LCHS2106 – CATAGEN Phase 1 Feasibility Study Public Version

CATAGEN LIMITED

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Glossary

CRL	Commercial readiness level
H_2	Hydrogen
IEA	International Environmental Agency
MRL	Manufacturing readiness level
R&D	Research and development

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Executive Summary

The following document details the work undertaken by CATAGEN during the LCHS2106 Phase 1 feasibility study in which the project goal was to "Complete the initial development and determine the feasibility of a low-cost thermocyclic hydrogen production reactor".

After the scene for the project is set in the introduction, the process of assessing the technologies that were considered is outlined and why the chosen hydrogen production method was selected.

Our solution for hydrogen production is then presented, followed by the testing results from the prototype reactors developed as part of work packages 4, 5 and 6. In this section, the capability of the reactor is assessed, whilst proving that hydrogen can be made via the selected method.

The Phase 2 demonstration project is then described and initial design plans are outlined for a demonstrator. These sections outline the aims for a Phase 2 project that would carry the technology to a level closer to being commercially ready, along with how a potential Phase 2 prototype reactor would be constructed.

This is followed by the key benefits that come with the technology and the technology affords three key benefits over what is the primary competing technology – electrolysis. Firstly, waste heat can be integrated into the system to reduce the overall energy cost. Secondly, the technology can be more easily scaled than electrolysis. One final benefit is that reactors such as that proposed for demonstration inherently have a high thermal inertia during operation. The thermal inertia provides a damping effect on any fluctuation on input energy availability and as such the process stream is impacted less than it would be in a low inertia scenario.

Case studies detailing different maturity levels of the technology were used to calculate levelized costs to provide a direct comparison to the primary competing technology, electrolysis. It was shown that with an optimised model, approximately 5 years of development beyond Phase 2 plus the integration of a waste heat source, that the cost of hydrogen could be reduced by 11.2%, compared to an electrolyser. Further to this levelized cost comparison, the electrical energy cost per kg of hydrogen was calculated to be 37.4% lower using CATAGEN's technology.

Finally, the potential for different business models that the commercial reactors would follow is discussed along with steps required to be undertaken before the rollout of the technology could occur. The actions that need to be completed to improve the commercial readiness levels (CRL) are also outlined as the technology navigates its way to market.

The Low-Carbon Hydrogen Supply 2 Competition funding has facilitated the technological advancement of hydrogen production technology. Through the funding, an alternative approach to electrolysis has been evaluated for hydrogen production, with this evaluation showing promising results. For queries around the work completed please contact:

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1. Introduction

The hydrogen economy is now at a crucial point. It is considered a vital avenue to fully exploit the benefits of renewable and sustainable energy. As the pace of decarbonisation is accelerating, the current market is demanding access to alternative energy sources that produce little or no carbon emissions. Hydrogen, particularly hydrogen produced using renewable energy and water (or ‘green’), has become increasingly sought after as a way to provide energy that does not produce emissions. Hydrogen is considered a “clean” fuel as when used in a fuel cell to generate electricity, water is the only product.

As well as this, the UK government has stated the aim of having 10 GW of low carbon hydrogen generation capacity by 2030, an ambitious target that requires a multitude of technologies and generation techniques to achieve, this is evidenced by the current shortage of electrolyser production capacity both within the UK and worldwide.

Hydrogen production as a form of alternative energy storage technology is mainly limited to small scale production using electrolysers. Thermocyclic hydrogen production has the potential to produce hydrogen at an industrial scale from renewable energy at a more competitive price per kg compared to electrolysers. Furthermore, it has the potential to have less impact on the environment over its operational lifespan than alternative hydrogen production methods such as electrolysis, biomass gasification, steam reforming, and solar thermal.

This project sought to determine the feasibility of developing new capabilities and technologies to combine with re-circulating gas reactor technology to yield a production machine and process for high-efficiency green hydrogen production.

2. Considered Technologies

2.1 Electrolysis

One of the main drawbacks of using electrolysis to produce hydrogen at a larger scale is that the cost of electrodes does not decrease as size increases, this is independent of the electrolyte. Repeating electrode units, or cells, is the only way to increase hydrogen production, this is a linear relationship, so doubling the size will in theory double the costs. This is not very favourable in terms of cost relative to the amount of hydrogen produced. Conversely, chemical reactors do scale favourably with size as the amount of hydrogen produced is directly linked to the mass of reactants and therefore the volume of the reactor. Chemical reactors are already readily available in very large sizes. As a result, thermochemical hydrogen-producing reactions will be more economically feasible, at larger scales, relative to the amount of hydrogen produced when compared to electrolytic cells.

