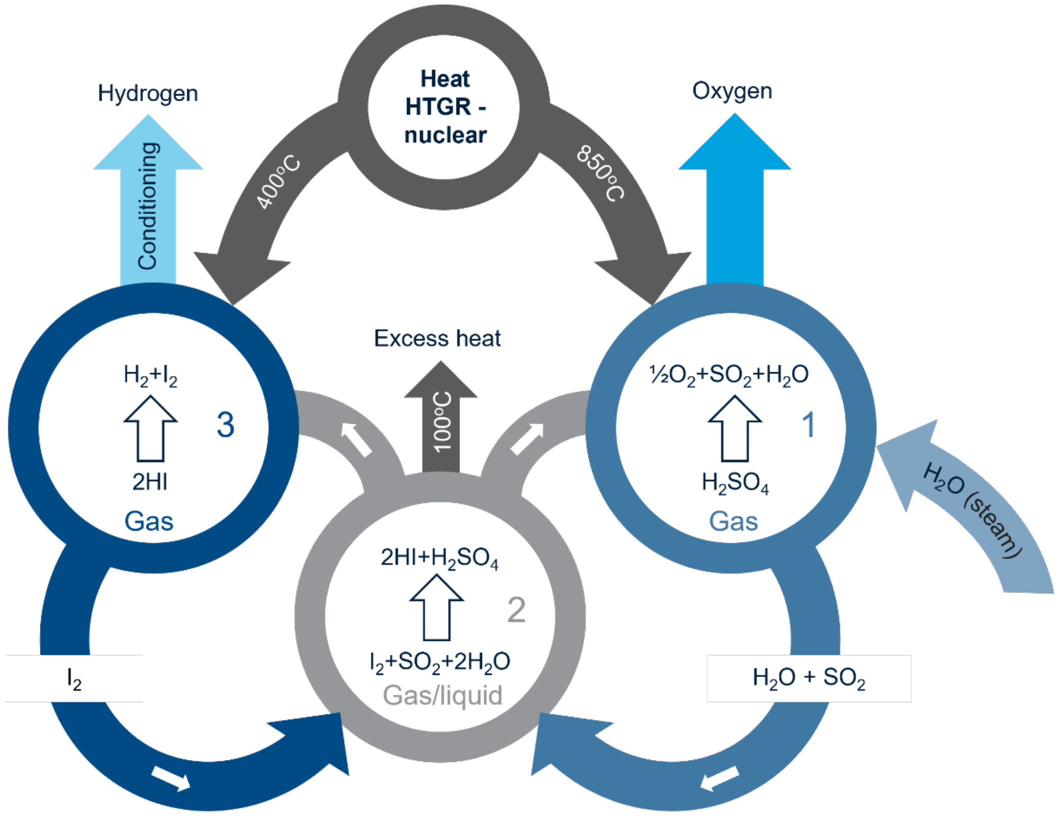

Figure 2: An overview of the S–I process illustrating the chemical reactions and energy inputs required for generating hydrogen.

The HyS process (sometimes referred to as the Westinghouse process) decomposes water into hydrogen and oxygen in two steps, each involving two reactions, requiring a high-temperature heat source and an electrolyser cell [14]. The reaction steps are illustrated in Figure 3, with the electrolyser steps on the left-hand side (Step 2) and the thermally driven processes on the right had side (Step 1). The hydrogen generation step involves electrolysis, but this occurs at a significantly lower voltage than with water-based electrolysers. Furthermore, the operating temperature and energy consumption is lower than for the S–I process, though at a chemical level the concept is like that process. The concept was developed in 1967 and the design was patented in 1975. The UK was active in research on this technology, and NNL has access to archived information. The TRL of the HyS process has been assessed as Level 4 due to the demonstration of the process in several laboratory studies.

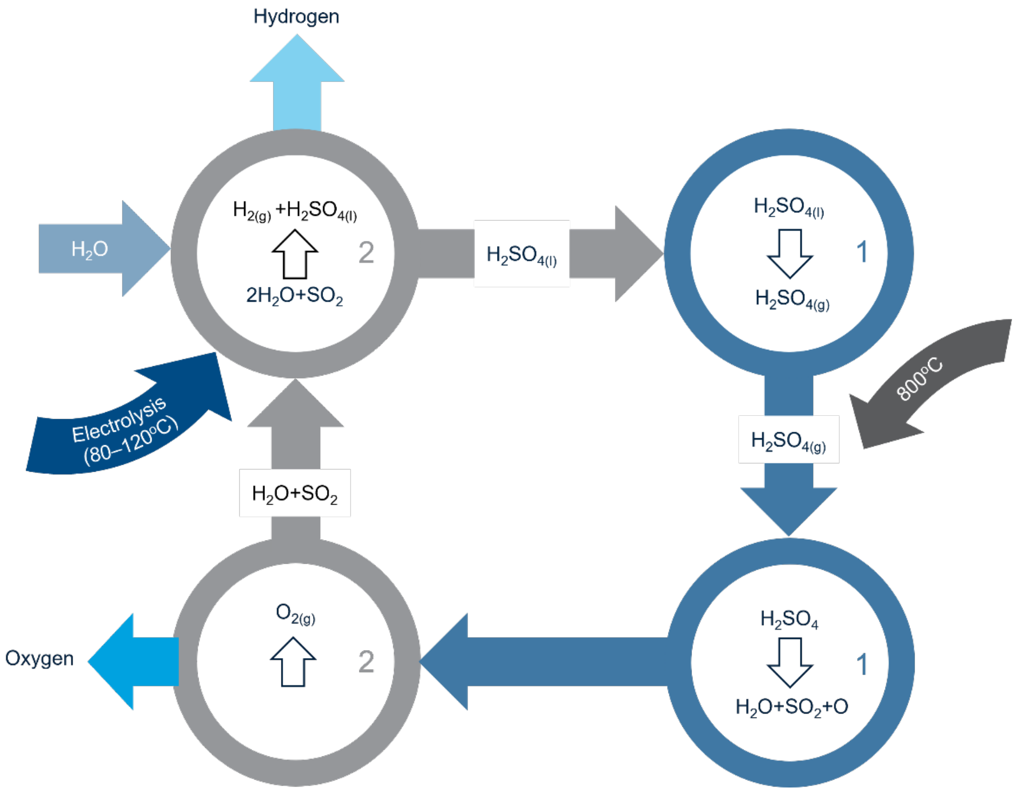

Figure 3: An overview of the reaction scheme for the Westinghouse hybrid sulphur process.

