CATAGEN

LCHS2108 –Complete the initial development and determine the feasibility of a low-cost liquid hydrogen fuel production reactor– Public Version

CATAGEN LIMITED

HEAD OFFICE 5 ELMBANK CHANNEL COMMERCIAL PARK, QUEEN'S ROAD, TITANIC QUARTER, BELFAST, BT3 9DT, NORTHERN IRELAND +44 (0) 28 90 455 100 info@catagen.co.uk catagen.co.uk

Glossary

CAD	Computer Aided Design
Capex	Capital expenditure
CH_4	Methane
CO	Carbon Monoxide
CO_2	Carbon Dioxide
CRL	Commercial readiness level
DAC	Direct Air Capture
FT	Fischer-Tropsch
FTE	Full time Employees
H_2	Hydrogen
kWh	Kilowatt Hour
MDO	Marine Diesel Oil
MRL	Manufacturing readiness level
N_2	Nitrogen
Opex	Operating expense
PTE	Part time Employees
RWGS	Reverse Water Gas Shift
WGS	Water Gas Shift
WP	Work Package

Executive Summary

This document outlines the findings from phase 1 of BEIS Low-Carbon Hydrogen Supply 2 Competition project LCHS2108 "Complete the initial development and determine the feasibility of a low-cost liquid hydrogen fuel production reactor". This document also includes a literature review, experiment set up, results and outlines a plan for a further demonstration project (Phase 2).

The project's aim was to produce liquid E-fuel (a carbon-neutral direct replacement fuel) from green hydrogen and carbon dioxide sources. E-fuel is any type of hydrocarbon (Methane, Petrol, Diesel etc.) that is produced from green sources. The project consisted of testing two reactions to understand their setup and operation while understanding if both reactions could be used together to produce E-fuel.

The first reaction was the reverse water gas shift reaction (RWGS) which used captured carbon dioxide (CO_2) and hydrogen (H_2) to create carbon monoxide (CO). Several conditions were tested to understand the best operating conditions to get the best conversion efficiencies.

The second reaction tested was the Fischer Tropsch (FT) reaction. This reaction used the synthetic gas, created by mixing the CO produced by the RWGS with other gases, to create a synthetic E-fuel. The testing was successful in producing liquid E-fuel under several different test conditions. Samples were sent for chemical analysis to further analyse the makeup of the produced liquid. The testing was also successful in producing gaseous hydrocarbons in the form of methane and propane.

This report outlines the results from above in greater detail but also looks at the feasibility of producing a large-scale reactor to produce liquid E-fuel to be sold. This study looks at what a large-scale reactor would look like by combining the abovementioned reactions.

The study looked at the market as a whole, considering the benefits of the products to the market. Barriers to entry of the market with roll-out potential and route to market were also assessed. This section is important to understand where the product sits in the market and how it can be implemented in a safe, timely and cost-effective manner.

Overall, the project's testing phase was successful with both reactions producing a significant amount of desired products. A good understanding of the testing process allowed for changes to be made for a potential stage 2 machine design. This knowledge additionally allowed for scale up calculations to be completed, proving the project's strong business case. Calculations showed the potential to create a cost effective E-fuel for a series of different applications. This production of net-zero fuel will supply the markets rising requirements for a fuelling method that does not contribute to carbon emissions.

The Low-Carbon Hydrogen Supply 2 Competition funding has facilitated the technological advancement of the technology described in this report. Through the funding, a high-density hydrogen based fuel production approach has been evaluated, which showed promising results. For queries around work complete please contact:

Dr Andrew Woods, CATAGEN CEO, andrew@catagen.com or
Dr Matthew Elliott, CATAGEN Principal Technologist, matthewe@catagen.com

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Author	Émer Duffy, Liam Mc Grane, Matthew Elliott
Approver	Matthew Elliott

Contents

1. Introduction

Pollutant emission content in the atmosphere is one of the most prominent challenges faced today with the rate of CO_2 production vastly outstripping the current capabilities for CO_2 capture and sequestration. As a result of this, methods of decarbonisation are vital to maintain the health of this planet. Green hydrogen solutions could hold the key to this.

Despite the importance of green hydrogen being widely recognised, it is limited by the lack of developments in H_2 storage methods which will be required before global implementation. Currently it is expected that these storage developments will take over 7 years before it is optimised fully for this level of readiness. E-fuel production could provide the answer to this problem.

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.

As of 2020, the transport sector in the UK produced almost a quarter of net greenhouse gas emissions. The current push towards the electrification of this industry is hindered by the limits to battery production and the time taken to change infrastructure of both vehicle manufacture and fuelling. There are additional problems particularly in the maritime and air transport industries for which decarbonisation may be difficult to solve solely by electrification.

The hydrogen economy is now at a crucial point. It is considered a vital energy storage strategy to fully exploit the benefits of renewable and sustainable energy. As the pace of decarbonisation is accelerating, the current market is demanding access to the green energy hydrogen has the potential to provide. However, the current infrastructure is unable to support this necessary growth.

