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University College Cork, Ireland Coláiste na hOllscoile Corcaigh





Technoeconomic evaluation of Power-to-Gas: Modelling the costs, carbon effects, and future applications

by

Shane McDonagh

A thesis submitted for the degree of

Doctor of Philosophy (Energy Engineering)

NATIONAL UNIVERSITY OF IRELAND, CORK

19/12/2019

Academic Supervisor

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Conducted within the of College of Science, Engineering, and Food Science under

Professor Liam Marnane

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Declaration

I hereby declare that this thesis is my own work and that it has not been submitted for another degree, either at University College Cork or elsewhere. Where other sources of information have been used, they have been acknowledged. I have read and understand the regulations of University College Cork concerning plagiarism.

Shaw McDonagh

Signed:

Date:

19/09/2019

Acknowledgements

As of writing this I've been a student for twenty-two years and two weeks, 82% of my life, it's starting to seem excessive. It's official though, I can go no further, I suppose I'll have to get a real job now and it's time to thank those who have helped me get here, for there's no such thing as a self-made man.

To my supervisor Jerry, thank you for your guidance and giving me the opportunity to work with some fantastic people. I may not have always filled you with confidence, but we got there in the end. To my colleagues, Richie for raising the bar, Conor for our lunch time debates, David for getting me started, and Paul for his instant replies, I am truly grateful. To all my colleagues¹, a great bunch who made this experience so enjoyable! And a special thank you to Tara, not all heroes wear capes.

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Last but not least, my friends, after all I picked you. Nothing is worth doing if you don't have someone to share it with, so thank you for bringing so much fun to my life. Especially to the "shlugs" as they are affectionately known, who kept the "days upon days of absolute craic" coming.

"Sure look, it'll make a good story?!"

¹ Aoife, Markus, Karthik, Richen, Enrique, Davis, Archie, Quishi, Benteng, Ketan, Maarten, Chen, Helen, Kyle, Jess, Zoe, Truc, Conor, Tarun, Parveen, Evan, Magdalena, and more.

Abstract

Power-to-Gas (PtG) splits water into hydrogen and oxygen using electricity. As the hydrogen can be used directly or combined with carbon dioxide to produce methane, it has been mooted as a versatile renewable fuel especially suited to reducing transport emissions. PtG's ability to flexibly consume electricity means that it can alleviate some of the issues associated with increasing amounts of variable renewable electricity (VRE) like wind, providing storage and ancillary services to the electricity grid.

The sustainability of PtG (both hydrogen and methane) was examined in terms of cost and emissions using various methods and for a range of scenarios. Cash flow models were used to calculate the levelised costs, and sensitivity analysis was performed on these. Electricity market models were used to optimise the cost of the electricity consumed, and also to control the carbon intensity of the gas produced, while wind speed data and simulations of the electricity system produced results on directly pairing PtG with VRE. Each chapter also includes analysis of PtG regarding potential barriers to its implementation and niche applications, suitable to all energy stakeholders.

Should zero cost electricity be available throughout the year it would result in a levelised cost of €55/MWh (55c/L diesel equivalent) for PtG (methane). However, in reality it is not viable to base PtG on otherwise curtailed or difficult to manage (zero cost) electricity alone, the resource is too small even at high VRE penetration; it is preferential to increase the run hours of gas production to a level that amortises the capital expenditure by bidding for electricity in the wholesale market. Results show that by optimising electricity consumption large savings in levelised costs can be achieved, but they are still dominated by electricity purchase (56%), followed by total capital expenditure (33%). The base levelised costs for PtG (methane) were found to be €124/MWh in 2020 which may fall to €93MWh in 2040, valorising the oxygen or grid services could reduce these by €19 and €37/MWh respectively.

The majority of the life cycle emissions from PtG are due to the source of electricity, but by operating at times of low-cost or high forecast wind power, these can be reduced. Cleaner hydrogen production (up to a 56% reduction in

carbon intensity) at a lower cost (up to 57% less) can be achieved when compared to hydrogen associated with the grid average. Synergistic effects that increased with VRE penetration were noted, meaning that ignoring emissions and instead minimising levelised costs using these controls still reduced the carbon intensity of the hydrogen produced by 5-25% for the bid price control and by 14-38% for the wind forecast control.

Direct connection to an offshore wind farm was also considered though results suggest that curtailment abatement alone will not drive investment in PtG; high hydrogen values are a necessity. To justify converting all electricity to hydrogen, a developer would have to anticipate 8.5% curtailment and be able to receive €114/MWh of hydrogen, or 25% curtailment and €101/MWh. Hybrid systems are preferable and increase project value when hydrogen is sold for €106/MWh or more, otherwise selling electricity alone is more profitable.

The strategies and configurations tested in this thesis allow for hydrogen/methane to be produced from electricity without exacerbating the mismatch of supply and demand. PtG has significant potential as a future source of low carbon transport fuel, especially in the haulage sector. However, in order to be competitive PtG systems must also valorise the ancillary services they provide and focus on optimising the consumption of electricity, as capital cost reductions alone are unlikely to sufficiently reduce levelised costs. The system wide benefits of PtG make it highly suitable for incentivisation especially in light of increased VRE penetration and ambitious renewable transport energy targets.

Thesis output

Chapters published as papers or currently under review in peer-reviewed journals and for which I am principally responsible:

Chapter 3:

S. McDonagh, R. O'Shea, D. M. Wall, J. P. Deane, and J. D. Murphy, "Modelling of a power-to-gas system to predict the levelised cost of energy of an advanced renewable gaseous transport fuel," Appl. Energy, vol. 215, no. January, pp. 444–456, 2018.

Chapter 4:

S. McDonagh, D. M. Wall, P. Deane, and J. D. Murphy, "The effect of electricity markets, and renewable electricity penetration, on the levelised cost of energy of an advanced electro-fuel system incorporating carbon capture and utilisation," Renew. Energy, vol. 131, pp. 364–371, 2019

Chapter 5:

S. McDonagh, P. Deane, K. Rajendran, and J. D. Murphy, "Are electrofuels a sustainable transport fuel? Analysis of the effect of controls on carbon, curtailment, and cost of hydrogen," Appl. Energy, vol. 247, no. November 2018, pp. 716–730, 2019.

Chapter 6:

S. McDonagh, S. Ahmed, C. Desmond, and J. D. Murphy, **"Hydrogen from offshore wind: Investor perspective on the profitability of a hybrid system including for curtailment,"** Applied Energy (Under review).

Articles published as papers or currently under review in peer-reviewed journals and for which I am only partially responsible:

Chapter 7: Contributions to the papers below have been synthesised into a chapter to provide additional context to this thesis.

Chapter 7.1:

R. O'Shea, D. M. Wall, **S. McDonagh**, and J. D. Murphy, **"The potential of power to gas to provide green gas utilising existing CO2 sources from industries, distilleries and wastewater treatment facilities," Renew.** Energy, vol. 114, pp. 1090–1100, 2017.

Chapter 7.2:

D. M. Wall, **S. McDonagh,** and J. D. Murphy, "**Cascading biomethane** energy systems for sustainable green gas production in a circular economy," Bioresour. Technol., vol. 243, no. June, pp. 1207–1215, 2017.

Chapter 7.3:

L. Janke, **S. McDonagh,** S. Weinrich, J. D. Murphy, D. Nilsson, P.A, Hansson, A. Nordberg, **"Modelling power-to-X applications in the Nord Pool electricity market: Effects of different bidding strategies on plant performance,"** Applied Energy (Under review).

Outreach publications:

- "Banning fossil fuel exploration is posturing not pragmatism", RTÉ Brainstorm, April 2018.
- "The unseen fight against climate change", RTÉ Brainstorm, October 2018.

Other engagement:

- Six invited speaker roles.
- Five engagement events.
- Five outreach programmes.
- Vice-Chair of world's largest student energy summit.

Contribution to the papers

Chapter 3: Modelling a power-to-gas system to predict the levelised cost of energy

I designed the study and conducted the research including analysis and interpretation, and I was responsible for producing the first draft (first author). My colleagues in University College Cork and I are responsible for updating reviewed drafts.

Chapter 4: The effect of electricity markets, and renewable electricity penetration, on the levelised cost of energy

I developed the hypotheses and was responsible for planning the research. Results from previous work by Dr. Paul Deane, a MaREI colleague, were used in preparing the study, as credited. I then conducted the research, interpreted the results, and produced the first draft as first author. My colleagues and I reviewed, edited and polished the manuscript.

Chapter 5: Are electrofuels a sustainable transport fuel? Analysis of the effect of controls on carbon, curtailment, and cost of hydrogen

I proposed and researched the study. I also designed the methodology and was responsible for data analysis and interpretation. I was responsible for producing the first draft (first author) and updating reviewed drafts.

Chapter 6: Hydrogen from offshore wind: Investor perspective on the profitability of a hybrid system including for curtailment

A colleague is responsible for the early concepts, I was then responsible for the planning, design, and execution of the study. I performed the majority of model development and carried out all data analysis and produced the results. I was the first author and prepared the first draft.

Chapter 7: Co-authored work

Chapter 7.1: The potential of power to gas to provide green gas utilising existing CO2 sources from industries, distilleries and wastewater treatment facilities

I was involved in the ideation, design, and data collection for this study.

Chapter 7.2: Cascading biomethane energy systems for sustainable green gas production in a circular economy

I helped to develop the scenarios explored and produced the graphics. I also contributed to and reviewed the manuscript.

Chapter 7.3: Modelling power-to-X applications in the Nord Pool electricity market: Effects of different bidding strategies on plant performance

I was involved in the design and research of the study. I developed the financial model, and I was also involved in preparing the first draft and the subsequent revisions.