HyTN identified that the development challenges for both of these processes are similar and therefore continued development of both provides a more resilient development path [6]. The challenges identified are summarised in Table 1, and it was considered that the most significant of these is the identification of catalysts to control and improve the chemical reactions. The role of a catalyst in any heterogeneous reaction is to provide an alternative mechanism by which reactants can be converted to products at a lower activation energy. Hence, catalysts can speed reactions up, promote preferential pathways to increase product yield and can also allow reactions to proceed at lower temperatures. This means that catalysis offers the potential to lower operating temperatures for thermochemical processes, enabling an increase in the overall thermal efficiency of the system. Lower operating temperatures will also improve the lifetime of the chemical reactors by reducing thermal degradation.

Development of catalysts is typically done by separating the relevant unit process being optimised into laboratory-scale rigs. This has been previously demonstrated through international developments on thermochemical hydrogen technologies which have focused on the optimisation of the unit processes in parallel with development of laboratory-scale closed-cycle demonstrators. Such an approach has guided the development and thinking of HyTNs proposed approach to Phase 2.

The UK has a strong pedigree in the development of catalysts, with world-leading capabilities across multiple sectors, including large-scale industrial manufacture of commercial catalysts and academic research. Engaging this capability in the development of thermochemical hydrogen production, coupled with the relative scale of the challenges faced in the commercialisation of this technology, could quickly put the UK into a world-leading position in the development of this step-change technology.

Table 1: Summary of process challenges and R&D solutions required to improve on currently available TRL 4 solutions.

Performance issue	R&D solution	R&D activities
High temperatures that are difficult to manage and shorten life of plant	Catalysts to change the reaction so it takes place at a lower temperature (e.g., acid decomposition reactions)	Bench-scale test rigs to test performance of catalysts Small-scale test rigs to test integral systems (between two or more coupled process steps) Process and chemical models
Undesirable side reactions that lower the efficiency of the process and generate problematic waste slurries	Separation technologies to remove undesirable products Catalysts (electrodes) to make the reaction scheme more favourable	Bench-scale test rigs to test the performance of separator technologies Bench-scale test rigs to test catalytic electrodes Small-scale test rigs to test integral systems (between two or more coupled process steps) Process and chemical models
Impure product streams	Separation technologies that remove contaminants from the product streams allowing for re-use/recycling of wastes	Bench scale test rigs to test membrane performance and degradation (heat, corrosion, erosion, radiation)
Short lifetime of critical components	New material and coatings to improve component lifetime	Novel materials testing, materials degradation (heat, corrosion, erosion, radiation)
Complex reaction schemes leading to challenges to safely controlling the process	Control systems allowing safe operation to be maintained when scaling up to production scale Better understanding of the operation envelope (phase diagram of the process)	Small-scale test rigs to test integral systems (between two or more coupled process steps) Laboratory-based R&D studies to measure thermodynamics of the reaction schemes Process and control systems models utilising artificial intelligence and digital twin technologies

3.2. Unit Process Development

Figure 4 highlights the three main reactions of relevance to the S–I and HyS processes:

- Catalyst systems for the decomposition of sulphuric acid
- Decomposition of hydroiodic acid
- The Bunsen reaction.

The HyTN feasibility study reviewed existing international literature for the development of these processes with detailed recommendations for what next steps can be taken to resolve outstanding challenges and suggested engineering designs for development rigs.