E-Fuels are a synthetic hydrocarbon, produced from sources of green hydrogen and carbon. These can act as an easily transportable green hydrogen carrier, due to their excellent energy density relative to gaseous H_2. They can be used as a direct “drop-in” substitute with today’s technology, having the advantage of using the same infrastructure as their fossil fuel equivalents, giving them the potential to be implemented almost instantly. This transition to E-fuels could provide a net-zero alternative to fossil fuels used currently, having the ability to dramatically change the profile of overall emissions.

Hydrogen produced from water and renewable energy (currently electrolysis is the dominant technology for this process) is combined with CO_2 to create synthetic hydrocarbons. This synthesis using hydrogen partially combats the struggle of hydrogen storage whilst also helping to reduce the current greenhouse gas emissions from the transport sector, which are almost entirely made up of carbon dioxide. This proposed E-fuel production method will include carbon capture to subsidise this by taking CO_2 from the atmosphere, or another green source, keeping the system in a closed loop.

1.1 Objectives of this technology

The goal of this Phase 1 project was to determine the feasibility of developing new capabilities and technologies to combine with current CATAGEN technologies to yield a reactor capable of producing a high density, easily transportable green E-fuel (such as a long chain hydrocarbon).

To achieve this goal, a number of feasibility questions need to be considered throughout the process:

1. Can RWGS and FT reactions be harnessed to efficiently produce a liquid green hydrogen-based fuel?
2. Is sourcing of green CO_2 for the production of the green syngas viable?
3. What is the expected operational cost of producing green syngas?
4. What is the expected operational cost of producing long chain hydrocarbon?
5. Can long chain hydrocarbon composition be accurately and repeatably controlled?

1.2 Considered technologies

The water-gas shift (WGS) and Fischer Tropsch (FT) reactions can be paired for the purpose of E-fuel creation. The major differences in these technologies come in the form of their reactors and catalysts.

The reverse water gas shift (RWGS) reacts H_2 and CO_2 to create CO and water (H_2O). The FT reaction combines H_2 and CO to produce hydrocarbons. Gas produced from the RWGS can then be used to feed the FT reaction. For future work, it is planned that both reactants will come from green energy sources with CO_2 being sequestered from atmosphere.

For the RWGS, catalysts are used to facilitate the reaction at high and low temperatures. Over the years, WGS reaction catalyst technology has advanced dramatically and has been suitably modified to assist the reaction even in the medium temperature range and achieve higher conversion.

Conventionally, WGS reactions have been performed by a pellet bed reactor followed by a heat exchanger. Heat can be applied from different heat sources depending on the application and available energy sources.

For the second half of the E-fuel creation process, Fischer–Tropsch catalysts are selected based on their choice of operating pressure and temperature which primarily drives the resultant product distribution.

For industrial Fischer Tropsch applications, the reactors come in several forms at present: the fixed bed, fluidised bed and slurry reactor.

For the success of this project captured CO_2 is required. Several methods were studied and explained in a previous project deliverable (Deliverable 3.1). It was concluded, carbon capture can be easily assimilated into E-fuel production through various methods. Solvents are the most mature technology for capturing carbon, but sorbents are currently the most commonly utilised for the purpose of synthetic fuels, however new emerging technologies associated with indirect capture through water possess a lot of promise. A lot of work is yet required to reduce the costs substantially enough to make this process entirely economical but with the substantial amounts of investment in this industry, a real emphasis has been placed on solving this issue and fast-tracking the process of large-scale carbon capture. CATAGEN is currently developing its own technology to capture CO_2.