Nomenclature

NTP: Normal temperature and pressure (N): $20^{\circ}C$ and 101.325kPa

The symbol $\boldsymbol{\eta}$ is used to denote efficiency

AD	Anaerobic Digestion	L _{diesel}	Litre of diesel equivalent by energy
AEL	alkaline electrolysis cells	LHV	Lower heating value
BM	Biological methanation	NGV	Natural Gas Vehicles
BoP	Balance of plant	NOH	Non-Operating Hours
CAPEX	Capital Expenditure	NPV	Net Present Value
CCGT	Combined Cycle Gas Turbine	O&M	Operation and Maintenance
CH ₄	Methane	OPEX	Operational cost
CM	Catalytic methanation	OWF	Offshore Wind Farm
CNG	Compressed Natural Gas	PEM	Proton Exchange Membrane electrolysis
CO ₂	Carbon dioxide	PHS	Pumped Hydroelectric Storage
DGA	Difference from Grid Average	PtG	Power-to-Gas
DSM	Demand Side Management	PtX	Power-to-X
ETS	Emissions Trading Scheme	RE	Renewable Electricity
EU	European Union	RED	Renewable Energy Directive (EU)
FFC	Fossil Fuel Comparator	SMP	System Marginal Price
FFH_2	Fossil Fuel derived Hydrogen	SMR	Steam Methane Reforming
GDP	Gross Domestic Product	SNSP	System Non-Synchronous Penetration
GHG	Greenhouse Gas	SOEC	Solid Oxide Electrolysis Cells
H ₂	Hydrogen	Syngas	Synthetic gas
HGV	Heavy Goods Vehicle	TRL	Technology Readiness Level
HHV	Higher Heating Value	TSO	Transmission System Operators
ISEM	Irish Single Electricity Market	VRE	Variable Renewable Electricity
LCOE	Levelised Cost of Electricity	WWTP	wastewater treatment plant
LCOH	Levelised Cost of Hydrogen		

1 Introduction

The aim of this chapter is to deliver an overview of Power-to-Gas (PtG) systems and provide context for each of the subsequent chapters, not to perform any exhaustive analysis. The chapter consists of an introduction, an exploration of the research questions, objectives, followed by an outline of the thesis. Each chapter also contains a brief introduction specific to that work.

1.1 The Power-to-Gas concept

The impacts of climate change and the harmful nature of fossil fuels are well established, with the Paris agreement (under COP21) setting a target of limiting the increase in global temperatures to less than 2°C [1]. To facilitate this, an 80% reduction in greenhouse gas (GHG) emissions by 2050 will most likely be required [2]. Two sectors produced nearly two-thirds of global carbon dioxide (CO₂) emissions from fuel combustion in 2014; by far the largest was electricity and heat generation accounting for 42%, while transport accounted for 24% [3].Therefore a reduction in GHG emissions will rely heavily on decarbonisation of the energy sector, and a push for sustainable energy solutions to meet increasing demand.

Energy policy has traditionally sought import reduction, cost optimisation, stability, and security but it is increasingly based on climate change policy. The European Union (EU), along with many other nations, has developed plans to transition away from fossil fuel reliance to more sustainable energy. The EU Renewable Energy Directive (RED) dictates that 32% of final energy consumption in the union be from renewable sources by 2030, with a sub target of 14% for transport [4]. From a legislative perspective, the responsibility for meeting this sub-target falls on transport fuel suppliers. Caps on first generation food crop-based biofuels and limited alternatives to liquid fossil fuels increase the difficulty of this goal and generate a demand for alternative low carbon fuels. Nevertheless, it is the responsibility of this generation to champion the energy transition, but also to recognise the opportunities associated with this change.

Introduction

In response to the challenge, and combined with the declining costs, renewable energy technologies are being rapidly deployed and continue to decarbonise the energy system [5]. By far the most progress has been made in decarbonising electricity, the technologies are more mature and arguably require much less systemic change, especially on the part of consumers. As transmission system operators aim to facilitate targets set under the RED, renewable technologies will be prioritised [4]. This is not an issue with dispatchable renewable electricity from biomass or hydropower; they fit well into the existing market and technological structures [6]. However, high levels of variable renewable electricity (VRE) are being integrated into the electricity grid too, in particular wind and increasingly solar whose output varies temporally and spatially with climatic conditions. At increasing shares these give rise to issues of grid balancing, stability, and lost energy, potentially affecting security of supply [6,7]; though they are still the most advanced existing options for affordable low carbon electricity and as such are vital for the transition.

Better forecasting and demand side management helps to alleviate the issues associated with VRE, but are insufficient alone [8]. Large scale and flexible energy storage options are seen as a means of reducing these issues, and will be required to ensure the reliability and safe operation of electricity supply [7]. The increasingly difficult task of matching supply with demand can lead to periods of curtailment (where supply exceeds demand) or congestion (where the grid cannot accommodate the energy), forcing the system operator to accept less VRE than it is possible to produce [6]. This is inefficient, although some levels of curtailment may remain even in optimised systems [9].

Storage options exist but display a wide range of technology readiness levels (TRLs) and potentials. The system benefits of storage can be a function of a wide range of important characteristics; ramp up and down times, partial load capabilities, life cycle costs, capacity, leakage, efficiency, geographic suitability, social acceptability, and access to existing infrastructure [10]. Pumped hydroelectric storage for example is mature and reliable but is restricted by geography, especially in Europe [11]. Other technologies such as compressed air energy storage, batteries, and flywheels, among others, have

2

been mooted as potential storage mechanisms in future electricity networks but none have emerged as an obvious front runner [12].

Power-to-Gas (PtG) is another potential energy storage solution, one that does not require favourable geography. Certain configurations also require relatively little infrastructural change. It is an emerging technology that converts electricity to hydrogen (H₂) by splitting water into its constituent parts via electrolysis. The hydrogen produced can be used as an alternative fuel or as a feedstock in chemical reactions, including synthesising other gaseous (methane and ammonia) and liquid fuels (methanol, dimethyl ether, hydrotreated vegetable oil, and Fischer-Tropsch diesel) [13,14]. The production of hydrogen is the key starting point or first step in each of these processes, and the sustainability of each largely depends on the source of hydrogen. This work focuses on PtG in terms of hydrogen and methane (CH₄), although the insights also apply to the vectors mentioned above.

PtG has been proposed as a means of not only storing excess electricity as a flexible energy carrier, but of adding stability to the grid, and as an alternative to excessive grid expansion [15,16]. These so-called ancillary services may attract a fee and reduce the necessity to "turn off" electricity power plants or "spill" renewable electricity [17]. Converting electrical energy to chemical energy (gas) allows for high capacity storage of difficult to manage energy, potentially through current gas grid infrastructure [18]. In this way it could help to decarbonise existing industry and heavy goods transport demand [19]. Given the advancements in VRE, and the advantages above, interest in PtG has grown.

Hydrogen may be used directly, or even injected into the natural gas grid but it is subject to strict limits [20]. Therefore, conversion to methane may be advantageous as to a large extent it avoids these limits. Unlike hydrogen, there is also a substantial established demand for methane. The Sabatier process is the exothermic reaction of hydrogen with carbon dioxide to produce methane. The reaction works with any sufficiently clean source of carbon dioxide though as it is renewable, biogas (mixture of CH₄ and CO₂ produced by decaying biological material) is a promising source of carbon dioxide. In this way PtG acts as an upgrading solution, offsetting the need for traditional scrubbing of the biogas [21].

The aforementioned renewable energy targets, cap on first generation biofuels, and lack of alternatives make the fuel produced highly suitable for use in the transport sector. Either directly as hydrogen, or injected to the natural gas grid as methane, gaseous fuel from PtG could be used as an advanced fuel in the difficult to decarbonise haulage sector [22]. In conjunction with guarantees of origin PtG could provide the required emissions reduction as compared to the fossil fuel displaced required by the recast RED [4]. Hydrogen fuel cell vehicles are developing quickly and are a promising future low carbon transport option, while natural gas vehicles are already increasingly replacing diesel [23].

In synthesis Power-to-Gas (PtG) converts electricity to hydrogen via electrolysis of water and provides the option of additionally upgrading biogas to biomethane [21]. Operating ideally, PtG facilitates higher shares of indigenous VRE by functioning as a means of grid balancing and energy storage [24], offsetting the need for energy imports and abating GHG emissions [17]. The end product is suitable as a heavy goods transport fuel to allow emissions reductions that are otherwise difficult to achieve. While we know this is technically feasible, what remains to be seen is if it is possible to do so economically, and to what extent the potential GHG savings can be realised.

1.2 Rationale for the thesis

With PtG mooted as a solution to balance increasing VRE production, provide energy storage and address difficult to decarbonise areas, among other benefits, this thesis investigates the economics, sustainability, and potential for the technology. The research within aims to provide information that could accelerate the uptake of PtG. The common thread in this thesis is the potential of PtG in future energy systems as a means of decarbonising heavy goods transport and meeting renewable energy targets.

1.3 Objectives

The objectives of this thesis developed throughout its preparation, adapting to new information and taking into account the results from preceding objectives or new studies. From the outset though the aim was to reduce the uncertainty in the financial modelling of PtG, identify opportunities and barriers to its implementation, and to provide information appropriate to industry and policymakers.

High level objectives are to:

- Develop a model of PtG costs and the breakdown of such.
- Identify and address areas where improvements would be most beneficial.
- Develop optimisation strategies for cost and sustainability.
- Evaluate interest in, and potential applications for, deployment of the technology.