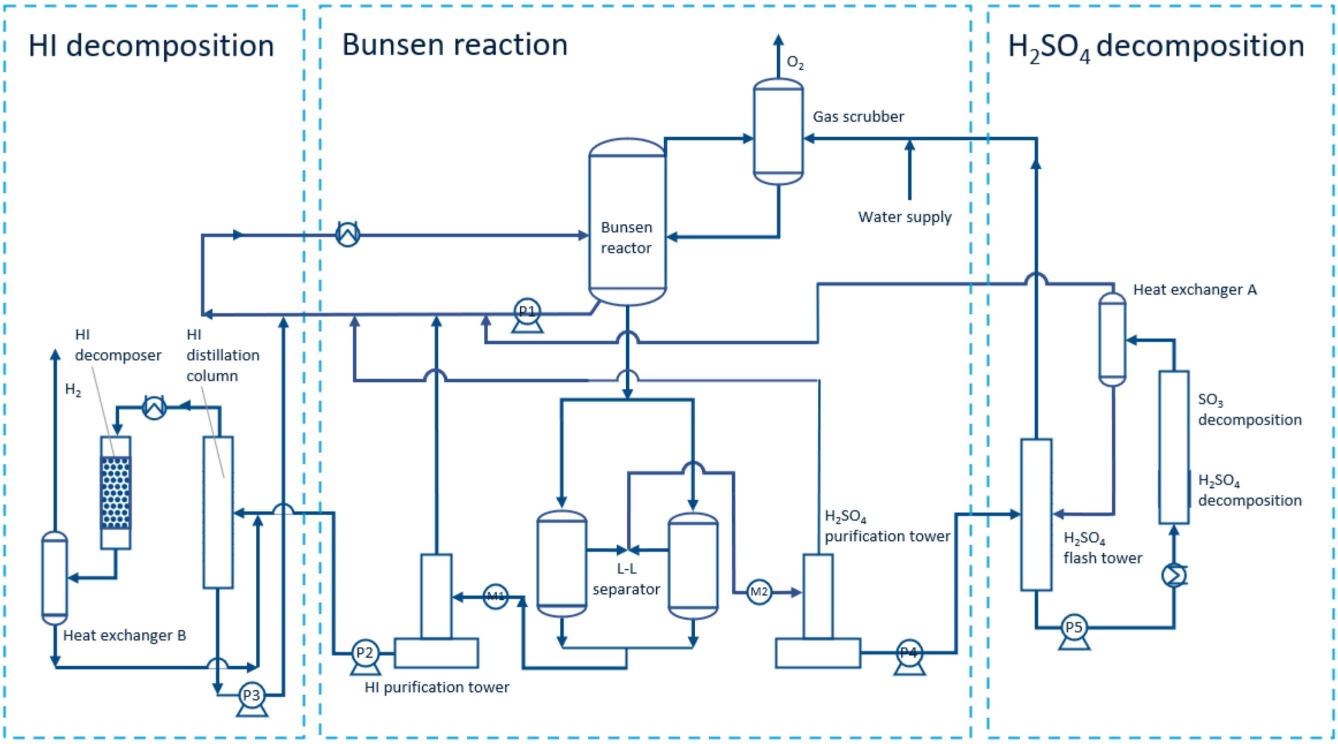

Figure 4: Detailed schematic of how different unit processes are integrated to form the S–I process. Some of the same processes are used for the HyS process [15].

HyTN proposes a collaborative approach to the development of these processes and the resolution of the other identified development challenges, whereby NNL acts as a central integrator of the technology working closely with specialist groups across the UK to resolve specific challenges. It is an approach that NNL has previously demonstrated successfully through the BEIS-funded Advanced Fuel Cycle Programme, where NNL acted as technical integrator across a broad range of advanced nuclear technologies [16]. There is a further potential opportunity to utilise NNL-managed, unique UK facilities to facilitate testing of uranic catalysts that have shown considerable potential in similar processes.

Partnerships with key UK universities and industrial partners across a range of disciplines, including catalysis, electrochemistry, separation science and corrosion science, will be key to leverage UK skills, infrastructure and capabilities to accelerate development of the technology.

NNL are currently exploring the use of an existing partnership with the Centre for Process Analytics and Control Technology (CPACT) to coordinate collaborations between NNL subject matter experts, academic and industry partners to support further R&D for HyTN Phase 2 [17]. Established as an interdisciplinary industry–university consortium to promote advanced process monitoring and control techniques, CPACT is made up of a broad range of academic, research institute and industrial members, and offers opportunities for collaboration across a range of disciplines. As a member of CPACT, NNL can leverage existing collaboration agreements, which means that projects can be initiated quickly, allowing the full benefit of experimental programmes to be realised.

Several key technical challenges around thermochemical processes relate to a need for optimised stable and resilient catalysts to accelerate reactions under extremely harsh processing conditions and promote reactions at lower processing temperatures. The HyTN project will take advantage of the UK's world-leading capability for the supply and design of catalysts to accelerate UK knowledge and understanding of the key processes to enable the UK to catch up with international efforts for thermochemical hydrogen production. As part of the current phase of the HyTN programme, NNL has initiated a dialogue with the UK Catalysis Hub [18]. The Catalysis Hub is a consortium of universities involved in catalysis research around the UK and focused on developing catalytic processes for more effective use of water and energy, waste minimisation, material reuse and reduction of gaseous emissions. The universities, small- and medium-sized businesses, and large business partners within the consortium have extensive catalysis expertise and routinely develop and operate catalyst testing rigs. They also offer extensive capability for catalyst characterisation and will be well placed to support further development of the technology.

As discussed in the preceding section, opportunities to leverage recent international developments on thermochemical cycle demonstrator facilities will be pursued to optimise an approach to the deployment of demonstrator rigs in the UK. This will include engagement with JAEA through the NNL/JAEA technical collaboration agreement to identify the current trajectory of research around the development of demonstrator rig facilities in Japan.

Apparatus for the development of these unit processes is further described in the HyTN Feasibility Study report, "Experimental Apparatus to Meet the Development Needs for Nuclear Enabled Thermochemical Hydrogen Production Technology", based on international experience.

Development of all the processes needs to focus not only on opportunities for improvement through selection of suitable catalysts, but also on materials for holding reactants and suitable control systems for managing the reactions, as highlighted in Table 1. By separating the system out into constituent unit processes, these additional aspects can be further developed with suitable partners, as outlined above, prior to development of an integrated solution.

In terms of the broader needs of the programme, the UK and the nuclear sector have extensive experience of developing digital twin technology. For example, the BEIS-funded programmes NVEC (Nuclear Virtual Engineering Capability) and FAITH (Fuel Assembly Incorporating Thermal Hydraulics) have already demonstrated the core principles of digital twin technology for pilot-scale test rigs. Broader skill sets will need to be exploited to provide the underpinning data to steer both the laboratory-scale test programme and modelling of the unit operations, and this will utilise capabilities drawn from across a number of UK chemical engineering research groups.

3.2.1. Catalyst Systems for Decomposition of Sulphuric Acid

The decomposition of sulphuric acid is a key reaction step in both the S–I cycle and the HyS cycle. It is not only the most energy intensive step, but also the highest-temperature unit operation in both the S–I thermochemical cycle and the HyS hybrid cycle and, as such, dictates the temperature requirements of the primary energy source.

The use of such high temperatures in combination with corrosive reaction conditions presents significant engineering, materials compatibility and process monitoring challenges. Reaction yield and selectivity are also barriers to industrialisation of the thermochemical production of hydrogen. Hence, the development of a catalytic system to reduce the temperature of the sulphuric acid reaction will be essential to moderate reaction conditions to address engineering and material compatibility issues, improve reaction yield and selectivity to enhance the overall process efficiency, and increase the flexibility of the technology for integration with lower-temperature heat sources.

Experimental rigs for this unit process will be utilised to further develop the sulphuric acid decomposition unit process as follows:

- Develop cost-effective catalysts that are active, selective, stable to the harsh operating conditions and promote the reaction at lower temperatures
- Provide data to support a detailed assessment of the reaction kinetics for use in modelling studies
- Provide flexibility to support testing of catalysts in a variety of forms with a range of feed compositions
- Allow a detailed assessment of the decomposition of sulphur trioxide into sulphur dioxide and oxygen in isolation and in combination with the preliminary acid evaporation and dehydration steps
- Support development and testing of on-line processing monitoring requirements for this section of the cycle.