1.3 This solution

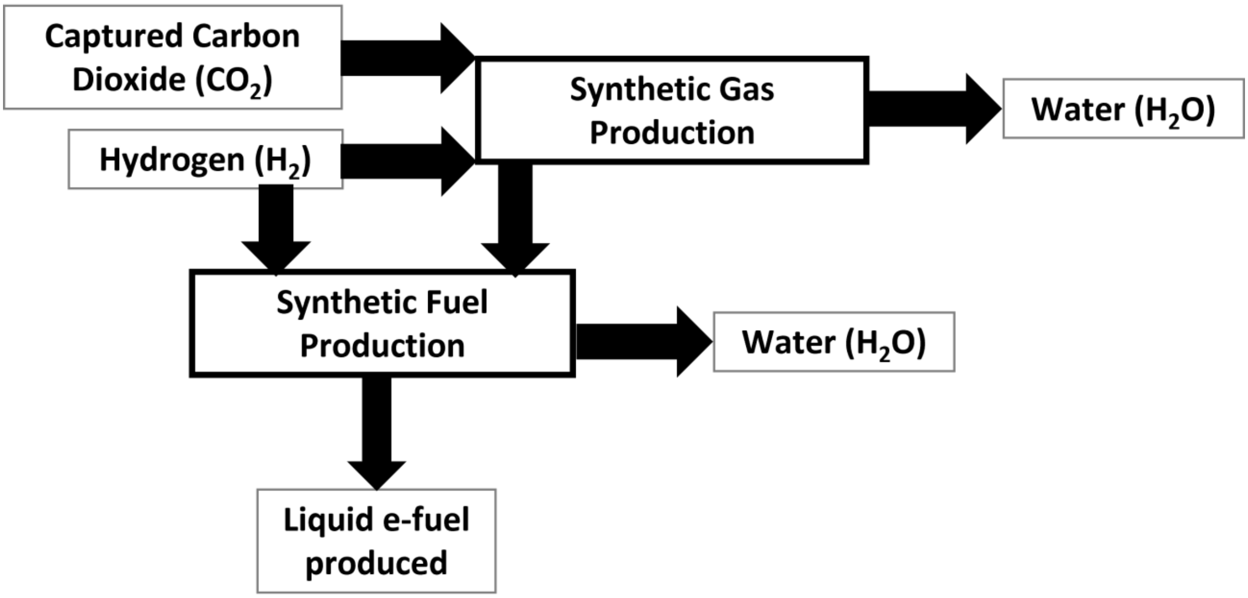

Figure 1: Proposed methodology for generation of E-fuel

The proposed methodology for generation of E-Fuel investigated in this wider research project is outlined in Figure 1 above and can be described as follows:

- Hydrogen is produced by a renewable or carbon neutral source – external to project.
- Carbon dioxide is captured, ideally from the air – external to project.
- The captured carbon dioxide and generated hydrogen are used to generate synthesis gas, through the reverse-water-gas-shift reaction (RWGS).
- The synthesis gas is converted to E-Fuels through the Fischer-Tropsch (FT) process.

The first phase of this process is the reverse water gas shift reaction. The RWGS reactor was built using CATAGEN technology. The input flow is controlled before passing through the reactor and exiting through an extraction system and subsequent gas analyser. Several different catalysts were tested as catalyst loading optimisation could provide key cost savings at full scale roll out.

The second reaction, Fischer-Tropsch, is suggested by literature that the choice of operating temperature primarily drives the product distribution.

The reactor is preceded by a heat source and followed by a condenser. The reaction vessel itself requires cooling as the FT reaction is strongly exothermic, with accurate temperature control in the reaction vessel identified as critical for sustaining reaction product quality. A condenser is then used to control the phase change of the hydrocarbons to form liquid E-fuel as the reaction products are typically in a vapour state rather than the required liquid.

1.4 Key benefits to our technology

- Liquid E-Fuel can be much more easily transported than gaseous H_2.
- Technology can produce a CO_2 net zero fuel which can be easily implemented with current infrastructure.
- Improvements with feedstock utilisation
- Proposed technology uses an energy efficient method to produce the aforementioned fuel.
- Technology is scalable/modular to suit broad range of applications.
- The reactor is designed to be tolerant to variable power supply e.g. renewable energy and capable of load following.

2. Experimental/ modelling results and conclusions of phase 1 project

2.1 Reverse Water Gas Shift (RWGS)

The water gas shift is a reversible reaction between carbon monoxide and water to produce carbon dioxide and hydrogen. The forward reaction in Equation 1 is moderately exothermic.

Equation 1

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

As we are employing the reverse water gas shift, it is an endothermic reaction and, as such, additional heat tends to shift the equilibrium to the left. The output of this process is highly dependent on gas mixture proportions injected as well as the ability for the reactor to reach suitable temperatures to achieve sufficient conversion of CO_2 and good selectivity to CO. As carbon dioxide is a stable molecule, a catalyst is required to activate the CO_2 molecule and facilitate a reaction with H_2. The prominent reaction parameters are temperature and feedstock composition. These conditions are the focus of the study for this reaction.

2.1.1 Test plan

To understand their effect on production rates, several parameters such as temperature, feedstock ratio, feedstock concentrations and background CO were altered during different test cycles. The temperature was evaluated to understand equilibrium shift and catalyst activity. The input gas proportions were varied to help find an optimal ratio between these for syngas production. These feedstock concentrations were evaluated to understand how a scaled reactor may operate optimally. As the end goal of this project is to design a recirculating gas reactor, background gases were added during some tests to understand the effect this would have on reaction conversion.

2.1.2 Results and Evaluation

2.1.2.1 Temperature

Temperature changes were seen to display the expected relationships with activity, diffusion rates and equilibrium conditions. Overall, the measured performance closely matched what would be expected based on the calculated thermodynamic equilibrium.

2.1.2.2 Feedstock ratio

Different feedstock ratios were used during testing. This testing looked to understand the effect of different feedstock ratios on CO production at different temperatures. It was seen that higher temperatures produced more CO. Different ratios of reactants give different CO outputs which matched the literature studied.