Detailed objectives are included in chapters 3 to 6 but can be summarised as:

- Create a bespoke model that calculates the levelised cost of energy (LCOE)² from PtG systems for a range of inputs, scenarios, and time periods.
- Assess the most appropriate PtG technologies (electrolysis and methanation).
- Identify relationships between PtG system value and various internal and external parameters through sensitivity and cost composition analysis.
- Examine electricity market data for trends that will affect PtG viability, such as operating on otherwise curtailed electricity, or the relationship with VRE.

² LCOE is a commonly used metric that allows comparison between energy sources and vectors, if the reader is unfamiliar with LCOE they should familiarise themselves before reading this thesis however, several notes and explanations have been included.

- Identify the electricity purchase strategies that minimise the LCOE of PtG or maximise its environmental benefits, and their effect on curtailment.
- Investigate valorising PtG services or identify a potential investor.
- Derive insights suitable for industry and policymakers on potential benefits and incentivisation of PtG.

1.4 Outline and link between chapters

The thesis consists of 8 chapters with the appendices and references inserted at the end of the associated chapter. It follows the academic paper model, also known as PhD by publications, whereby a number of published (and/or under review) journal articles which can be read independently or as a whole, are brought together to form a thesis.

Chapter 1 introduces the topic, providing sufficient background for the reader to proceed to chapter 2, a literature review. Chapters 3 to 6 are original works of research, and chapter 7 is a short synthesis of co-authored works relevant to the thesis, each produced over the research period. Chapters 3 to 6, appear as per the published (or under review) manuscripts with some minor modifications to harmonise abbreviations, reduce repetition, and improve the reading experience. Each chapter builds upon the previous in terms of identifying remaining research questions and exploring solutions. The thesis is held together by the theme of producing renewable fuels from electricity either as a finished product or as a necessary step in synthesising other higher hydrocarbons or alternative energy carriers. There is a self-contained bibliography for each chapter.

A summary of the rationale of chapters 2 to 7 is given below, revealing the link between chapters and the evolution of ideas throughout the research:

Chapter 2: Literature review

As PtG touches on many issues, chapter 2 contains a wide-ranging literature review. It includes reviews of policy, technology, and PtG benefits and

drawbacks. Concepts that are not studied in detail in the thesis, but that act to guide research questions and are vital in understanding the potential future role of PtG are outlined. The PtG concept has been mooted for a number of years, but the rate of publication on detailed systems analysis has increased over the duration of this thesis. As such a significant number of works have been published after the papers were published. The more recent articles will be referenced within the introduction and brief literature review of the chapters to which they apply, along with the more detailed insights from literature required for that particular work.

Chapter 3: Modelling of a power-to-gas system to predict the levelised cost of energy of an advanced renewable gaseous transport fuel.

This study uses a discounted cash flow model to determine the LCOE of PtG with methanation for various cost scenarios in 2020, 2030, and 2040. The composition and sensitivity of these costs are investigated as well as the effects of incentives and supplementary incomes. The aim was to reduce the large uncertainty in levelised costs that exists in the literature and identify the key drivers of the LCOE. This work was required to provide a platform from which other works could develop and to inform further investigations.

Chapter 4: The effect of electricity markets, and renewable electricity penetration, on the levelised cost of energy of an advanced electro-fuel system incorporating carbon capture and utilisation

Electricity purchase proved to have a key influence on LCOE. It is also an area with much room for optimisation. The relationships between electricity bid price, the average cost of electricity, and capacity factor (run hours) were established. How these relationships changed with VRE penetration and the effect on LCOE of PtG with methanation was evaluated. Three models; 2016 at 25% renewable electricity penetration and 2030 at both 40% and 60% penetration levels were tested with the aim of minimising the LCOE in each

case. This study also sought to evaluate the viability of PtG based on otherwise curtailed or difficult to manage energy alone.

Chapter 5: Are electrofuels a sustainable transport fuel? Analysis of the effect of controls on carbon, curtailment, and cost of hydrogen.

The previous chapters demonstrated that high run hours were essential to produce competitive PtG but could lead to periods of consuming high carbon intensity electricity, sacrificing optimum sustainability for economic improvements. VRE intermittency leads to variations in price, carbon intensity, and curtailment over time. Therefore, two electricity purchase controls that aim to increase sustainability in advance of a fully decarbonised electricity system, without requiring policy changes were tested in models of 40% to 60% VRE. (1) Set a maximum price the plant will pay for electricity in order to avoid consumption during peak demand. (2) Dictate that the plant may only run above a minimum forecast VRE production to reduce carbon emissions.

Chapter 6: Hydrogen from offshore wind: Investor perspective on the profitability of a hybrid system including for curtailment

This chapter investigated combining an investment in PtG with offshore wind to try and reduce issues of curtailment. This concept would ensure a truly renewable gas and decrease pressure on the electricity network by directly connecting to the electricity source. To access investor interest in PtG, as measured by changes to the project net present value, two scenarios are compared to selling electricity alone. (1) Converting all of the power produced to hydrogen, and (2) a hybrid system of exporting high value electricity to the grid and producing hydrogen from low value electricity. Various levels of curtailment, hydrogen values, and investment costs are considered. Modelling was achieved using historic wind speed data, and simulated models of hourly electricity price and system load.

Chapter 7: Summary of insights from co-authored work

The author contributed to three additional articles during their PhD degree, included to demonstrate the additional knowledge required to make the detailed conclusions found in Chapter 8.

Chapter 7.1: The potential of power to gas to provide green gas utilising existing CO₂ sources from industries, distilleries and wastewater treatment facilities

Potential sources of carbon dioxide are assessed for their suitability to the PtG process using multi criteria decision analysis.

Chapter 7.2: Cascading biomethane energy systems for sustainable green gas production in a circular economy

The potential role of PtG in the wider renewable gas system is explored, including integration with biogas upgrading and improved gasification.

Chapter 7.3: Modelling power-to-X applications in the Nord Pool electricity market: Effects of different bidding strategies on plant performance

A model of the electricity market is built using Neural Networks and two bidding strategies are tested aiming to deliver hydrogen at a minimum cost or to customer demand. Various aspects of the configuration are examined.

Chapter 8: Conclusions

The thesis ends with a chapter that aims to summarise the findings of the previous chapters and provide detailed conclusions on many issues. These

insights are suitable to industry and policymakers as the results are contextualised and some key debates within PtG are commented upon.

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2 Literature Review

Chapters 3 to 6 also each contain a brief contemporary review of literature relevant to the specific topic within the introduction, such that the reader is able to follow the methodologies without extensively referring back to this chapter. As this thesis was conducted over three years, included in these reviews are additional literature specifically relevant to that chapter, which have been published since this work began. In this way the thesis as a whole reflects the progression in the state of the art.

The aim here is to detail the motivation, various technologies, technical constraints, potential role, and areas of interest with respect to Power-to-Gas (PtG). The concept is expanded upon and sufficient information is provided to follow the remainder of the thesis.

2.1 The Power-to-Gas concept in brief

Many future low carbon or net-zero emissions systems significantly feature in the conversion of electricity to hydrogen via electrolysis (PtG) [1–3]. It has been proposed as a means of storing excess electricity [4], adding stability to the grid [5], as an alternative to grid expansion [6], and most widely to produce a substitute for fossil fuels [7].

The technology does not require favourable geography [4] and can offer high storage capacity and discharge times, especially if injected in to the natural gas grid [8].

Operating ideally, it may help to balance intermittent renewable electricity however, as a means of storing and re-generating electricity, it currently suffers from low efficiency and high cost compared to alternatives [9]. Focus on advanced transport fuels or using hydrogen as a low carbon chemical feedstock may be preferable.

Besides hydrogen and subsequent upgrading to methane, PtG is the key enabling technology behind alternative energy carriers such as ammonia, dimethyl ether, and methanol. The hydrogen requirement of the FischerTropsch process and hydrotreated vegetable oil may also be satisfied this way. These products are often collectively termed PtX, electrofuels, or advanced fuels [10]. Insights from this work are applicable to each. The hydrogen pathways are varied but they all rely on sustainably producing significant volumes of hydrogen.

Herein, this work focuses on PtG in terms of hydrogen (as a proxy for all PtX) and methane (as the incumbent fuel) and their near future applications.

2.2 Power-to-Gas policy

PtG policy is examined from an Irish and European perspective. Europe is leading the development and deployment of the technology [11] and has made significant effort to legislate for its use. The European Union's (EU) Renewable Energy Directive (RED), which dictates much of the renewable energy policy, has changed significantly between 2009 and today (September 2019); successive recasts of the Directive have addressed the potential of PtG.

2.2.1 Policy goals

PtG is included in the directive using the term gaseous fuel from non-biological origins. The RED recognises its ability to aid grid balancing while providing low carbon transport options where fossil fuels is difficult to displace. It is also promoted to diversify the fuel mix, due to its low land use change, and its waste to energy/circular economy characteristics. Specific attention has been paid to ensuring only renewable or difficult to manage electricity is converted (see section 2.2.2.1).

Successful implementation of PtG could leverage advances in decarbonised electricity in providing benefits to the heat, and to a greater extent the transport sector above and beyond electric vehicles (EVs). PtG acts at the interface of electricity storage, transport, and gas policy and therefore is particularly reliant on coherent policy.

More generally, the RED is a top down approach to integrating renewables. It provides relatively technology neutral high-level targets updated to reflect changes in technology, markets, and knowledge. It recognises that strategic decisions are required in order to accelerate the energy transition. Where markets are addressed it is to allow smoother cross sector/border trading of renewables such as through the guarantees of origin scheme whereby a consumer can show the energy they used was produced from renewable sources via traded certificates [12].

2.2.2 Targets and rules

The RED includes a binding target of cutting total emissions in 2030 by at least 40% compared to 1990, and a separate target of increasing renewable energy to 32%. Within this transport fuel suppliers are obliged to ensure that renewable energy holds at least a 14% share of energy in transport by 2030 in each member state. Traditional, "first generation" biofuels such as corn ethanol are capped at a 7% contribution as they compete for land with food; therefore, more innovative advanced fuels are required.