2.2 Thermochemical cycles

Multiple thermochemical cycles were evaluated, and the one chosen was based on multiple factors including: hydrogen production, energy requirements, feedstock materials, and overall process efficiency. The thermochemical cycles that were reviewed initially include:

- Carbon monoxide/dioxide cycle
- Cerium oxide cycle
- Hybrid sulphur cycle
- Hydrogen chloride cycle
- Indium oxide cycle
- Iron oxide cycle
- Molybdenum oxide cycle
- Silica oxide cycle
- Sulphur ammonia cycle
- Sulphur bromine cycle
- Sulphur iodine cycle
- Tin oxide cycle
- Tungsten oxide cycle
- Zinc oxide cycle

2.3 Literature Review

The first main deliverable completed for the Phase 1 project was to complete an analysis of the available literature on the chosen process, in total over 50 papers were reviewed. This was used to inform the prototype build for each reaction to be tested during Phase 1 and the experiment scope that was to be completed at CATAGEN. It also provided CATAGEN with an understanding as to what scale the technology had been tested to in the past and where CATAGEN could add the most value.

Most of the key challenges that require solving for the feasibility of this technology were uncovered during this process and they include:

- Pre-treatment of reactants and products to improve overall process efficiency.
- Supplying the high energy demand required for the process in an environmentally and economically friendly way.
- Evaluating several different reactor designs.
- Achieving a low energy cost relative to the amount of H_2 produced.

3. Our solution

For our proposed solution to be a sustainable source of green hydrogen the energy supplied must come from a renewable source. The aim of the Phase one study was to design a multi-reactor system, and an accompanying experimental plan for each reactor to replicate results found during the initial literature review. Additionally, the experiments would evaluate how CATAGEN's reactor design compared to previous examples and provide insight on the long-term suitability of the system setup and materials of construction.

During the feasibility study each of the reactors were investigated separately to better understand the individual reactions that the overall process comprised of. The learning from these experiments will provide the foundations for further research activities in Phase 2. Each of the reactors successfully converted their respective reactants into the desired products while keeping the number of undesired by-products below detectable levels. As a result, each of the experimental plans for the multiple reactor systems were deemed as successful.

Some of the reactors' designs were based on a combination of several already-proven technologies. For these systems the goal was to see how integrating different design attributes could lead to an overall improvement in reactor efficiency. The results of the experiments showed that by combining different aspects from already proven technologies the CATAGEN design was able to improve upon the current designs found in literature. This will provide the starting point for further modifications and experiments in Phase 2.

4. Experimental results and conclusions

The experimental campaign completed at CATAGEN during Phase 1 aimed to show that all reactions within process can operate in isolation, confirm literature findings, whilst also learning about the intricacies of the process beyond the information attained from the literature review.

For this, each of the reactors had an experimental plan developed to better understand the difficulties in recreating literature results, and to gain an understanding of chemical properties, and material compatibilities.

Overall, the experimental plan conducted at CATAGEN successfully demonstrated each of the reactions within the process with hydrogen being produced, demonstrated they progressed as expected, and added to the existing knowledge base. The hydrogen production rate reached peaks of at least 14g/hr. This proved the core feasibility of each of the reactions and demonstrated CATAGEN's ability to not only recreate experiments found in literature but to improve upon them and analysis the results. One of the main findings was that CATAGEN's reactor design improved the conversion efficiency of the initial chemical process by reducing mass transfer limitations that occurred in previous reactor designs that were found in literature.

5. Description of the demonstration project

Globally, the International Environmental Agency (IEA) estimates that the current demand for 70 Mt of hydrogen will grow to over 200 Mt by 2030 with the majority of this growth coming from carbon neutral and carbon zero sources such as electrolysis and blue hydrogen production. This further emphasises the need for innovative solutions that can increase the generation capacity of green hydrogen that will further develop hydrogen economies at scale, a role that this technology is ideally placed to play.
Within the demonstration project, the aim is to build a demonstrator system which would have much more capability to produce hydrogen than the Phase 1 prototype. Efficiency gains would be implemented to improve the cost effectiveness, such as the use of industrial waste heat/simulated waste heat. As the system is a thermal and chemical process, offsetting the thermal energy required has a significant impact on the hydrogen production cost. Renewable energy will also be used to power the demonstrator as to generate green hydrogen.