2.1.3 Evaluation of Performance (WGS)

Overall testing was a success in creating syngas in suitable amounts for the next stage of the project. Background gases were found to have a negligible effect on the syngas yield. Further testing would need to be completed to understand the effects of different catalyst loadings, and gas concentrations.

2.2 Fischer Tropsch (FT)

The Fischer Tropsch reaction (Equation 2) is a chemical catalytic process that causes a syngas mixture of hydrogen and carbon monoxide molecules to participate in a polymerisation reaction by means of an active metal to create a synthetic fuel made up of water and hydrocarbons.

Equation 2

$$CO + H_2 \rightarrow C_xH_y + H_2O$$

The FT synthesis product spectrum consists of a complex mixture of linear and branched hydrocarbons and oxygenated products. The main products are linear Paraffins and Olefins. Fuels produced with the FT synthesis are high quality due to very low aromaticity and zero sulphur content.

2.2.1 Test plan

The major reaction parameters for Fischer-Tropsch are temperature, pressure and syngas proportions. The impact of residual gases was also considered in these tests to see its effect on product output and scaling of yield with feedstock additionally was studied to help give better estimates on scaled up production. Catalyst temperature was closely monitored due to the highly exothermic nature of the reaction.

Post condenser, all liquid was collected in the product vessel. Any carbon chains still in vapour form were vented through an extraction line, where they were sampled with a gas analyser. Final liquid samples were sent to a 3rd party to undergo chemical analysis to understand the makeup of the final product to help understand how test conditions affect fuel quality.

2.2.2 Results and Evaluation

2.2.2.1 Temperature

Changes to production of different lengths of hydrocarbons were observed as anticipated with changes to the reaction temperature. In addition to this, higher production rates were seen at temperatures that were previously identified to be optimal.

2.2.2.2 H_2/CO ratio

Before testing began, possible syngas proportions were decided upon to ensure stoichiometric flow for the FT reactions. This analysis enabled the identification of optimal conditions which matched predictions and generated more liquid product than other tests run.

2.2.2.3 Additional findings

Testing results showed several unexpected outcomes. A gas analyser was used to measure gaseous products. Observations showed that large amounts of shorter chain hydrocarbons, particularly methane, were produced. This gas could either be used as a final product or utilised elsewhere as high-quality feedstock.

2.2.2.4 Evaluation of Performance (FT)

From the study, all testing conditions were successful in producing both liquid and gaseous E-fuel (both considered useful products). The tests completed at the previously identified optimal condition produced a higher volume of products, with the yield of hydrocarbon product from tests increasing exponentially with feedstock concentration.

Whilst reactant concentration and system pressure were accurately controllable, further work is required to maintain other reaction variables. This will help produce single (user specified) species products, along with expected improvements in yield. Further, a fractional distillation step should be used to separate the various fractions based on their boiling point – a common activity in the petrochemical industry for fossil fuels

The conclusions of the completed testing were positive. Moving forward more work is required with control of the system to help produce more singular output during testing.

Overall, the production rate of long chain hydrocarbons was slightly lower than anticipated based on the performance data provided by the catalyst supplier. Further optimisation of catalyst form factor and size could help address challenges, in this case the catalyst was procured based on availability rather than peak performance.

3. Description of the demonstration phase 2 project

The CATAGEN E-fuels reactor combines green hydrogen and captured carbon to create localised green fuel production. The reactor will utilise renewable energy to keep the process environmentally friendly and economical and can use current fossil fuel infrastructure for distribution and storage, minimising downstream infrastructure disruption, reducing costs, and removing barriers to adoption by end users.

Phase 2 of the CATAGEN E-fuel reactor development will have a large focus around consortia engagement and pilot scale development. These partners will enable refinement of the system design to meet industry needs as well as integration with renewable energy that can further optimise the performance of reactor. These partners are expected to facilitate the system to be fully integrated on site, allowing the CATAGEN system, from renewable energy generation to carbon capture and green hydrogen production right through to E-fuel production, to occur in the one place.

In terms of the hydrogen economy, this allows localised levels of generation, with one of the main requirements for E-fuels being renewable energy, which is readily available in many places across the globe. This locality of supply addresses the major issue associated with energy security. It also tackles hydrogen economy obstructions like carbon footprint tracking, as presently, there are difficulties assessing the carbon intensity of green hydrogen. This is primarily hindered by the variety of definitions and colour gradings with a lack of standard classifications. The CATAGEN system allows companies and individuals to see exactly where the fuels are made from capture through to storage and end use and removes complexities associated with distribution.