A sub target of 3.5% advanced biofuels by 2030 is also stipulated, however member states may exempt suppliers should they instead produce electricity for transport or renewable liquid and gaseous transport fuels of non-biological origin, such as PtG. Therefore, suppliers must choose to either use PtX (hydrogen as a finished product or as a feedstock for electrofuels), or produce advanced biofuels (from feedstock listed in Part A of Annex IX) in order to meet EU targets [13].

Minimum greenhouse gas emissions (GHGs) savings, which are calculated against Fossil Fuel Comparators (FFCs) of 94 and 80gCO_{2eq}/MJ for transport and heat respectively, are required to be deemed sustainable and to count towards a member state's targets as a renewable fuel. The wording and less stringent targets of the RED imply that where options are suitable to both heat and transport, transport should be preferred owing to the relative lack of affordable alternatives.

2.2.2.1 Using electricity in producing fuels

The minimum GHG savings from the use of PtG (hydrogen) is 70% from 1 January 2021. This can be achieved by direct connection to a renewable electricity source, or through grid connection and the trading of guarantees of origin for the electricity consumed. When standard grid electricity is consumed, one must use the average value of renewables on the grid from two years previous in calculating GHG savings, as is the case with EVs. Therefore, PtG would only be renewable in an electricity grid with an excess of 70% renewables; cognisance of hydrogen conversion efficiency must be included in the assessment of hydrogen GHG savings. Future iterations of the RED aim to include PtG used to alleviate electricity grid congestion as fully renewable, and implement "temporal and geographical correlation" between production and consumption with fuel suppliers "adding to the renewable deployment or to the financing of renewable energy" [13].

2.2.2.2 Recycled carbon fuels

The rules and targets with respect to recycled carbon fuels (PtG methane) can be complex. Confusion exists as no minimum GHG savings applies yet (due in 2021), and there is no credit for using biogenic or external sources of carbon. Thus, one must assume that when calculating the GHG savings the process emissions are a function of the electricity consumed in producing hydrogen plus any other sources of emissions. Within the RED, member states are not obliged to include renewable PtG methane where the carbon dioxide source comes from fossil fuels, presumably to discourage all use of fossil fuels [13].

A minimum GHG saving of 65% is required for biogas or bioliquids in transport from 1 January 2021. When upgrading biogas using PtG, the carbon produced in hydrogen generation plus the carbon emitted in biogas production (fertilising, harvesting, processing) form the total emissions. Again, no credit applies for utilising the carbon dioxide content of biogas but a sufficiently low carbon hydrogen source would increase the GHG savings of biogas per unit of energy produced (see section 2.5).

Gaseous fuel from PtG, injected to the natural gas grid, could be used in natural gas vehicles and in conjunction with guarantees of origin provide the

required GHG saving (65% with biogas, 70% with fossil carbon). GHG emissions associated with hydrogen production remains the key issue [13].

2.3 Electrolysis

Electrolysis is a mature technology with commercial electrolysers available, but with high investment and operating costs. The relative low-cost of the steam reforming of natural gas mean it only accounts for a small proportion of the world's hydrogen production [14]. However, "green" hydrogen from renewable electricity may feature in future decarbonised energy systems. Electrolysis is common to all PtG applications as it allows for the conversion of electrical energy and water, into hydrogen and oxygen, as in Equation 2.1.

$$2H_2O \xrightarrow{\text{yields}} 2H_2 + O_2 \tag{2.1}$$

Hydrogen production occurs in the electrolysis cells. Though it may vary slightly depending on the technology, cells generally contain water, electrodes, and an electrolyte material crossed by an electric current. Hydrogen and oxygen are produced separately, at the cathode and anode respectively. The electrolyte material ensures the transfer of ions from one section (typically referred to as a cell) to the other, which are separated by a membrane. The cell size is limited by the ability of the membrane to withstand the electric current [9]. Electrolysis cells are therefore piled into stacks that make up the core of an electrolyser and hence are somewhat modular [15]. Each unit also contains a water pump and cooling system, electrical auxiliaries, hydrogen purification, and instrumentation. The removal of impurities damaging to the electrolysis cells can be achieved either by systems within the unit or by a centralised system and distributed to each electrolyser. More thorough descriptions of the process can be found in past literature [16,17].

2.3.1 Technologies

Although this work is more techno-economic and systems modelling based, it is necessary to know the characteristics and technical limitations of the available electrolysis technologies. The three technologies examined represent the most suitable electrolysis systems for PtG now, in the medium term, and in the future. Individual chapters outline the specifications used for that particular model.

2.3.1.1 Alkaline electrolysis (AEL)

AEL remains the most developed electrolysis technology suitable for large scale PtG applications with several manufacturers positioning themselves as potential providers for the PtG market [15]. AEL operates at 70-90°C, and at atmospheric or elevated pressures using a 20-40 wt% aqueous alkaline solution (NaOH or KOH) as the electrolyte to transfer electrons through hydroxide anions as needed to dissociate the water. Depending on the scale and operating conditions the efficiency of AEL varies between 66 and 74%; the system can operate at loads of 10-150% for limited times at reduced efficiencies, and has a restart time of 10-60 minutes [9]. Hydrogen purity is typically 99.5% [15]. High maintenance costs can potentially occur due to the corrosive nature of the alkaline solutions [18]. Although continuously developing, increases in system performance are likely to be marginal given the existing maturity of AEL. Additional cost reductions can come from market growth (with maximum reduction envisaged at 10 to 20% of the final price). Similar reductions can be assumed in the required capital expenditure due to technical innovations [15,18,19]. A more detailed assessment of the current and future capabilities of AEL has been outlined in past literature, however the state of the art is constantly moving [18].

2.3.1.2 Proton Exchange/Polymer Electrolyte Membrane (PEM)

PEM electrolysis is a more recently developed technology that is currently used in small scale applications in industrial markets. However, PEM electrolyser manufacturers are very active in the development of the technology for PtG applications with demonstration units operating up to 2MW [15,17]. The technology uses proton transfer polymer membranes that act as both the electrolyte and the separation material between the different cells of the electrolysis stack. PEM operates at 60-80°C and is capable of operating at pressures up to 100 bar with newer units expected to far exceed that [20]. The quoted efficiencies for PEM vary between 67 and 82% with future advances beyond this expected [16,18]. PEM electrolysis offers very fast shut down and
start up times from both transient and cold operation, a part load range of 5-100%, and high purity (99.99%) hydrogen [21,22]. Long-term degradation of the cells is a technical barrier to commercialisation of this technology, however improvements are expected [19,23]. The use of platinum group metals may also hinder development due to cost and scarcity.

2.3.1.3 Solid Oxide Electrolysis Cell (SOEC)

Other emerging technologies such as solid oxide electrolysis (SOEL) may be considered in the future [24].

SOEC, also known as high temperature electrolysis, is still at an early stage of development with the investment costs yet to be distinguished and no commitment to producing MW scale units in the medium term. SOEC operates at high temperature (700-800°C) using ceramic materials for both the electrolyte and electrode materials; the high temperature reduces the electrical input required for the water to dissociate. The significant advantage of SOEC technology is its high efficiency (typically 80 to 90%). The high temperatures also limit system flexibility as they are not stable against fluctuating or intermittent power [18]. The biggest challenge to the viability of SOEC is the fast material degradation and limited long term stability of operation [25].

Future integration with an exothermic reaction (for instance, catalytic methanation) would allow for heat recovery to produce steam for the electrolysis stack and could theoretically lead to efficiencies above 100% [26]. However, at present, SOEC is considered to be at a low TRL [9,15].

2.3.1.4 Comparison and suitability to PtG

The choice of technology is multi-dimensional but what is certain is that future system needs to improve if they are to be part of a cost-effective energy transition. To best suit PtG applications electrolysis would dynamically operate over a wide range of partial loads, have high efficiencies and gas purity, with a small footprint and low costs. Research and developments are focused on innovations that will improve flexibility, current density, efficiency, durability, and the output pressure of AEL and/or PEM. Over time, such advancements are expected to deliver improved economic performance [27]. For the periods being analysed (2020-2040) SOEC is considered to be too immature and

therefore modelling its performance would be speculative. Although continued technological improvements may question the dominance of AEL and PEM [27].

Trade-offs between AEL and PEM exist in terms of efficiency, cost, and flexibility. Immaturity means PEM electrolysers currently have higher capital and maintenance costs, a significant short-term benefit to AEL however, further development is expected to reduce investment costs significantly, in line with or below that of AEL [27]. Given the technological improvements being made and the rates at which they are occurring for the respective technologies, for a given specification, a point will be reached where the performance of PEM surpasses AEL. Therefore, becoming the principal technology for PtG systems [17].

PEM has been specially designed for flexible operation which significantly reduces start-up times from cold or warm standby [28], reducing the associated energy penalty and potentially leading to higher annual performances of PtX systems [29]. AEL is a mature technology with limited ability to increase performance [17].

2.4 Utilisation of hydrogen

As a versatile energy carrier and feedstock for many chemical processes, the results of this thesis can be applied to any use of the hydrogen produced [1]. However, the author considers the PtG and back to power route to be too inefficient (maximum ca. 45%), not currently warranting investigation given the advancements in alternative storage technologies [30]. Greater impacts may be seen should the hydrogen be used elsewhere.