The development of the demonstration project for the CATAGEN green hydrogen generator has three main aims:

1. The technology works at pilot scale in an optimised setup that allows the technology to be commercially viable
2. The process can be integrated into existing infrastructure/industry
3. The solution can generate hydrogen at a cost that is competitive or cheaper than current alternative solutions

To do this, engagement with potential consortia partners has already begun to identify ideal collaborators and the optimal way to demonstrate the feasibility of the technology. This will also enable investigation of how the technology can be optimised.

6. Design of demonstration

The purpose of this section was to ascertain an early design schematic for a demonstration scale reactor, required for Phase 2. Understanding this as early as possible is critical due the Phase 2 project framework. This work allows the Phase 2 work packages surrounding reactor design to gain a head start in their works and optimises the decision processes surrounding the demonstrator.

Early in the project, a thorough literature review was conducted to better understand the intricacies of the technology. This initially informed the design of the basic prototype reactors, but some of the information gathered was not implementable into the Phase 1 project due to its constraints. As well as these lessons, learnings from the experimental campaign conducted at CATAGEN were also implemented into the Phase 2 design. Various aspects of the technology were modelled to understand where the largest efficiency gains could be made and these were used as key aspects that had to be included in the Phase 2 design.

The outcome of this work was an initial, complex schematic for a Phase 2 hydrogen production reactor. It incorporates processes from the Phase 1 experimental campaign and proposed processes that are deemed necessary to make this technology feasible. It also provides an early estimation of footprint, utility requirement and a bill of materials that would be required, which subsequently allows for estimated total project costs to be calculated. The proposed demonstration project will cost in the region of £5 million. This has been estimated based on the proposed design and prior experience in reactor builds (both in and outside of LCHS2106). Knowing this ahead of time streamlines the Phase 2 demonstrator design and allows for the demonstrator build to occur more quickly. The approximate breakdown of costs are given below, with the majority of these associated with the build, operation and analysis of the demonstrator.

Category	% Cost
Project Management	5%
Engineering Design	10%
Build, Operation, and Analysis of Demonstrator	25%
Materials	32%
Subcontract Labour	28%

7. Benefits & Barriers

Work was completed in this section to assess the benefits and challenges associated with this technology and quantifying them to understand how they compare to existing technologies, such as electrolysis. This was done to assess how feasible it is for this technology to be cost-effective, and ultimately whether it is worth the potential investment.

First, the benefits of the technology were identified and detailed. These largely tied in with the fact that this technology was a thermochemical process. This was done through the research completed in the literature review and also via modelling work completed during the project. Alongside this the main challenges of the technology, to which there are many, were identified over the course of the Phase 1 project. Again, these were collected throughout the literature review, but some were also encountered through the experimental campaign.

Following these benefits and challenges being identified, case studies were simulated using the model developed within the project to ascertain levelised costs for hydrogen production under different technology maturity levels that had some of the key challenges solved. These case studies including solving issues such as feedstock purity and reducing the electrical energy requirement through the integration of industrial waste heat. Optimising the reactor through these problems requires further research and development (R&D) through Phase 2 and beyond. Assumptions also had to be made around electrolyser performance levels, with best estimates from BEIS Green Hydrogen Production literature used[1].

The assumptions made on both sides of the counterfactual assessment resulted in uncertainties in the cost comparison between technologies. Increased certainty regarding the levelised cost of H2 production using this technology will only be realised at demonstration phase and beyond, with this uncertainty unavoidable at present. Further consideration should also be given to the production costs across the load range of the equipment, rather than taking a single point analysis of energy cost.

This section demonstrated that, with further development, it was feasible to produce hydrogen in a cost-effective manner using this technology, as was demonstrated by the levelized cost of hydrogen calculated. It was shown that there is the potential to produce hydrogen cheaper than what could be achieved via a standard electrolyser of a similar magnitude.

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[1] Department for Business, Energy and Industrial Strategy, Hydrogen Production Costs 2021, 2021, .

8. Costed development plan

The aim of this work was to outline an initial project plan in developing a demonstration reactor and ascertaining an early estimate as to how much funding and resourcing would be required for a Phase 2 project. These steps are required as there is a small window between the end of Phase 1 and the potential beginning of a Phase 2 project, so understanding the requirement for a Phase 2 project as early as possible ensures a smooth transition.