3.2.2. Decomposition of Hydroiodic Acid

One of the critical steps in the S–I cycle is the hydrogen iodide (HI) decomposition reaction. This reaction is only slightly endothermic but is the slowest reaction in the S–I cycle (i.e., the rate limiting step) and shows poor thermodynamic equilibrium since it is not entropically favourable (it is a homogeneous gas phase reaction). Additionally, the products form an azeotrope, which means that the composition of the decomposition products does not change as the reaction progresses. As a result of the slow kinetics and thermodynamic limitations, considerable energy consumption is incurred through the separation and recirculation of the unreacted species, making the use of a catalyst with high performance and low cost essential to unlock workable reaction rates. Since this reaction is supposed to proceed under highly corrosive conditions at elevated temperature, a corrosion-resistant catalyst with high thermal stability will be required to promote HI decomposition for thermochemical hydrogen production.

Furthermore, HI decomposition is also the efficiency-determining step in the S–I process owing to the low conversion rate of HI decomposition into hydrogen at chemical equilibrium (22% at 400°C). This low conversion increases the quantity of recycled materials in the HI decomposition section, thereby increasing the thermal burden and decreasing the thermal efficiency of the process. The development of a membrane-based hydrogen separation process can open up the possibility of increasing the conversion of HI decomposition and is recommended within Phase 2.

The experimental rigs proposed for HyTN Phase 2 will be utilised to further develop the HI decomposition unit process as follows:

- Develop cost-effective catalysts that are both active and stable, and promote the reaction at lower temperatures
- Provide data to support a detailed assessment of the reaction kinetics for use in modelling studies
- Further develop hydrogen selective membrane reactor technology to overcome the thermodynamic limitations of the HI decomposition reaction and enhance conversions
- Develop reactor systems which integrate highly active and stable catalysts with highly selective hydrogen separation technologies
- Support development and testing of on-line processing monitoring requirements for this section of the cycle.

3.2.3. The Bunsen Reaction

The Bunsen reaction is a key component in both the S–I water splitting cycle for hydrogen production and the more novel hydrogen sulphide splitting cycle for hydrogen and sulphuric acid production from the sulphur-containing gases. As such, the reaction has been the subject of intensive research and development in the last 10–15 years.

Experimental rigs will be utilised in HyTN Phase 2 to further develop the Bunsen reaction unit process as follows:

- Investigate processing conditions to further optimise the conventional Bunsen reaction where large volumes of water and iodine reactants are required to drive the reaction
- Develop and optimise the electrochemical Bunsen reaction using a proton exchange membrane to physically separate the two acid phases to minimise demand for large volumes of reactant and avoid additional energy-intensive processing steps
- Investigate the use of alternative solvents in the Bunsen reaction for the selective extraction of HI from the reaction products to improve separation of products in the absence of excess volumes of reactants and improve cycle efficiency
- Support development and testing of on-line processing monitoring requirements for this section of the cycle.

3.3. HyTN Phase 2 Programme

NNL proposes to develop a virtual demonstrator programme in HyTN Phase 2, incorporating delivery of hands-on experiments in multiple partner organisations to develop and resolve some of the outstanding challenges associated with thermochemical hydrogen production. NNL will then incorporate this learning, in an iterative process, into the design and build of a centralised modular demonstrator at a suitable facility within the UK via a digital twin. By implementing this iterative process, NNL will allow learning from the unit processes to be incorporated into the whole system design and enable a more impactful demonstration system. The approach is outlined in Figure 5.

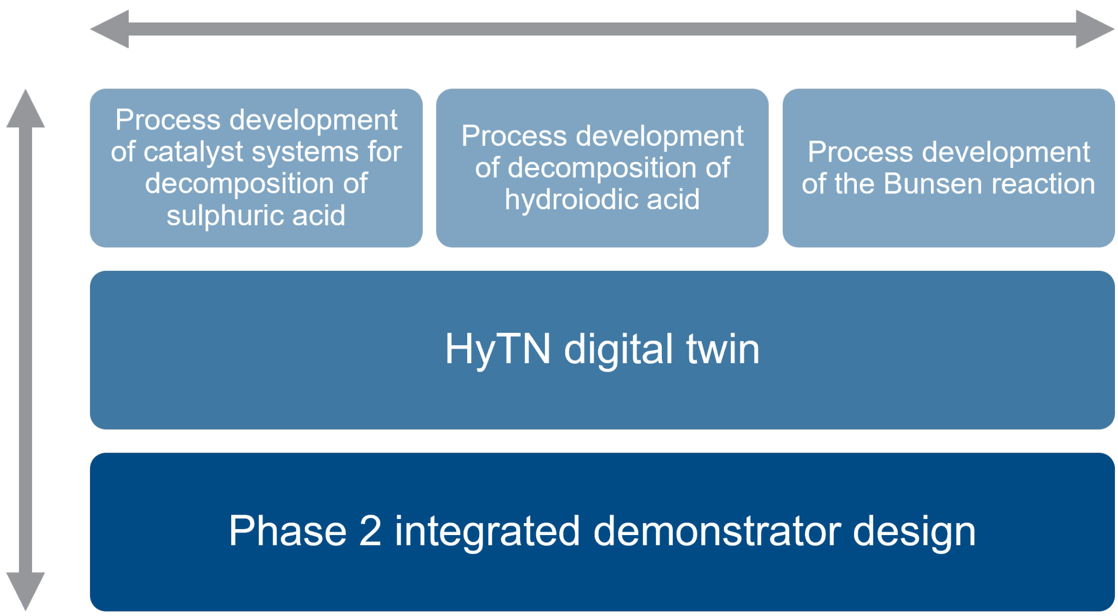

Figure 5: Outline of how process development in HyTN Phase 2 will be integrated through a digital twin to drive the Integrated Demonstrator Design.

To incorporate learnings and understand their impact on the development of the technology, HyTN will implement a digital twin of the process. Where new developments of catalysts and processes are created in the unit processes, these will initially be incorporated into the digital twin to assess their impact on the whole process. This will then be used to guide the construction of the full demonstrator system.