This would be a major step forward in the development of the hydrogen economy strategy as today, electrolysers are the backbone of the hydrogen economy. Despite this, there are notable setbacks to electrolyser usage, or usage of pure hydrogen fuels, in the form of desalination, long lead times and material shortages, energy supply and most notably storage. It is expected that developments in hydrogen storage have a timeline of approximately 7 years for full industrial level implementation. The hydrogen storage and transport challenge must be solved, or at least partly overcome, before there can be widespread roll out of hydrogen fuelled vehicles or applications, which itself would have to follow widespread roll out of infrastructure – this takes the 7 years into a longer timeframe. The further conversion of this hydrogen into the form of E-fuels allows for much easier storage in large volumes and facilitates the possibility of storing this fuel – essentially enabling carbon sequestration in a denser method than the technique of piping carbon underground and the associated risks with this method that is presently used. Further, E-fuels in fact would be able to utilise existing infrastructure to expedite their roll out and could even be blended with fossil fuels in the first instance to facilitate decarbonisation.

The project goals of phase 2 have been highlighted below. Some have been explained above and others will be further explained in the text below.

- Design a single system that is capable of producing E-fuel using the two reactions (RWGS and FT) outlined in Phase 1 in an economical manner using green energy sources. The technology itself is feedstock and energy agnostic, but is ideally suited to and net-zero applications to produce net-zero products.

- Create a system that is capable of producing a range of different hydrocarbons chain lengths which gives control to the user over product selection and allows for separation of the various products.
- Study and understand carbon sequestering technologies and understand how they can be implemented into the system.
- Develop a final E-fuel product that can be sold to market as an alternative to current liquid fuel sources. This will involve testing of product purity ensuring it adheres to current fuel standards.

4. Design of demonstration

The system design proposed for Phase 2 demonstration comprises two reactors in the one system, a RWGS and a FT reactor, along with a series of additional electrical components, and other balance of plant equipment. The reactors are also supplied by CO_2 and H_2 feedstock from large storage tanks and tube trailers respectively – ideally these would be supplied by hydrogen production and carbon capture equipment on site, but to deliver best project value these high-cost pieces of equipment are replaced by their product only.

One control system is also proposed for the joint operation of each of the two sub-reactors and systems – the primary function is this is to maximise energy utilisation at a renewable site with the interim storage vessels providing some degree of de-coupling of the systems.

The gas supplies to the RWGS reactor are connected through gas regulators. The RWGS reactor will operate at a pressure and temperature suitable to the selected catalysts. These conditions will be user selected. The target gas mix is delivered through the heat source where the heated gas is then passed through the RWGS catalyst. Before exiting the reactor to a holding tank, the reaction products are passed through a cooler which allows the water produced by the RWGS reaction to be removed.

The Fischer-Tropsch reaction in phase 2 will operate at different pressures and temperatures than that tested in phase 1 , (FT temperature and pressure will also be user selected). Additional components to optimise the reaction and stabilise conditions will be added. There will also be added mechanisms for the purpose of increasing safety of disposal, energy efficiency and to facilitate the decoupling of the two key processes.

Gaseous Feedstock is passed through the FT reaction zone. Controlling certain variables within the reactor bed was a challenge in the Phase 1 project as additional measures necessitated by H_2 safety considerations may have limited the reaction.

Downstream of the FT reaction zone there will be a variety of reaction products. The function of the post-processing equipment is to capture the useful products and remove waste products.

A second phase separation step follows this, where the liquid products are then continuously pumped out of this into temporary storage tanks before further separation through periodic fractional distillation.

The energy cost of producing and capturing the H_2 and CO_2 is high, comprising the bulk of the overall energy cost of the E-fuel. As such, there are CO_2 and H_2 separation steps added into the post processing, these are to be designed as part of the Phase 2 project.

The CO_2 and H_2 depleted reactor off-gas may contain gaseous products, whilst this is not the desired primary output from the reactor, this has high value, as a solution to decarbonise the natural gas grid for instance. The gaseous products must be separated from the off-gas, the technology for which is proposed to be identified during the Phase 2 project.

Overall, the proposed Phase 2 demonstrator will utilise H_2 and CO_2 feedstock to generate both liquid E-fuel and E-methane at a renewable energy site.

It is important to note that any products produced in the liquid or gas phase will need to be analysed to understand if they meet the current fuel requirements before they are released to market. Currently this will require analysis from a 3rd party lab. It is hoped that in the future CATAGEN could complete these certifications internally.

5. Benefits & Barriers

5.1 Benefits

The objective of the feasibility study was to evaluate a means of producing a higher energy density, more easily transferrable hydrogen-based fuel than hydrogen alone. The feasibility testing has shown that this can be achieved through RWGS and FT using CATAGEN’s technology. From the range of data collected in phase 1, the phase 2 technology should be able to produce a range of different liquid E-fuels to match the user's requirement. The outputs will be controlled by different operating conditions. Test conditions can also be controlled to create gaseous products such as methane if required.

The process of converting into hydrogen also have several energy benefits. Methane has >3 times the energy per unit volume of hydrogen at equivalent pressure. This also applies to longer chain hydrocarbons, where there is 10 times the energy per litre than hydrogen stored at 350 bar.