Project work packages have been decided upon through a combination of lessons learnt from Phase 1, key challenges discovered that require specific attention and previous experience in reactor builds. The timeframe for the project necessitates concurrent completion of activities. The project critical path is driven by the design, build and testing of the reactor. Project costs have been estimated based on the proposed design and prior experience in reactor builds (both in and outside of LCHS2106). Given current market volatilities these may change between submission of this report and any Phase 2 application.

The result of this work is a project plan that comprises of 13 work packages across a 102 week period. The reactor build work package commences early in the project, with civil engineering works to prepare the location for reactor and storage tank installation. Upon receipt of the reactor materials and components, reactor build and assembly will be completed, primarily through skilled sub-contract labour. Once the reactor has been built, commissioning activities to validate the safe operation of the demonstrator will be complete.

The end of the project involves final reporting on the project outcomes, with a final work package included for sign-off and review for all project deliverables and documentation lasting 1 month. As a final comment on the project timeline, other activities have been moved forward where possible to help de-risk the project delivery.

Alongside the demonstration project (funding permitted), additional activities to enhance the manufacturing readiness level (MRL) and CRL for the technology are planned. The purpose of these activities is to enhance the business proposition, and to allow a commercially viable solution to be developed sooner.

9. Rollout potential

In order to understand the rollout potential once the demonstration project has completed, an early assessment of business use cases along with a pathway to rollout for the technology was required. Then, it was crucial to understand the risks that could impede this potential rollout so that these challenges could be addressed during the development of the demonstrator. Potential usages for the technology beyond demonstration were mapped out to understand what options were feasible in rolling out the technology.

The CATAGEN thermocyclic reactor can be both standalone and fully integrated into other industrial activities. The rollout of units has the potential to create several different business models and costs of production. The thermocyclic nature of the CATAGEN system makes it a prime candidate for co-location with GW scale wind and solar assets worldwide. A key challenge in the implementation of these large-scale renewable systems is the full utilisation of available energy. Without mitigatory steps excess energy will be lost through curtailment and constraint. The CATAGEN technology can be utilised as a complementary technology to utilise the excess energy. Additionally, the ability to generate large quantities of green hydrogen effectively could aid in the speed of development of renewable assets in areas where there is high renewable energy potential but a lack of sufficient electrical infrastructure by capturing the energy in the form of green hydrogen without the need for grid infrastructure development. This creates a new potential pathway to renewable energy development that does not rely on slower infrastructure development where wind and solar farms can be used to generate green hydrogen first and as electrical infrastructure comes online at the site can transition into both electricity export and green hydrogen generation.

However, rollout of the technology could be inhibited by a number of risks if these are not adequately addressed or mitigated. Several risks have been identified that could hinder the rollout potential that will require further R&D in the demonstration project. These include feedstock optimisation processes, optimising reaction efficiencies and identifying/procuring of suitable materials. As well as this, there are risks surrounding the competitiveness of the hydrogen produced. Considered risks include a significant improvement occurring in electrolyser efficiencies or the unsuccessful integration of industrial waste heat.

These several use cases demonstrate the flexibility of the CATAGEN system to integrate with both existing industrial processes and emerging developments in the renewable energy sector and so highlight the potential of the technology to rapidly deploy across many of the largest industries globally.

10. Route to market assessment

The CATAGEN thermocyclic hydrogen generator will require several significant steps to progress through CRL development; pilot scale demonstration, business model(s) development and application optimisation, MRL development and business model validation.

The progression to reach these steps has already begun during Phase 1 with the development of the system, as well as basic market awareness and value propositions being developed in parallel with the technology. Further progression of CRL will be dependent on the deployment of the demonstrator system with input from a consortium partner to fully align the technology with the market as well as optimisation of the technology to meet end-user demands.

This will prove the technical viability with what is in effect a simulated 'beachhead' customer and allow for refinement of financial models and technology optimisation. As well as this, the development of the system MRL will be necessary to ensure that the market demand for this technology is met and the scale of production is appropriate for the market.

As this system offers green hydrogen as a product, an energy vector, the total addressable market for this technology is incredibly large; with market potential across all areas of the energy sector including as an alternative to fossil fuels. Currently, there is a shortage of technologies that can use hydrogen as a fuel source. This creates a barrier to market but as industry pushes towards net zero targets, more hydrogen-based technologies will become available.