Within this programme, development is focused on the S–I process, noting that the same key steps, when resolved at a unit level, will enable further development of the HyS process. Whereas the physical combined demonstrator will be an S–I rig, NNL will maintain a HyS digital twin to aid further development of that process should it become favourable compared to the larger ultimate benefits forecast for S–I.

The proposed programme recognises the significant amount of work still required to further engage industry in the prospect of thermochemical hydrogen production. Unique IP could be generated within the programme through the identification of suitable catalysts, process control systems and materials for containers. Within the programme, NNL will lead development of an IP and commercialisation strategy designed to benefit from any native IP developed. This would make use of expertise both internal and external to NNL, and provide the basis for engaging future commercial developers and partners.

NNL would seek to identify commercial organisations to further develop thetechnology following on from a Phase 2 programme. NNL believes that a focused,short-term investment in thermochemical technology can excite both the commercial sector and research sectors in the potential of the technology, and unlock futurefunding to support future development. An interim indication of estimated costs for the next phase of technology development is approx. £6 million - this is provided in this report without any commitment and is for the purpose for phase 1 project requirements only. Key components are c.£3 million for 'unit process development' and c.£2million for 'integrated process development'. These figures will need evaluating prior to commencing the next phase of technology development.

One of the factors affecting the attractiveness of the technology for development will always be the potential price points on deployment. Within HyTN Phase 2, continued work will refine the forecasting of the price point, based on both improvements to the estimating methodology and improved knowledge of the structure of future processes, using the HyTN digital twin. The route to market development would continue within the programme, focusing on how selected high-value products and refinery scale operations can come to ultimate fruition.

Thermochemical hydrogen generation technology is not only dependent on the hydrogen production technology, but also the availability of advanced nuclear reactors as a heat source for the process. In fact, both technologies are interdependent on the availability of the other and HyTN will be aligned with the BEIS AMR research, development and demonstration (RD&D) programme, which is also being led by NNL.

4. Benefits and Challenges

HyTN is focused on the development of a low-TRL, potentially high-reward hydrogen production technology. The UK Hydrogen Strategy already recognises that the technology is unlikely to reach maturity before the mid-2030s, however, successful development could overcome a number of challenges associated with the future deployment of electrolytic hydrogen production.

When compared to proton exchange membrane (PEM) or alkaline electrolysis, thermochemical technologies demonstrate significant potential for improvements in efficiency. Table 2 summarises the forecast peak efficiencies that could be attained by a range of technologies, based on NNL's modelling of the processes. Normalised heat is used to provide a fair comparison of the total system efficiency for the different technologies, noting the use of both heat and electricity in some cases.

Table 2: Energy required to produce 1 kg of hydrogen (assuming a uniform reactor thermal efficiency of 40%) [19].

Technology	T (°C)	Electricity (MJ)	Heat (MJ)	(Efficiency) Normalised Heat (MJ)
Alkaline Electrolysis	40–90	190	0	**475**
PEM	40–90	187	0	**467**
Solid Oxide Steam Electrolysis	500	129	26	**348**
	850	96	71	**312**
S–I Cycle	720	0	174	**174**
HyS Cycle	720	58	148	**293**

Compared to alkaline/PEM electrolysis, steam (solid oxide) electrolysis could increase hydrogen production by up to 50% from the same reactor with a process which has a moderate TRL. Yet the S–I thermochemical cycle offers a potentially significant gain: an increase of 170% in hydrogen production compared to electrochemical processes. The HyS process offers up to 59% more hydrogen than electrolysis.

When this step change in efficiency is accounted for in economic analysis of the technology options, it results in an equivalent step change in forecast unit cost. Figure 6 shows the impact of this technology, assuming early deployment in 2035 and benefiting from learning from experience through to 2050. This builds on data presented in HyTN's economics report to provide a simplified comparison of key data [3]. Selected efficiencies of 80% (maximum) and 60% (mid) are provided, with data points taken for 1st of a kind (2035), 10th of a kind (2040) and 50th of a kind (2050) to reflect the learning process. As highlighted in the economic analysis of the HyTN feasibility study, further work is required to refine this model, including incorporation of updated expected cost data for the nuclear heat source, which can be supported through the parallel BEIS AMR RD&D programme in Phase 2.

Achieving the lower cost base for hydrogen production from S–I or HyS requires a significant market for the technology, which has been laid out by the HyTN project's analysis of potential future markets across the energy spectrum [4]. This report has already discussed the opportunity for low-cost hydrogen to provide a replacement feedstock for future synthetic hydrocarbon plants that underpins the future opportunity.