2.4.1 Grid injection of hydrogen

A significant advantage of PtG as a form of energy storage is the change of the energy carrier from electricity to gas, allowing for large-scale storage through existing gas grid infrastructure [20]. Though it is possible for hydrogen to be injected directly into the gas grid several issues would arise since the existing natural gas grids were designed for methane [31]. Pipelines used in the natural gas grid have not been designed to withstand the specific properties of hydrogen such as higher permeation and corrosion than natural gas. For safety reasons, hydrogen concentration in the gas grids must be controlled. The amount that can be injected is also limited by gas quality regulations, as hydrogen has approximately one third the volumetric energy content of methane (12 v. 36 MJ/m³) and end users, especially power generation, may be intolerant of this [22,32]. Mass balancing-based certification (akin to electricity guarantees of origin) of the gas would also be complex. In Europe the maximum hydrogen content allowed by national standards for biomethane injection into the grids generally varies from 0.1-10% in volume depending on the country limits up to 20% have been discussed [33,34].

Therefore, power-to-hydrogen for grid injection requires further work to define and standardize the allowable limits and is not feasible in the short-medium term in many regions.

2.4.2 Use in transport or chemicals

With limited alternatives, transport is a particularly difficult sector to achieve emissions reductions in; the EU suggest anything from a potential increase of 20%, to a reduction of 9% in transport emissions by 2030 in their roadmap to a low carbon [35].

As electric vehicles are likely to dominate the private passenger fleet, the best route for PtG in transport is to displace diesel in heavy commercial long distance vehicles, be that as hydrogen or other PtX products [36]. The superior mass/volume compared to batteries, growing restrictions on particulate emissions, and associated proposed bans on diesel powered engines facilitate this [37]. Captive fleets are especially suited to early adoption of PtG where more predictable vehicle usage, stronger influence of policy, and increasing deployment of refuelling infrastructure facilitate its uptake [36,37]. It has been shown that hydrogen fuel cell vehicles can under certain conditions outperform other transport options under multicriteria analysis including efficiency, emissions, and cost [38]. This result is further enforced by the limited potential

of electric or hybrid options (other highest performing fuel options in [38]) for long haul HGVs [39]. The chance to couple the transport and electricity sectors without exacerbating the mismatch of supply and demand is also attractive possibly through the establishment of hydrogen fuelling stations, where it offers high storage capacity and discharge times [20].

Without tighter restrictions or higher costs on emissions, the low market price of fossil fuel derived hydrogen remains a large barrier to implementation in the chemical industry. Fossil hydrogen price varies with scale (volume sold) and purity. Large, medium, and small application scale prices may be €1.5-2.5/kg, €3-4/kg, and above €4/kg respectively [14]. Current literature indicates that those prices are difficult to achieve with PtG even in ambitious scenarios [40].

2.4.3 Hydrogen compression and storage

Once produced hydrogen must be compressed and stored unless it is being injected into the grid. The volume and pressure depend on the source and end use, for example compression up to 500 bar is required for transport applications because of the low volumetric energy density of hydrogen compared with diesel (ca. 3.5kWh/mn³ vs. 10MWh/m³). Storage allows for decoupling of demand and supply, and buffering when the hydrogen is being processed further as the electrolysers are generally operated intermittently [18]. Suitable methods of storage include compressed gas tanks, cryogenic compressed liquid hydrogen tanks, and metal hydride storage [18]. The cost of hydrogen storage is poorly defined but certainly high, and depending on plant setup can make up a significant portion of total capital [41].

2.5 Power-to-Methane

Thanks to the natural gas grid PtG systems (when the vector is methane) have superior capacities and discharge times to other storage options, circumventing the limitations of hydrogen injection. The grid also allows for trading of "green gas" certificates (guarantees of origin) through mass balancing, meaning industry demand for clean energy can be satisfied with the help of existing infrastructure and producers may receive a premium [13].

Methane production is achieved by the reaction between carbon dioxide and hydrogen, via the Sabatier process as described by Equation 2.2.

$$CO_2 + 4H_2 \xrightarrow{\text{yields}} CH_4 + 2H_2O(g) - 164kJ.mol^{-1}$$
 (2.2)

A secondary reaction between carbon monoxide and hydrogen, under the same conditions and catalyst, is also likely to occur due to the decomposition of carbon dioxide as described in Equation 2.3 [42].

$$CO + 3H_2 \xrightarrow{\text{yields}} CH_4 + H_2O(g) - 206kJ.mol^{-1}$$
 (2.3)

Both reactions are highly exothermic. High pressures favour methane production, whilst high temperatures limit it thus, there is potential for the utilisation of waste heat. The reaction is thermodynamically limited to 74% efficiency (LHV: CH₄ (10.494 kWh/m³) / (4 x H₂ (3.543 kWh/m³)).

2.5.1 Source of carbon dioxide

The ideal source of carbon dioxide is biogenic, relatively pure, and located close to the PtG facility, reducing the energy penalty for capture and transport and improving the system GHG balance. However, methanation is capable of utilising any source of carbon dioxide that has been sufficiently scrubbed of impurities and potential catalytic poisons such as chlorine compounds or hydrogen sulphide [18,43]. Several industries generate relatively pure sources of carbon dioxide that could also potentially be used such as distilleries and wastewater treatment plants [44] thus, avoiding the high energy penalty associated with direct air capture or capture from flue gases.

Methanation has also been proposed as an alternative to traditional upgrading of biogas, where rather than separate and release the carbon dioxide content of biogas, it is combined with hydrogen to produce additional methane [45]. This could potentially offset the cost of traditional upgrading with the additional opportunity to utilise the waste heat. It is anticipated that in the periods analysed, biogas systems will become much more prevalent.

2.5.2 Technologies

Two established methods of methanation are possible, biological and catalytic; neither technology can be considered mature in the application to PtG. Comprehensive reviews of both can be found in literature [18] as well as details of ongoing and completed PtG projects [43].

2.5.2.1 Biological methanation

Biological methanation (BM) is a process whereby methane is produced using hydrogenotrophic methanogenic archaea that consume both hydrogen and carbon dioxide. The reaction is anaerobic and takes place in an aqueous solution, at atmospheric pressure, and at temperatures between 20 and 70°C [46]. BM has the potential to be a lower cost option due to simple reactor designs, low pressures, and low temperatures [47]. BM can be in-situ (using the existing methanogenic archaea present in an anaerobic digester) or ex-situ (reaction takes place in an external vessel specifically inoculated with methanogenic archaea). For PtG applications the high gas flow rates, mixing requirements, required purity, and controllability make the ex-situ process more suitable [48].

However, several barriers to higher efficiencies exist for ex-situ BM. The solubility of hydrogen in the reaction medium is greatly hindered by the gasliquid interface. This is addressed by higher mixing rates which increases the parasitic energy load [18,48]. BM is also susceptible to undesirable mixing of unreacted gases with product gases in the reactor (back mixing) and dilution of the reaction medium due to the formation of water in the reaction (washout) (Equations 2.2 and 2.3) [18].

There is no biologically dictated minimum load in terms of hydrogen throughput and immediate load change from 100 to 0% can be made without effecting the process [17]. Effective resumption of BM has been demonstrated after 560 hours of stagnant operation without harmful consequences, indicating high flexibility [17]. However, the practical minimum load (approximately 10%) occurs when the energy required of the stirrers exceeds that of the methane being produced [17]. A high tolerance for impurities and gas composition variation make the coupling of biogas from anaerobic digestion with BM particularly apt [46].

2.5.2.2 Catalytic methanation

Catalytic methanation (CM) is a thermochemical process which takes place at high temperatures (200 - 700°C) and at higher pressures between 1-100 bar. It is a mature technology as applied to the petrochemical industry or gas purification [43]. In large-scale and continuous operations, the most common technology is the adiabatic fixed-bed reactor; smaller scale or intermittent operation (as with PtG) can be achieved with isothermal reactors [47]. The heat released must be controlled to avoid catalyst degradation and maintain a forward reaction and is also the focus of much research [15,18]. Recent experiments using a nickel catalyst have produced conversion efficiencies of 99.06% when reacting at 20 bar, 450°C, and stoichiometric carbon dioxide to hydrogen ratios [49].

Operational flexibility is a key issue with CM as load changes may induce runaway heating or cooling of the reactors, and a complete shutdown requires flushing with an inert gas or hydrogen. A minimum load of 40% or temperature of 200°C to avoid such issues is desired, to prevent the formation of catalytic poisons, and to allow for fast restarts [17,18]. CM requires a high purity feed gas and thus, biogas from anaerobic digestion must be cleaned upstream prior to use [18].

2.5.2.3 Comparison and suitability to PtG

Much faster rates of production are achieved with CM as compared to BM due to the favourable conditions, presence of a catalyst, and absence of a gasliquid mass transfer resistance [43,50]. CM processes also have a lower power requirement per unit of gas produced than that of BM [18].

Process flexibility must also be considered. As the electrolysers can be operated more dynamically than the catalytic methanation reactor there is a need for a minimum volume of hydrogen storage as a buffer, a highly expensive system component [41]. The smaller or less dynamic the catalytic methanation reactor, the larger the required hydrogen storage to ensure a consistent feed of gases [43,46]. CM is far less flexible but cheaper than BM and more susceptible to economies of scale [17]. BM is highly flexible and has no minimum load [18]. Thus, the nature of the hydrogen supply and other gas flows also have a major influence on the choice between BM and CM.

BM is much more tolerant of impurities than CM, where the nickel catalysts may be poisoned over time leading to higher maintenance costs [18], perhaps making it more suited to upgrading biogas from difficult or contaminated feedstocks.

As discussed later, CM provides an opportunity to utilise waste heat, beyond its own thermal demand BM does not [51].