Hydrogen has been present in natural gas pipelines for decades. In this situation, it was considered an 'impurity' of the gasification of coal as it reduced the energy content of the gas mixture (town gas) and caused premature wear of some components at high concentrations.

This presents an emerging route to market in modern energy systems of displacing the use of natural gas in the gas network by replacing some of the gas content with green hydrogen. It is estimated that approximately 20% of the total gas content by volume could be replaced with green hydrogen without detrimental effects on the transmission network or existing boiler systems. But due to the lower energy content of hydrogen gas per unit volume compared to natural gas due to its lower density, this 20% vol addition represents only 7% of the energy content of the gas. It is estimated that approximately 4 times the volume of hydrogen gas would be necessary to produce the same energy content as natural gas. This route to market is currently being explored mainly in the UK and other parts of Europe where there is a large dependency on gas networks for industry and domestic heating and as such represents a potential route to market and export opportunity for the CATAGEN technology as a supplier of this green hydrogen.

Additionally, there are several categories of job creation associated with the deployment and successful commercialisation of this technology:

- Direct Technology Development and Manufacture
- Technology Support and Deployment
- Synergistic Sector Growth

These three categories represent a range of roles including:

- Mechanical, Chemical and Electrical Engineering
- Manufacturing and Deployment Logistics Crew
- Welding, Plumbing and Maintenance Crew

- Sales, Marketing and Administrative Support roles
- Wider sector growth roles e.g., increased demand for renewable energy jobs and transmission network roles

In addition, the potential for green hydrogen production assists in the decarbonisation of many industries. This can help to future-proof jobs in areas such as public transport, construction and power generation by offering a zero-carbon alternative to entire industries currently dependent on the use of fossil fuels. The impact of this technology could be globally significant in aiding in the creation of a hydrogen-based world energy system and can aid in ensuring the sustainability of jobs across a multitude of businesses.

Through the development of green hydrogen production, there is also the opportunity to reduce the carbon emissions of industries such as the aviation industry (currently responsible for 8% of UK transport emissions annually) as well as the public and private mobility sector by adopting fuel cell electric vehicles such as buses and passenger vehicles. This zero-carbon solution can help ensure these vital industries do not further contribute to human-induced global warming and present an alternative way to harvest renewable energy from intermittent sources such as wind and solar by 'locking up' the excess wind in chemical form, further increasing the viability of intermittent renewable assets as part of the wider energy network.

11. Dissemination

Ongoing dissemination activities have occurred in parallel to technology development throughout the project lifespan. These activities have included individual and group site visits for stakeholders including: government (national, regional, and local level), supply chain partners, potential customers and consortium members. Additionally, CATAGEN staff have attended a range of events to raise public and industry awareness of the project and obtain independent feedback concerning the suitability of the technology for different market segments and industries.

12. Conclusions

The goal of this Phase 1 study was to "Determine the feasibility of developing new capabilities and technologies to combine with known re-circulating gas reactor test technology to yield a production machine and process for high efficiency green hydrogen production.". Whilst different hydrogen production methods were assessed, one technology was selected for further development based on a number of criteria.

A Phase 1 prototype was built, commissioned and tested with the goal of ascertaining a better understanding of the technology. The testing proved that the reactor could be used to yield hydrogen. The experiments completed at CATAGEN have provided a greater understanding for the intricacies of the technology and have informed the design of a Phase 2 reactor.

Alongside the practical elements of Phase 1, modelling activities were completed to understand what further R&D activities would be required to reduce the cost of hydrogen produced from a demonstrator. CATAGEN were able to highlight the key problems that require solving, with some potential solutions identified that require further research.

The potential efficiency gains identified in Phase 1, allow levelized costs to be calculated which demonstrate that CATAGEN technology has the potential to produce low cost and low carbon emitting hydrogen.

Overall, the Phase 1 LCHS 2106 project has successfully demonstrated that through further R&D activities, a low cost thermocyclic hydrogen production reactor is feasible. This has been demonstrated through:

1. The testing of the Phase 1 prototype reactor that prove hydrogen can be made via this process.
2. The modelling deliverables that establish, by targeting specific issues, significant efficiency gains can be made that reduce the overall cost of hydrogen production.
3. Evaluating potential partnerships that can add value to the system that will decrease the energy cost of hydrogen.