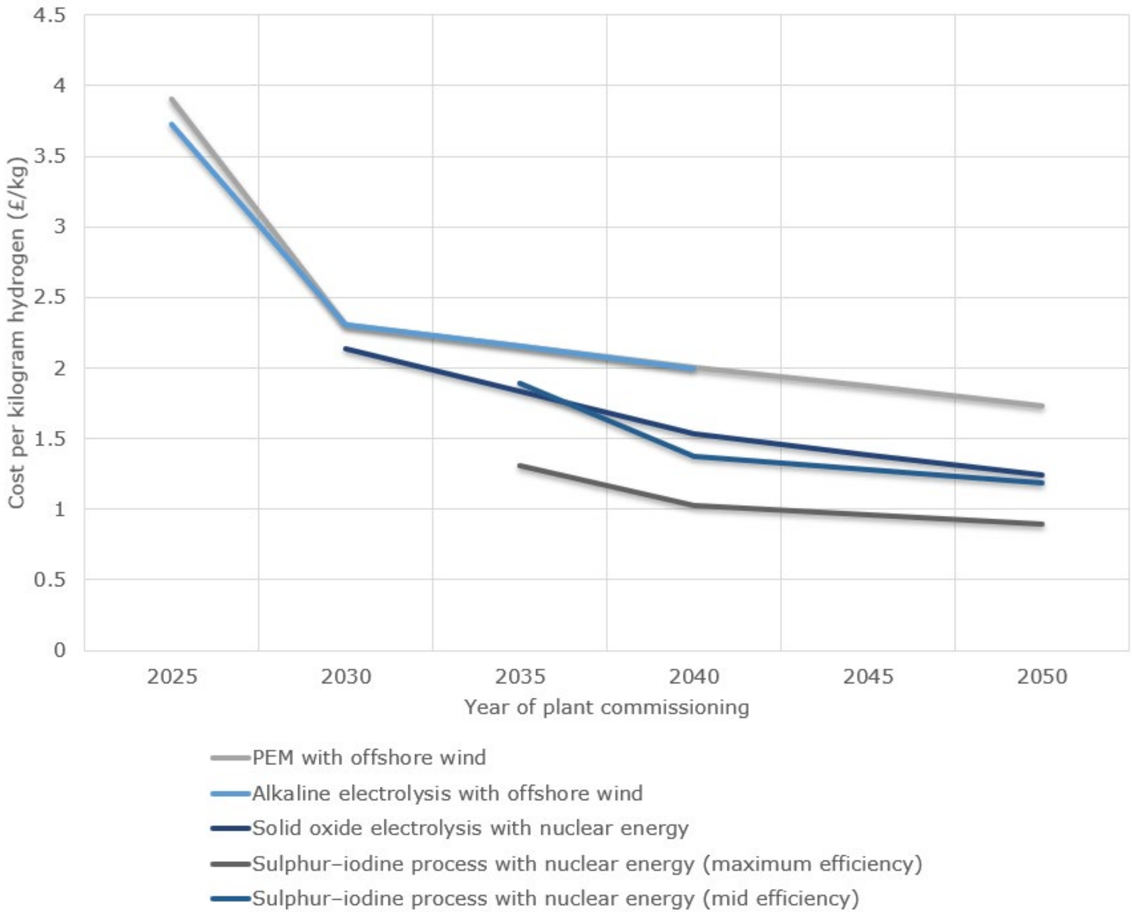

Figure 6: Comparison of forecast costs for the S–I process and a range of comparative electrolysis technologies. Nuclear-related cost data is taken from NNL's proprietary economic model whilst offshore wind-related processes are taken from [20]. All costs are quoted in 2016 values.

Thermochemical hydrogen production is a long lead time technology, not expected to be available at a commercial scale until the late 2030s. As such, the benefits and opportunities of the technology are not only in supporting the decarbonisation of hard to decarbonise sectors (such as aviation, shipping and hydrocarbon manufacture) but also as a replacement to transition technology. The typical lifetime for many energy plants is twenty to thirty years, therefore transition deployments, such as early deployment of CCUS-enabled hydrogen production will be coming up to needing replacement in the late 2040s [21]. Technologies that can further decarbonise low-carbon technologies will be crucial at that point to achieving net zero.

By coupling with nuclear AMRs, thermochemical technologies embed themselves as a long-term solution for successive generations. Typical global nuclear reactor lifetimes are around 60 years, meaning less need to replace infrastructure on a shorter timescale.

Thermochemical technologies should be significantly more scalable in terms of single unit capacity than electrolysis technology, therefore they should be better suited to this challenge. The scalability is driven by the typical route to scale up of chemical processes. Whilst electrolysis would be scaled up by deploying multiple small-scale electrolysers, thermochemical technologies could be scaled up for bulk production, similar to how current generation refineries are operated. In a similar vein, many of the components of the system are likely to have different suppliers compared to an electrolyser supply chain, increasing resilience of the technology option in scale-up.

Research into catalysts for thermochemical technologies is focused on identifying catalysts that reduce the capital cost, which are mostly focused on complex oxides [6]. Delivering this would offer a benefit compared to electrolyser technology, where availability of materials to construct cells is likely to be a future rate limiting factor for the deployment of the technology.

This report has previously highlighted a number of the challenges associated with the development of thermochemical hydrogen production, which are further detailed in supporting reports "Review of future market demand, applications and technology options for large scale hydrogen production from nuclear energy" and "Experimental Apparatus to Meet the Development Needs for Nuclear Enabled Thermochemical Hydrogen Production Technology" [4] [6]. Key technical barriers to commercialisation are listed in Table 1.

Wider to the technical challenges, achieving the full potential of thermochemical hydrogen production is complemented by the parallel development of multiple ancillary processes. This could include both the development of suitable advanced nuclear technology as a heat source, but also the commercialisation of direct air capture and the subsequent integration with synthetic hydrocarbon production. There is growing interest in deploying nuclear energy to support hydrogen and synthetic hydrocarbons, as evidenced by the publication of the UK Hydrogen Fuel Cell Association position paper on Nuclear Enabled Hydrogen [22]. To further understand this, NNL is proposing an ancillary technology review within HyTN Phase 2 which will also seek to develop further engagement with organisations experienced in the commercialisation and deployment of similar technology.

5. Route to Market

HyTN Feasibility project report "Hydrogen production from Thermochemical-Nuclear Coupling: Routes-to-Market Assessment" outlined a number of markets through which thermochemical hydrogen production could play a role in a future net zero economy [7]. This built on the analysis from "Review of future market demand, applications and technology options for large scale hydrogen production from nuclear energy" [4]. Whilst both lay out a clear ultimate demand for hydrogen and the benefits that thermochemically produced hydrogen could bring, navigating a viable route to large scale adoption presents other challenges. Figure 7 outlines some of the key factors affecting a route to market for the technology through to 2050.