2.5.3 Utilisation of methane

The use of methane is much more common than hydrogen, with vast infrastructure dedicated to its transport and consumption. Methane from PtG is a drop-in fuel that can satisfy the demand for renewable energy options from industry already connected to the natural gas grid. EU law also dictates that alternative transport fuel infrastructure be built and specifically recognises the benefits of renewable and natural gas [37]. Uptake of renewable methane faces much less resistance than hydrogen and its consumption would not require active decisions, similar to blending ethanol and petrol/gasoline.

2.5.3.1 Grid injection of methane

The high selectivity of the methanation process leads to a methane content of approximately 95% in the product gases. The actual figure is dependent on the technology [18]. However, this still results in an energy content less than that of natural gas due to the lack of higher hydrocarbons [18]. In smaller quantities, the gas produced by PtG can be compressed and injected into the transmission grid without issue but in some instances the addition of propane may be required to meet the gas grid specifications, particularly when injecting into the distribution network [15,32]. Customers have been guaranteed a composition within tight limits, such as the Wobbe index, which predicts the

flame height in natural gas burners. Power generation is especially susceptible to change in the composition of natural gas [33].

2.6 Environmental impact and co-products

Several studies have concluded that the majority of the climate impact of PtG can be attributed to the electricity consumed in the electrolysis step [52–54]. Parra et al [55] indicated that electrolysis and its associated energy consumption contribute more than 90% of the potential environmental impacts (climate change, particulate matter, ozone depletion, eutrophication) of PtG with the electricity generation method being the most sensitive parameter. Similar results were found by Collet et al. and Reiter et al. who determined low carbon electricity was mandatory to achieve a sustainable production of PtG [56,57]. As such, reductions in the carbon intensity of the electricity consumed are analogous to reductions in the environmental impact of PtG.

2.6.1 Production of heat

Heat is produced in both the electrolysis and methanation processes and represents an opportunity to improve the GHG balance and economics of several process related to PtG.

Recoverable heat from electrolysis is technology dependent but generally less than 15% of energy input (60% of losses) [51]. Valorisation of this heat depends highly on local conditions, such as access to district heating, as it is low grade heat (less than 80°C). The effect of heat recovery on system economics may be small as the volume and value are low, though if it displaces fossil fuel heating it may have a high impact on GHG savings. It may also provide thermal energy for an anaerobic digester (biogas production) or feed water heating, improving plant efficiency [29].

BM has little opportunity for exportable heat recovery, instead satisfying its own thermal demand to a large extent and possibly that of the anaerobic digester, again improving plant efficiency. On the other hand, up to 80% of heat generated in CM is recoverable [51]. This means that sufficient high grade (greater than 200°C) thermal energy is produced from the cooling circuit to preheat the feed gases, with sufficient energy left to run a steam turbine or use elsewhere; this increases the process efficiency and allows for cost savings [36,48]. An economic alternative use would be to heat the anaerobic digester and to pasteurise the digestate (end product suitable for use as a biofertiliser but which may contain pathogens) [58].

The significant heat demand of amine scrubbers (carbon dioxide removal from gaseous mixtures) can be satisfied in this way too [9]. Effective means of valorising this heat may be the deciding factor in methanation technology choice. Although it is not necessary to include in every analysis, awareness of these opportunities will help to identify niche applications where PtG could thrive.

2.6.2 Utilisation of oxygen

As per Equation 2.1, significant volumes of oxygen are produced during electrolysis and could constitute an additional income if there is an established demand (e.g. medical industry). This value is not proportional to the hydrogen produced though, even at moderate uptake of PtG the market may quickly reach saturation. This means only a portion of the oxygen may be valuable. Therefore, valorisation is highly dependent on local conditions (distance and demand).

That is not to discount potential uses of a pure oxygen stream. Integration or co-location with gasification would reduce costs and increase output syn-gas quality [59]. In wastewater treatment oxygen can greatly reduce the energy consumption and increase effectiveness of the extended aeration process [60].

Should the oxygen displace that produced by conventional methods (e.g. cryogenic or vacuum swing absorption), it may also have an environmental benefit. This benefit can represent an effective increase in electrolysis efficiency of 5% [61] and may mean oxygen from PtG is more attractive to environmentally conscious consumers.

2.7 Electricity supply

The electricity system market structures and regulations were designed around large thermal generation plants and predictable, non-responsive demand patterns [62]. In general, it is accepted that current technical and market structures are only partially capable of efficient integration of variable renewable electricity (VRE) [63]. Wind and solar, will make up the majority of this VRE generation, as they are the current state of the art technologies available at the required scale [3]. From an exergetic perspective electricity should always be deposited as electricity on the grid (highest efficiency). However, as VRE levels continue to increase their intermittency will pose challenges for the grid with regards to balancing, inefficient production, stability, and periods where supply exceeds demand, meaning this is not always preferable or possible. [62,64].

Specifically, the nature of VRE means that net system load (difference between demand and production) may change rapidly. Given this, the speed at which load following units are capable of ramping up/down to compensate must increase and the extent to which they can do this (range between minimum and maximum dispatchable generation required in a day) must also increase. This is known as ramping speed and ramping range [65]. Cross-sectoral technologies such as electric vehicles also affect the demand and supply profile, exacerbating these issues and potentially affecting security of supply [64]. Obviously then, data analytics and demand side management must play a future role in deciding when electric vehicles are charged and likewise when electricity is drawn down to produce hydrogen.

In the short to medium term the energy transition may be smoothed by the use of PtG, allowing the integration of more renewables and joining other currently less well-connected systems such as heat and transport [9]. PtG does not require favourable geography nor perhaps large infrastructural changes in countries with existing gas networks, and can access existing markets [8]. The social acceptability of gas infrastructure is generally high as compared to electrical infrastructure as represented by overhead power lines [9]. The extent to which PtG can offer solutions to these issues is a function of the technology and dependent on the specific problem.

2.7.1 Storage requirements

Increased interconnection is often very cost effective in addressing the challenge, particularly at lower penetrations of VRE [6]. It is a logical and prudent investment for grid managers, though its effectiveness will ultimately be limited by demand profiles [66].

Large scale and flexible energy storage options are seen as a means of reducing the negative effects of VRE [67]. Presently deployed solutions are insufficient should significant dispatch down of VRE be avoided. Storage could represent a serious limit on the expansion of renewables. For those researching future low-carbon energy systems, PtG can mitigate some of the traditional storage requirements and provide a low carbon alternative fuel or feedstock in areas where decarbonisation is difficult [68]. Converting the hydrogen back into electricity is not encouraged due to the low efficiency, in this respect PtG differs from most other storage options. Thus, PtG is most beneficial for times of overproduction, and may not have significant benefits in times of underproduction from VRE in term of grid balancing. Operating ideally, PtG facilitates higher shares of indigenous wind, wave, and solar energy offsetting the need for energy imports and abating GHG emissions [55].

2.7.1.1 Alternative storage options

Thermal storage of electricity is not considered here as its value is highly regionally dependent, whereas storage in the form of electricity and transport vectors are somewhat ubiquitous [67].

Storage of difficult to manage electricity has typically been achieved through pumped hydroelectric storage (PHS) systems. It is a mature technology well known to provide fast power balancing. Currently installed capacities are much less than the anticipated future requirements, and it is limited by geography, especially in Europe [69]. Compressed air energy storage (CAES) requires favourable geography too and so its usefulness is limited. As well as environmental concerns, social acceptance issues plague large storage projects. Other large-scale options which are further from commercialisation include molten salts, superconducting magnetic energy storage (SMES), and flywheels [67].

Batteries are currently expensive, especially at scale, and more especially for long periods of in northern Europe with little wind. Materials and gradual discharge are of concern [30]. They do though offer potentially high efficiencies and solve problems of grid stability by also discharging when VRE production is low, something PtG cannot do. In energy storage terms alone, this may mean they are preferred in many situations for short term storage in the future [30].

2.7.1.2 Curtailment and constraint

Curtailment here is defined as when a generator is asked to produce less than they can or were scheduled to, due to system wide demand being less than production. Constraint is similar but is due to insufficient local grid capacity.

The difference is important as grid expansion greatly alleviates constraint, but does much less to alleviate curtailment [70]. Constraint is also eased by introducing storage or flexible demand behind the congestion point.

In order to avoid significant curtailment, the flexibility solutions of a high VRE electricity system will need to be different from those in today's system. Unlike large scale thermal generators, VRE does not have mechanical inertia. The turbines (rotating mass) of synchronous generators act to smooth out rapid frequency change, by resisting acceleration (positive or negative) caused by a rapid net system load change. Wind and solar, connected to the grid through inverters, do not provide the same resistance [62]. Therefore, a limit to the amount of non-synchronous (i.e. wind and solar) generation in the mix at one time is often used. In Ireland for example, this is known as the System Non-Synchronous Penetration (SNSP) limit, and is given in Equation 2.4 [71].

$$SNSP = \frac{Non-Synchronou\ Generation + Net\ interconnector\ Imports}{System\ demand\ + Net\ Interconnector\ Exports}$$
(2.4)

System demand here includes storage therefore, increased storage such as PtG increases the SNSP limit. As there exists an upper limit of SNSP, curtailment is most likely to occur when wind and solar generation is high relative to system demand. Ireland is currently testing a world leading SNSP of 70%, intending to achieve 75% by 2020.

2.7.2 Electricity markets

Electricity is a commodity that is bought, sold, and traded but by its nature is difficult to store therefore being produced on demand unlike many other commodities that can be easily stocked. Furthermore, supply and demand vary continuously and cannot be perfectly forecast.

An electricity market is a system that enables trading where bids and offers use demand and supply principles to set the price, markets may extend beyond national boundaries or regions may exist with a single country. Wholesale transactions (bids and offers) are typically cleared and settled by the market operator or a special-purpose independent entity, knowledge of the trade must be provided to the transmission system operator (TSO) in order to balance generation and load. Electricity is traded in a variety of markets, but these markets can be broadly broken into fully regulated and partially deregulated.