A further benefit is in the potential for the synthesised hydrocarbons to be a direct drop-in for their fossil-derived equivalent. Discussions with various stakeholders throughout the duration of the project have shown that there is a desire for such a product across a range of industries. For each case a transition to solely hydrogen fuel would necessitate substantial changes to equipment or obsolescence of existing equipment and infrastructure. E-Fuel, such as that which could be produced through the CATAGEN approach, could not only facilitate immediate decarbonisation of these applications (rollout permitting) but also remove the requirement for equipment upgrades, which avoids the embedded carbon associated with such activities.

5.2 Barriers

For this process to be a success, there are several barriers and engineering problems which must be overcome. The FT process is a very exothermic reaction, and the hydrocarbon product is very dependent on test conditions such as temperature and pressure. Phase 2 will incorporate measures to combat these and reduce their influence on the reaction. Such approaches would allow different amounts of heat and pressure extraction throughout the reaction vessel, which will help maintain more consistent conditions throughout.

During the FT process a range of hydrocarbons will be produced, as found during Phase 1. The process can also produce unwanted products such as water and alcohol, some of this is unavoidable given the release of oxygen from the carbon monoxide feedstock, but some by-product formation can be avoided. It is important to understand the correct operating conditions for desired products and be able to control the reactor with a well-designed control system. Further to this, it is also important that the various products can be accurately separated from one another into their various categories, to overcome this challenge it is proposed that a fractional distillation approach is used downstream of the FT reactor.

With final products, distribution into the market could be a potential barrier. All fuels that enter the market must adhere to international fuel standards, which is a challenge in itself. Beyond the demonstration project physically distributing the fuel to either: a refinery or end user would also pose a challenge.

Several of the utilities required for E-fuel production may also be a barrier during the development phase. Large amounts of reactants (CO_2 and hydrogen) and large amounts of energy will be required for production. Current energy and gas costings (particularly CO_2) are also a barrier which must be overcome, in order to deliver good project value.

5.3 Metrics

Comparisons of E-fuel as a hydrogen carrier to hydrogen alone are complicated by a number of factors, including availability of technology with which the fuel can be used, the application for which it is to be used, transport and distribution of the fuel among others. This section therefore seeks to provide some quantitative values around the relative production cost and energy density of E-fuels produced by the technology under evaluation. These values have been removed from this document due to commercial sensitivities.

When considering E-fuel production there are four key factors: hydrogen cost, carbon dioxide cost, RWGS cost and FT cost. In practice for both Phase 1 and 2 the feedstock was / is planned to be supplied from a 3rd party rather than produced at site in order to manage costs and deliver project value.

- RWGS testing costs are determined based on the energy required to heat the feedstock from ambient temperatures to the target operating temperature. The extent of the RWGS and therefore the reaction products were calculated based on equilibrium conditions as the Phase 1 testing showed that performance could closely match these.
- FT testing costs are determined based on the energy required to reach the desired temperature and pressure. An exact value for performance cannot yet be determined with high certainty, hence the requirement for multiple evaluation cases. Also included in the FT energy costs are balance of plant operating costs.

The value of the RWGS reaction products is entirely dependent upon what they can be used to generate in the FT reactor.

It was initially proposed at the outset of the project that these long chain HCs which are liquid at STP were the only desirable product from the FT reactor. Current market trends along with insight from stakeholder engagement has identified that there is also a use for E-methane, and as such this is classified as a useful output for the purposes of the overall E-fuel production analysis.

6. Costed development plan

A plan for the proposed demonstration project is outlined below from a high level, and included in the appendices in greater detail. The main premise of the project is to build and test an E-fuel production system which utilises renewable energy to generate a carbon-neutral, energy dense, hydrogen carrier. These research and development activities comprise 12 work packages across the 102-week period beginning 14/2/23.

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 itself.

The design of the reactors (WP2) is scheduled for the beginning of the project, where upon completion, the majority of the system components should be specified, ahead of the procurement activities. The predominant cost for this activity is labour related, however additional costs are budgeted for software licensing (reactor simulation and CAD modelling), along with chemical engineering and H&S consulting.

Following the intensive design phase, procurement of material and components for the reactor build is scheduled. This has been guided by learnings from the phase 1 project, where global supply chains are less reliable than in the past. Included in the WP is a period to allow for competitive tender for high value items to ensure good project value, along with an additional period to allow for extended component lead times. CATAGEN are currently experiencing longer lead times for control and electronic equipment, and as such the procurement of these components is included in WP6, allowing extra time for delivery. A high proportion of the project material costs will be accrued throughout this work package.

The build of the RWGS and FT reactors is contained in WP5. This 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 complete, 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. This will include: I/O testing, simulated operation to validate control software, and initial testing of each of the sub-reactors. The program then moves to reactor testing, wherein the performance will be validated, with evaluations of efficiency, product quality and overall functionality tested. This testing, followed by an extended program, will incur substantial material costs owing to the cost of acquiring initial feedstock for the reaction, along with the electrical cost of operating the equipment. Given the lead times for carbon capture and hydrogen production equipment, it is unlikely that these could be available to support the demonstration. This may therefore mean that external supplies of hydrogen and carbon dioxide are required for testing. This will be clarified prior to submission of any Phase 2 application, with the project plan adjusted accordingly if there are technologies available.