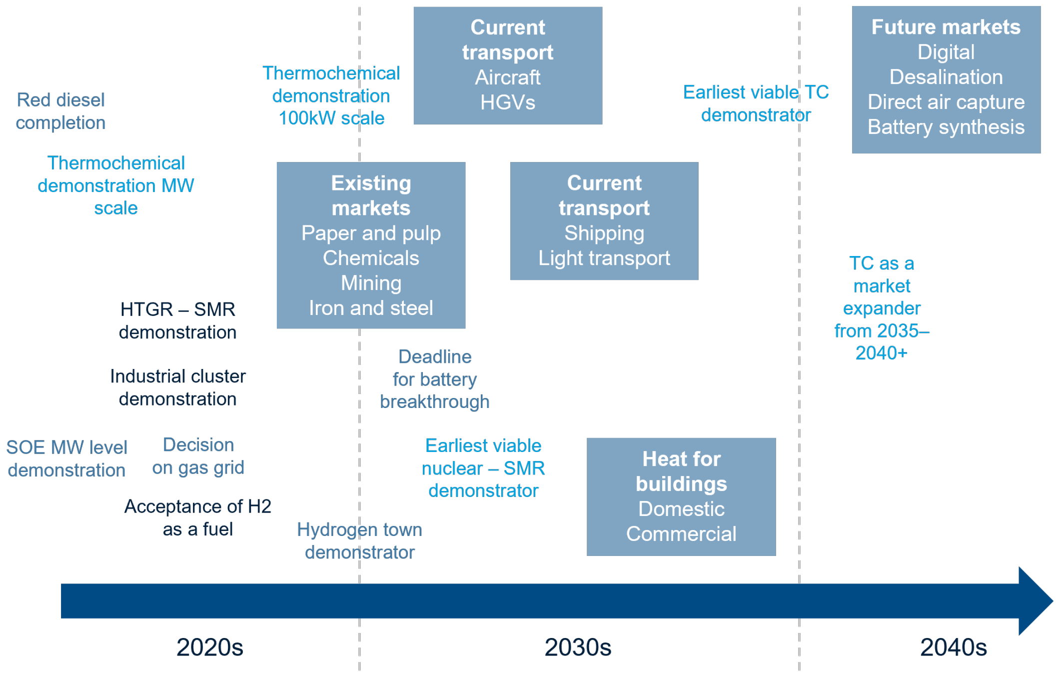

Figure 7: Predicted path to market maturity [23] [24] [8] [25] [26] [27].

As has already been outlined in this report, NNL believes that the UK is well placed to develop unique IP on thermochemical hydrogen production, leveraging a world-leading capability in catalyst development and process control. Furthermore, HyTN Phase 2 aims to engage commercial entities in the development of the technology, with a commercialisation strategy and licensing approach to be fully defined in Phase 2.

Given the long timescales required for commercialisation of thermochemical hydrogen production, this will mean that HyTN Phase 2 will act as a launchpad for future development. A focused development effort could bring the UK into line with international progress and stimulate academic and commercial interest, opening up routes to traditional R&D funding. Alongside this, ongoing development of AMR technology will be interdependent with viable applications and, as such, will benefit from further development of this technology. The milestones for this progression are as follows.

- **TRL 4–6**
  - Laboratory-scale testing of a range of early TRL thermochemical processes
  - R&D investment available to academia and industry through government funding, including conventional innovation routes
  - Partnership with the supply chain established to find solutions to problems encountered
  - Undesirable high-temperature effects of thermochemical process surmounted in both chemical and nuclear reactors
  - Demonstration of viable thermochemical technology at 100 kW scale
- **TRL 7–8**
  - Demonstration of viable thermochemical technology at 1 MW scale
  - Design of hydrogen plant using UK IP
  - Saleable thermochemical technology patented, and terms agreed for a consortium to exploit it with a reactor vendor partner, chemical partner, government endorsement, user group and supply chain
  - Investment secured for build of thermochemical hydrogen demonstrator
  - Inactive coupling of technology at test reactor level successfully trialled
  - Inactive demonstrator coupling of this technology trialled
- **TRL 9**
  - Commercial deployment alongside advanced nuclear technology

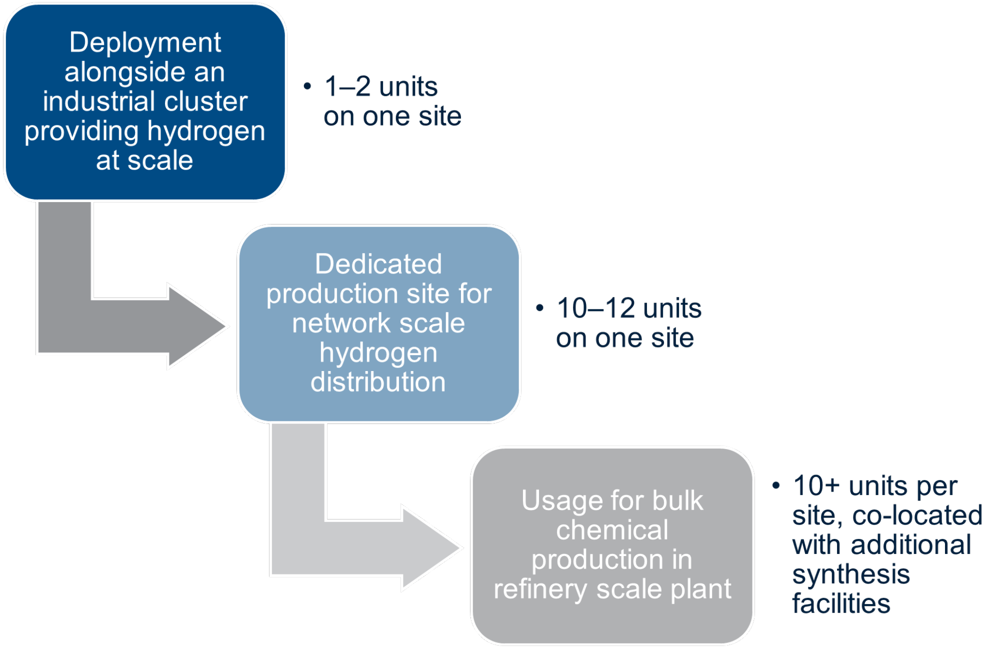

Figure 8: Outline of how hydrogen production would be scaled up at different types of sites alongside AMR nuclear technology.

When it comes to higher-TRL, commercial-scale rollout, NNL believes there is a route to rapid expansion of the market through the late 2030s and 2040s. This would need to be in lock step with the deployment and rollout of AMR technology, but as an enabler for higher value products from AMRs, there will be a symbiotic dependence to the rollout of both. Figure 8 describes how this rollout could progress through that timeframe, with a single unit AMR rollout to support industrial operations in the late 2030s, moving to dedicated hydrogen production for gas grid usage before moving to full integration with chemical production facilities in the 2040s. It is important to note that these latter stages would exhibit a step change in deployment approach for accompanying nuclear facilities, which is expected to dramatically reduce capital costs of the solution.