In general, in a fully regulated market a single entity provides electricity to a region, that is the generation and sale is provided without competition but subject to government regulation. This kind of market is becoming less common and being replaced by markets that encourage competition.

In a partially deregulated market, transmission, distribution, and wholesale trading are generally controlled by state bodies but generation, and supply to the consumer are competitive. The aim is to provide safe, efficient, and affordable electricity. A wholesale electricity market exists when competing generators offer their electricity output to retailers or large independent consumers. Purchasing electricity directly from generators is a relatively recent phenomenon and is mostly commonly associated with "green" energy for large commercial bodies seeking to reduce emissions. For a large user like a PtG plant, wholesale electricity offers the most economical solution, requiring participation in the market. Disadvantages include market uncertainty, membership costs, set up fees, and organisation costs, as electricity would need to be bought regularly, however, the larger the electrical load, the greater the benefit to buying wholesale. Common components of a competitive

deregulated market are day ahead markets where large quantities are traded, intraday markets to satisfy hourly fluctuations, and other markets that offer balancing and frequency control services at a shorter time frame (see 2.7.3).

This work focuses on competitive wholesale markets (common in OECD) while the results are also largely applicable to all open competitive generation markets.

2.7.2.1 System price variability

The system marginal price (SMP) is the hourly or half-hourly wholesale price of electricity. It includes for the cost required to meet the forecast demand and additional costs associated with start-up or operating as a reserve that a generator will need to recover. The SMP is set by the marginal costs of the last generator online to meet demand, primarily done through day-ahead auctions that aim to meet forecast demand at the minimum cost (other mechanisms exist as discussed above). In general, the SMP is lowest when there is more than sufficient generation capacity online to meet demand, and the more expensive generators do not need to run. When the amount of generation online to meet demand is scarce, the resulting SMP is higher, as higher cost generators are called upon [72].

The SMP is influenced by renewable and zero marginal cost generators [73]. Electricity markets seeking to increase the share of VRE may offer them priority dispatch on the electricity grid [13]. Curtailment of VRE is often a last resort in times of excess generation. Therefore, strong positive correlation has been found between increased shares of VRE and the periodic availability of low-cost electricity [74]. Furthermore, with increasing shares of VRE in the energy mix, electricity markets and prices become less predictable. It leads to price volatility as the generation mix changes throughout the days or weeks [75,76], which in turn also means that the carbon intensity of the electricity generated can vary substantially temporally. In particular, sudden and unexpected price peaks and emerging seasonality of prices at daily, weekly and yearly level have been observed [77].

2.7.3.2 Electricity purchase strategy

Much of the focus of PtG research has been on utilising surplus [78] or otherwise curtailed VRE [6,79]. However, the perception that large quantities of low-cost or curtailed electricity will be consistently available is not reflective of electricity market data or market desires [17,48]. Instead it is a resource reflective of inefficiencies that states will aim to minimise over time. Therefore, if significant volumes of gas are to be produced PtG will instead have to purchase electricity from the spot market (or local market mechanism), where large quantities of electricity are traded. Different operational strategies may then have a significant influence on the profitability of PtG and can be controlled by the PtG operator.

2.7.3 Ancillary services

Secure electricity system operation is achieved with a mix of power plants responding to the variable but largely predictable daily, weekly, and seasonal variation in demand. Three types of plants typically meet this demand, known as baseload (constant demand), intermediate load (daily variation in demand), and peaking (peak demand). The same or other power plants also provide operating reserves to meet unforeseen increases in demand, faults with other plants or the grid, and other contingencies. This range of services, many of which can be performed not just by generators, are called ancillary services [65]. This is a simple explanation and not an exhaustive list, in fact as grids expand and VRE increases the range of services sought by transmission system operators also increases [80].

PtG is a highly scalable flexible consumer with significant potential as an alternative to traditional grid expansion or storage. PtG facilities show the potential to provide some of these ancillary services to the grid, enabling further stable integration of VRE into the electricity mix [5]. However, they do not yet directly benefit from this or receive "free" electricity, with some rare exceptions [81,82], though this is the subject of much discussion [9,64,83]. Receiving a fee for these services has been identified as vital in aiding PtG economic viability [9], though the policy changes required make it difficult to

model. Income of this nature is technically feasible but speculative. As an advantage of PtG its importance will grow over time.

2.7.3.1 Frequency control

Electricity system frequency is controlled by the speed of the rotating mass of generators. The ability to respond to small, unpredictable changes to the system load, that in turn alter system frequency, is known as frequency regulation/control [65]. It requires units that can rapidly change output, or in the case of PtG input. AEL is not yet flexible enough to offer this service (new models are being designed with this in mind), but PEM electrolysers have demonstrated an ability to ramp up and down quickly enough to provide frequency control [19,84].

2.7.3.2 Demand side management

Similar to frequency control, PtG demand side management (DSM) would involve turning on and off the system to aid grid balancing, but it is much less time sensitive. DSM has shown great potential to alleviate electricity grid issues and integrate VRE [85,86]. PtG could absorb excess electricity generation and remove the requirement to "turn off" electricity power plants. For example, with day ahead DSM, PtG could be asked to run at times when forecast VRE generation is high, and turn off when it is low, receiving electricity at a discounted rate. This demand elasticity effectively decreases the instantaneous SNSP and increases system flexibility [63].

2.7.3.3 Effects on electricity price

PtG interacting with the electricity market may have benefits for generators and transmission system operators. By creating demand in low-load hours off peak prices increase, and by removing it in high-load hours the cost of balancing at peak demand decreases. For generators this has the potential to offset some of the decreased revenue due to periods of suppressed electricity prices [73]. It does also mean that the more PtG installed, the fewer low-cost or otherwise curtailed units of electricity are available. A study in Ireland found that the profitability of VRE increased when PtG was present [87], opening the possibility of investment by a cooperative of VRE generators.

2.8 Conclusion

PtG has the potential to leverage the successful integration of renewable electricity against our increasing transport emissions. In doing so it may also help to mitigate some of the issues associated with intermittent renewables. Although hydrogen is versatile, its use in transport is still in its infancy, leading to interest in upgrading it to methane to access existing markets. Several business models could be developed that aim to optimise PtG income from various sources, such as a hydrogen filling station simultaneously offering ancillary grid services, or a wind farm seeking to valorise reduce curtailment. PtG therefore sits at the intersection of gas, electricity, and renewable energy policy, and warrants serious investigation in terms of its economic and environmental sustainability and the role it could play in future energy systems.

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3 Modelling a power-to-gas system to predict the levelised cost of energy³

Abstract

Power-to-gas (PtG) has been mooted as a means of producing advanced renewable gaseous transport fuel, whilst providing ancillary services to the electricity grid through decentralised small scale (10MW) energy storage. This study uses a discounted cash flow model to determine the levelised cost of energy (LCOE) of the gaseous fuel from non-biological origin in the form of renewable methane for various cost scenarios in 2020, 2030, and 2040. The composition and sensitivity of these costs are investigated as well as the effects of incentives and supplementary incomes. The LCOE was found to be €107-143/MWh (base value €124) in 2020, €89-121/MWh (base value €105) in 2030, and €81-103/MWh (base value €93) in 2040. The costs were found to be dominated by electricity charges in all scenarios (56%), with the total capital expenditure the next largest contributor (33%). Electricity costs and capacity factor were the most sensitive parameters followed by total capital expenditure, project discount rate, and fixed operation and maintenance. For the 2020 base scenario should electricity be available at zero cost the LCOE would fall from €124/MWh to €55/MWh. Valorisation of the produced oxygen (€0.1/Nm₃ profit) would generate an LCOE of €105/MWh. A payment for ancillary services to the electricity grid of €15/MWe for 8500h p.a would lower the LCOE to €87/MWh. Price parity with diesel, exclusive of sales tax, is achieved with an incentive of €19/MWh.

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3.1 Introduction

The Paris agreement (under COP21) has set a target of limiting the increase in global temperatures to less than 2°C. To facilitate this, an 80% reduction in greenhouse gas (GHG) emissions by 2050 will most likely be required [1,2]. The reduction in GHG emissions will rely on decarbonisation of the energy sector, and a push for sustainable energy solutions to meet increasing energy demand through leverage of existing and future technologies.

As transmission system operators (TSO) aim to facilitate targets set under the Renewable Energy Directive (RED), renewable technologies will be prioritised [3]. The ensuing decarbonisation of the energy system will increase the amount of variable renewable electricity (VRE) on the electricity grid, posing challenges for the grid with regards to balancing, stability, and periods where supply exceeds demand [4,5]. Thus, the storage, flexibility, and balancing capabilities will need to increase with increased installed capacity of VRE, to ensure the reliability and safe operation of electricity supply [6,7]. Large scale and flexible energy storage options are seen as a means of reducing curtailment, inefficient production, and protecting security of supply [8].

Storage of otherwise curtailed electricity has typically been achieved through pumped hydroelectric storage (PHS) systems, a mature technology but one that is restricted by geography [9]. Other technologies such as compressed air energy storage and battery storage have also been mooted as important storage mechanisms in future electricity networks. Power-to-Gas (PtG) is an emerging technology that can utilise otherwise curtailed electricity and convert it to hydrogen (H₂) via electrolysis of water. The hydrogen can then be further combined with carbon dioxide (CO₂) to produce methane (CH₄) via a Sabatier reaction. The ability of PtG to absorb excess electricity and remove the requirement to "turn off" electricity power plants or "spill" renewable electricity facilitates VRE and allows for the provision of ancillary services [10,11]. It has been proposed as a means of storing excess electricity, adding stability to the electricity grid, an alternative to excessive grid expansion, and producing a substitute for natural gas [12–14]. Operating ideally, PtG facilitates higher shares of indigenous wind, wave, and solar energy offsetting the need for

energy imports and abating GHG emissions [8,11]. A significant advantage of PtG as a form of energy storage is the change of the energy carrier from electricity to gas (either H₂ or CH₄), potentially allowing for large-scale storage through existing gas grid infrastructure [6].