The final elements of the project involve final reporting on the outcomes of the project, with a final work package included for sign-off and review for all project deliverables and documentation. During the final reporting, the reactor is scheduled for decontamination and potential decommissioning, with the concurrent approach taken necessitated by the short project timeframes.

As a final comment on the project timeline, other activities have been moved forward where possible to help de-risk the project delivery. This includes the control system development (WP6) and certain elements of the reactor builds. Also included in the workplan is a testing package on the original phase 1 reactor. The main objectives of this testing plan are to deepen the understanding of how finer changes in operating parameters effect the performance, with a planned upgrade to the reactor cooling design for instance to allow a more detailed evaluation of temperature and temperature profile through the reactor. The outline project plan has been developed with the project team's experience of Phase 1 in mind. This is evident in two key areas, supply chain and reactor commissioning. Additional time has been allocated for component lead time, with extra time also allocated specifically for commissioning, rather than this being included in the testing period. Further, key suppliers and contractors will be made aware of the key dates early in the project to allow them to allocate resource and commit to timeframes early, to help ensure they can support on time delivery of the project.

Project costs have been estimated between £4.5 - 5 million based on the proposed design and prior experience in reactor builds (both in and outside of LCHS2108). A financial breakdown is given in Table 1. Given current market volatilities the, estimated costs may potentially change between submission of this report and any phase 2 application.

Table 1: Phase 2 Financial breakdown

Category	Percentage cost
Project management	5%
Engineering Design	10%
Build testing analysis	22%
Reporting	2%
Material	32%
Subcon	29%

The material and subcon costs are associated with the design, build, installation and safe operation of the reactor. Key materials include electrical heating elements, control electronics, raw material for pipework and reaction vessels, catalyst, and a gas separation membrane deigned to help remove gas products from the FT outlet stream prior to recirculation. Key contributors to the subcon costs include electrical panel build and enclosure, fabrication of reaction vessels and other equipment, electrical supply works and civil engineering activities. The costs have been redacted from this document to protect commercially sensitive information.

7. Rollout potential

As this system produces hydrocarbons from CO_2 and green H_2, the demand for this technology from consumers is high as with CO_2 sourced from the fast carbon cycle (e.g. the atmosphere, biogenic sources etc) this creates a net zero hydrocarbon solution that is compatible with existing internal combustion engines and boilers. This presents many opportunities for use of the hydrocarbon products in the transport sector, as well as heating and heavy industry. The requirement for rollout of the system to meet these needs will require qualification of the hydrocarbons produced to meet the required octane ratings for specific fuel applications such as gasoline and kerosene. The testing of the hydrocarbon products has been included in the suite of tests undertaken as part of this project. Once the quality and optimal configuration in terms of energy efficiency is known for the system, rollout and target of the aligned market sectors (e.g. gasoline, kerosene, blends with existing fuel stocks) can be addressed and exploited.

As the system can also be used to transform green hydrogen into a more familiar, energy dense, and easily stored chemical, the technology also represents a solution to green hydrogen generation at renewable energy sites such as solar and wind farms. The higher energy density storage and ease of transport helps to overcome one of the main issues with decentralised green hydrogen production; storage.

8. Route to market assessment

The CATAGEN E-fuel system will require several significant steps to progress through CRL (Commercial readiness level) development; pilot scale demonstration, business model(s) development and application optimisation, MRL (manufacturing readiness level) development and business model validation.

The progression to reach these steps has already begun during Phase 1 with the development of the E-fuels system, as well as basic market awareness and value propositions being developed in parallel with the technology. This means that the system currently sits in the 3-4 CRL range. Further progression of CRL will be dependent on deployment of the pilot device 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 technology viability with a ‘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 a net zero hydrocarbon as a product, the total addressable market for this technology is incredibly large; with market potential across all areas of the oil and gas sector including diesel and gasoline. As this technology offers the same chemical product as fossil fuels but in a net zero fashion using CO_2 recovered from the atmosphere, where it then returns to after use.

This creates a disruptive effect in the industry but presents large liquid fuel users such as the marine (200 million litres of MDO annually) and the haulage sectors (a $4 trillion industry) a route to net zero that does not require retrofitting or replacement of existing assets and so removes a large financial barrier to their decarbonisation pathways. As an example of the potential carbon savings this technology represents, the maritime sector alone produces approximately 2% (1.056 billion tonnes of CO_2) of the world’s CO_2 emissions so addressing 10% of this demand would represent approximately 156 million tonnes of CO_2 prevented from entering the atmosphere.

As these examples show, the crucial need for development of a route to market will be demonstration of the technology and identification of the most favourable operation setup to minimise the cost of the E-fuels produced by the system. These questions can be addressed by pilot demonstration and the ongoing parallel development of MRL and CRL of the product, a role CATAGEN is approaching global supply chain partners to assist with as consortia members.