A typical scale of deployment for thermochemical and nuclear technology will be in the range of 200–300 MWth, which equates to generating approximately 1 TWh-H_2/yr (see 'Micro' SMR or AMR in [7]). Drawing on previous analysis by the HyTN project for potentially addressable markets, Table 3 highlights the cost of generating the hydrogen feedstock using thermochemical hydrogen and the total market value for those end-use sectors in 2019.[3] Analysis suggests there is a strong potential for commercial value generation from the technology, should it be viable at the price points identified by this study and the scale of demand is such that cost reduction through building of multiple units is viable.

Particular attention should be paid to the relative scale of a market and cost of generating equivalent hydrogen for that market with thermochemical technology. Whilst not a perfect comparison, it is clear that costs of generation with thermochemical technology could be well within existing market costs, reducing the economic impact of moving to net zero.

Not only is there a strong economic opportunity from just the market value of hydrogen that could be generated with thermochemical technology, the HyTN feasibility study has also generated the potential for significant carbon dioxide savings and job creation from deployment of the technology.

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[3] 2019 has been selected as a baseline year so as to avoid influence by major market transients such as COVID-19 and the 2022 global oil and gas supply crunch

Table 3: Total, estimated maximum and estimated central energy demand in key "hard to abate" sectors and cost of generating energy equivalent with thermochemical-nuclear technology. Extracted and updated from [4] [7] [1].

	DUKES Total Non-Electric 2019 Market Value £bn	Annual Demand (TWh/yr)[4]			Lower Marginal Cost of Generation[5] (£bn/yr)		
		DUKES Total Non-Electric Energy Consumption	HyTN Estimated Maximum	HyTN Estimated Central	DUKES Total Non-Electric Energy Consumption	HyTN Estimated Maximum	HyTN Estimated Central
Industry	4.2	125	105	25	2.8	2.4	0.6
Transport	8.3	195	140	75	4.4	3.2	1.7
Other (incl. Home Heating)	21.7	430	210	100	9.7	4.7	2.3
Total	**34.2**	**750**	**455**	**200**	**16.9**	**10.3**	**4.6**

[4] Note that DUKES values selected here are intended to represent the whole market. Total market scale is included to give a sense of the proportion of a market HyTN is expected to be able to address. HyTN figures are based on in-depth analysis by the HyTN project, presented in [7].
[5] All market value calculations based on lowest forecast cost of hydrogen generation as per [3].

6. Conclusions and Recommendations

Thermochemical production of hydrogen enabled by nuclear power could prove to be a step-change technology that accelerates decarbonisation of the UK and global energy system beyond 2040. The HyTN feasibility study has shown that the technology has the potential to achieve a marked increase in efficiency (Table 2) and unit hydrogen costs could be as low as £0.89/kg.[6] Such price points are validated by publicly available reports which outline routes to deployment that achieve prices as low as $0.90/kg[7] [2]. By utilising the heat from a nuclear reactor, and a chemical catalyst driven process for generating hydrogen, thermochemical technology could provide a significantly more scalable solution than other zero carbon hydrogen production technologies.

Thermochemical production from hydrogen has been demonstrated at TRL 4 by multiple organisations internationally, including NNL's recommended processes, the S–I and HyS processes. NNL's research has outlined a route for development that requires focusing on the smaller sub-units of the process in order to resolve outstanding technical challenges and enable the further commercialisation of the technology. A route for the delivery of HyTN Phase 2 that implements a range of engineering demonstrators to resolve these challenges and integrates the results of the development into a digital twin model of the HyTN process that can be used to shape a full integrated rig has been set out.

Delivering HyTN Phase 2 using this approach could enable the UK to capitalise on world-leading experience in the development of process catalysts and process control. Successful demonstration is likely to result in unique UK IP for the technology. Beyond generating unique IP, the technology also offers the potential to expand the role of nuclear energy in a future energy system, supporting the development of the UK nuclear sector.

HyTN has outlined a range of markets that thermochemical hydrogen production can support, covering hydrogen as an energy vector, for export markets and as a feedstock for synthetic hydrocarbons. A viable route to completely decarbonising the feedstocks for similar facilities would close the gap to reducing Scope 3 emissions from future products and energy vectors where a carbon element is unavoidable, allowing the use of direct air capture to create carbon-neutral fuels for a net zero energy system.

NNL is recommending a rapid programme of development for HyTN Phase 2 that would engage world-leading capabilities in the development of a potential step-change technology. An investment to deliver this programme is expected to raise interest among wider stakeholders and offer opportunities for private and academic research investments to drive forward commercialisation of the technology in lock step with the commercialisation of advanced nuclear reactors.

[6] Price base date: 2016
[7] Price base date for external source: 2019

7. Abbreviations

AMR	Advanced Modular Reactor
Cu–Cl	copper–chlorine
ESME	Energy System Modelling Environment
GBP	Great British Pound
GDP	Gross Domestic Product
HI	Hydrogen Iodide
HTGR	High Temperature Gas Reactor
HyS	Hybrid Sulphur (also known as Westinghouse process)
HyTN	Hydrogen from Thermochemical and Nuclear
IP	Intellectual Property
MWh	Megawatt Hours
NNL	National Nuclear Laboratory
ROM	Rough Order of Magnitude
S–I	Sulphur-iodine
t	Tonnes
TRL	Technology Readiness Level
TWh	Terawatt Hours
UKJ-HTR	UK-Japan High Temperature Reactor
USD	US Dollars

8. Definitions: Technical Readiness Levels

Research	TRL 1	Basic principles observed
	TRL 2	Technology concept formulated
	TRL 3	Experimental proof of concept
Development	TRL 4	Technology validated in laboratory
	TRL 5	Technology validated in relevant environment
	TRL 6	Technology demonstrated in relevant environment
Deployment	TRL 7	System prototype demonstration in operational environment
	TRL 8	System complete and qualified
	TRL 9	Actual system proven in operational environment

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