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 net zero fuels 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 net zero alternatives 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 this net zero E-fuel there is also the opportunity to reduce the carbon emissions of industries such as the marine sector (which produces approximately 2% of the global emissions) and the aviation industry (currently responsible for 8% of UK transport emissions annually). This net zero solution can help ensure these vital industries do not further contribute to human induced warming and allows current assets to be used to end of useful life; removing two of the main barriers to adoption of more sustainable energy systems, the capital cost and the present scarcity of available units.

9. Dissemination

Category of Activity	Title and Description of Activity	Stakeholders Engaged	Date
Identification of Market Need and Potential Economic buyer of product	*Presentations and Facility Tour*	*Market engagement meetings and identification of potential project collaborators (Stake holder details have been withheld for commercial sensitivities)*	*Various Dates in Project*
Identification of Collaborators and Renewable Energy Park Developers (Consortia Building)	*Presentations and Facility Tour*	*Market engagement, meetings and identification of potential project collaborators (Stake holder details have been withheld for commercial sensitivities)*	*Various Dates in Project*
Identification of New Potential Supply Chain Partners (Consortia Building)	*Presentations and Facility Tour*	*Market engagement meetings and identification of potential project collaborators (Stake holder details have been withheld for commercial sensitivities)*	*Various Dates in Project*
Attendance to Trade Shows	*Networking and Market Analysis*		*May 2022*
Attendance to Trade Shows	*Networking and Market Analysis*		*June 2022*
Dissemination to Energy Industry Experts	*Presentation of CATAGEN NET ZERO Technologies*	*(Stake holder details have been withheld for commercial sensitivities)*	*June 2022*
VIP Event Hosted at CATAGEN	*Presentation of CATAGEN NET ZERO Technologies*	*(Stake holder details have been withheld for commercial sensitivities)*	

The primary focus of the dissemination activities during Phase 1 were to build relationships with potential customers and collaborators for future activities. Many of these engagements were not solely focussed on E-fuels, but in each case they were a point of discussion, particularly for the mobility and energy suppliers. These activities have been successful. Beyond the end of the Phase 1 project, further demonstration activities are anticipated, including a technology showcase with a variety of key stakeholders, and technical publications and/or whitepapers to share a summary of the findings and outputs from the work.

10.Conclusions

The goal of this project was to "Complete the initial development and determine the feasibility of a low-cost liquid hydrogen fuel production reactor". Two reactions were utilised to complete this; the reverse water gas shift (RWGS) and the Fischer Tropsch reaction.

The RWGS reaction was complete successfully on a test reactor with CO being produced. Test results showed how differences in test conditions effected the production rate of CO. Background gases were found to have a negligible effect on the CO yield proving that the CATAGEN technology can be effectively implemented in future. Further testing would need to be completed to understand the effects of different catalyst loadings and gas concentrations. Additional research will be required to understand life span of the catalysts used at the proposed temperature. The temperature resistance and useful life of other catalyst types may also be researched. Furthermore, testing of the FT was completed successfully. This testing had to be complete on a custom-built rig with a new control system designed. Testing produced both liquid and gaseous E-fuel (both considered useful products). Testing of reactant quantity was limited due to safety concerns with hydrogen. More work will be required on the control system and reactor design to maintain more constant test conditions. This will help produce single (user specified) species products with little requirement for post process refining. As a result of these restrictions, the ability to repeat experiments was hindered.

Several modelling activities were also completed to examine the cost and product rollout. Numerous scenarios show the potential to deliver a cost-effective product. Several of the requirements needed for each scenario have or currently are being researched in CATAGEN, such as the hydrogen feedstock from several sources.

Progress has already been made on an assessment for route to market with market awareness and value propositions being developed in parallel with the technology. With the advantage of the E-fuel being a drop-in replacement, this is seen as a major benefit by a lot of potential customers as they strive towards net zero goals. From market assessment, the total addressable market for this technology is huge, with potential across all areas of the oil and gas sector, including diesel and gasoline.

The technology does however, come with some potential risks, which will have to be addressed in phase 2.

A detailed project plan has been developed for the phase 2 project. This has taken into consideration all learnings from phase 1 and other learnings from other BEIS projects on going in the company. Special emphasis will be put on component lead time and machine commissioning time.

Overall, the Phase 1 LCHS2108 project has successfully completed its objective to determine the feasibility of producing green syngas and high-density, easily transportable green E-fuel. This has been demonstrated through the following:

1. Testing of the phase one FT reactor was successful in producing both liquid and gaseous hydrocarbons. This was confirmed 3rd party chemical analysis and the use of our internal gas analyser.

2. The RWGS test rig was also successful in producing suitable amounts of CO from CO_2 and H_2 under several different test conditions, with ideal test conditions chosen for stage 2.

The energy cost and modelling show the potential for an economic business case to allow for the production of a cost-effective product.