PtG systems (when the vector is methane) have superior storage capacities and discharge times to that of PHS through use of the natural gas grid [15]. For instance, the French national gas grid alone has a capacity of over 100TWh [16]. PtG does not require favourable geography nor large infrastructural changes in countries with existing gas networks [17]. Notable exceptions include the coupling of existing underground natural gas storage facilities with PtG to create Underground Storage of Hydrogen and Natural Gas (UHNG). In cases such as this, when the favourable geography exists it is taken advantage of [18]. Gaseous fuel from non-biological origin produced by PtG is designated as an advanced third-generation biofuel; such advanced biofuels are heavily promoted within the EU framework due to their low land use change, potentially low carbon intensity, and waste to energy/circular economy characteristics. Transport fuel suppliers are obliged to provide an increasing share of advanced renewable transport (excluding first generation biofuels from food crops), rising from 1.5% in 2021 to 6.8% in 2030. At least 3.6% of this must be from advanced biofuels (including gaseous fuel from non-biological origin) [3]. Gaseous fuel from PtG, injected to the natural gas grid, could thus be used as an advanced transport fuel in natural gas vehicles (NGVs) and in conjunction with guarantees of origin provide the required 70% emissions reduction as compared to the fossil fuel displaced (required by the RED and proposed amendments to ensure sustainability of biofuels beyond 2021) [19-21].

The state of the art in LCOE (Levelised Cost of Energy) of PtG (methane) systems may be viewed in Table 3.1. A number of technology reviews of PtG with respect to working principles, relative advantages and disadvantages, and trends in technology have been provided in past literature [10,22,23]; estimates of system costs have also been detailed [10,22,24–27]. However, much uncertainty still remains with cost estimates varying substantially [6,23,24,26,28,29] from €75 to €600/MWh CH₄. It is the view of the authors' that anticipated cost reductions in the literature have not materialised to the

extent predicted. The concept that electricity that would have been curtailed being available at a low-cost is not reflective of current electricity market data [22,30]. The innovation in this paper is that it advances upon previous cost estimates using a discounted cash flow model of the lifetime of a plant which accounts for maintenance costs and frequency,

commissioning/decommissioning, fixed and variable operational expenditure and maintenance (OPEX), and real-world electricity market data. It also uses a plant lifecycle that optimises the replacement schedule of the components and the latest cost estimates for these.

Table 3.1:	State of the art in LCOE	of PtG systems
		-

LCOE	Assumptions (Year of reference)	Run hours	Electricity	Ref
(€/MWh _{CH4})		(p.a.)	cost	
			(€/MWh)	
600	Integration with a lignite power plant. 80MW _e input. (2012)	1200	N/A	[31]
190 – 316	Heat and O ₂ utilisation not included. (2014)	3000	25	[16]
132 – 245	Biological methanation as novel upgrading. Compression and grid injection (2016)	N/A	50	[32]
141 – 236	Heat and O ₂ utilisation not included. (2013)	8600	45	[22]
210	Coupled with 5 MW biogas production. No heat or O ₂ valorisation. (2014)	3000	50	[30]
185	10MW _e input. Tax free electricity. Compression and injection included. (2015)	7800	60	[25]
170	10MW _e input. Tax free electricity. Compression and injection included. (2015)	8600	40	[25]
143 – 150	PtG upgrading, biological methanation with and without prior CO ₂ separation. (2016)	7920	100	[33]
92 - 113	Heat and O_2 utilisation not included. (2050)	3000	25	[16]
95	10MW _e input. Tax free electricity. Compression and injection included. (2015)	6100	15	[25]
75	Revenue of €10/tonne O₂ included. (2015)	5000	50	[24]

The objectives of the paper are to:

- Assess the most appropriate technologies (electrolysis and methanation), and their associated specifications for use in a PtG system.
- Create a bespoke model that calculates the levelised cost of energy (LCOE) for PtG systems for a range of inputs, scenarios, and time periods.
- Investigate the relationships between various parameters and system LCOE through sensitivity analysis and examination of the cost composition of these.
- Calculate the required incentives to reach price parity with diesel as a transport fuel, and the effect sale of oxygen (produced through electrolysis) or grid services may have on LCOE.

3.1 Methodology

3.1.1 The Power-to-Gas (PtG) system

In this study, PtG is defined as the combination of electrolysis, to produce hydrogen, and methanation, to generate methane (by reacting CO₂ with hydrogen). In the envisaged system, the methane could be compressed and injected into the natural gas grid. It was also considered that the operation of the PtG plant may require temporary storage of hydrogen. Estimates for the variables outlined in Figure 3.1 and used in the model are based upon an extensive literature review and are referenced appropriately. Where several estimates existed, or there were large differences in the quoted values, average figures were calculated and used. Similarly, where estimates were found for time periods outside of those being investigated, figures were extrapolated backward or forward. It is postulated that this method of avoiding the use of a single set of figures minimises the risk of over or under accounting for costs specific to one piece of research, and allows for more accurate approximations of component costs and performance. Values in currency other than Euro were converted using a currency converter [34] and corrected to

2016 euros using inflation calculators [35,36]; as such the results are reported as 2016 Euro.



BoP (Balance of plant); OPEX (operational cost); CAPEX (cost of capital) Replace (replacement of components during plant life). Calculation of Land Capital cost (Equation 3.5) is detailed in Appendix 3.1.

Figure 3.1: Inputs and variables included in the model to calculate the LCOE of the produced gaseous fuel.

3.1.1.1 Electrolysis

Electrolysis is the key enabling technology for PtG. It is a mature technology with commercial electrolysers available on the market. Electrolysis allows for the conversion of electrical energy and water, into hydrogen and oxygen (O₂), as in Equation 3.1.

$$2H_20 \xrightarrow{\text{yields}} 2H_2 + O_2 \tag{3.1}$$

Hydrogen production generally occurs in the electrolysis cells with each cell usually containing water, electrodes, and an electrolyte material crossed by an electric current. Hydrogen and oxygen are produced separately, at the cathode and anode respectively. The electrolyte material ensures the transfer of ions from one section (typically referred to as a cell) to the other, which are separated by a membrane. The cell size is limited by the ability of the membrane to withstand the electric current. Electrolysis cells are therefore piled into stacks that make up the core of an electrolyser and hence are somewhat modular [25]. Each unit also contains a water pump and cooling system, electrical auxiliaries, hydrogen purification, and instrumentation. The removal of impurities damaging to the electrolysis cells can be achieved either by systems within the unit or by a centralised system and distributed to each electrolyser. More thorough descriptions of the process can be found in past literature [22,37–40].

Electrolysis only accounts for a small proportion of the world's hydrogen production due to the associated high investment and operating costs, and relative low-cost of the steam reforming of natural gas [38]. However, for future decarbonised energy systems "green" hydrogen from "surplus" renewable electricity is required for sustainability. The three technologies examined further in this paper are alkaline electrolysis cells (AEL), proton exchange membrane (PEM) electrolysis, and solid oxide electrolysis cells (SOEC). They represent the most suitable electrolysis systems for PtG now and in the future.

3.1.1.2 Alkaline electrolysis cells (AEL)

As of 2015, AEL was the state-of-the-art electrolyser and the only available electrolysis technology suitable for large scale PtG applications with several manufacturers positioning themselves as potential providers for the PtG market [25]. AEL can operate at atmospheric or elevated pressures and uses an aqueous alkaline solution (NaOH or KOH) as the electrolyte to transfer electrons through hydroxide anions as needed to dissociate the water. Depending on the scale and operating conditions the efficiency of AEL varies between 66 and 74%; the system can operate at loads of 10-150% for limited times, and has a restart time of 10-60 minutes [25,29]. High maintenance costs can potentially occur due to the corrosive nature of the alkaline solutions [10]. Although continuously developing, increases in system performance are likely to be marginal given the existing maturity of AEL. Additional cost reductions can come from market growth (with maximum reduction envisaged at 10 to 20 % of the final price). Similar reductions can be assumed in the required capital expenditure (CAPEX) due to technical innovations [7,10,25]. A more detailed assessment of the current and future capabilities of AEL has been outlined in past literature [7,10].

3.1.1.3 Proton exchange membrane (PEM)

PEM electrolysis is a more recently developed technology that is currently used in small scale applications in industrial markets. However, PEM electrolyser manufacturers are very active in the development of the technology for PtG applications with demonstration units operating up to 2MW [7,22,25,30]. The technology uses proton transfer polymer membranes that act as both the electrolyte and the separation material between the different cells of the electrolysis stack. PEM can operate at atmospheric pressure, and is also capable of operating at higher pressures than AEL [6]. The quoted efficiencies for PEM vary between 67 and 82% with future advances beyond this expected [7,29]. In terms of suitability to PtG, PEM electrolysis offers very fast shut down and start up times from both transient and cold operation, a part load range of 5-100%, and higher purity hydrogen [41,42]. Long-term degradation of the cells is a technical barrier to commercialisation of this technology, however improvements are expected [7,29].

In the choice between PEM and AEL electrolysers there exists a trade-off between system efficiency and cost. Given the technological improvements being made and the rates at which they are occurring for the respective technologies, for a given specification, a point will be reached where the performance of PEM surpasses AEL. PEM electrolysers currently have higher CAPEX than AEL due to lower technology readiness level (TRL). However, further development of the technology is expected to reduce investment costs significantly, to below that of AEL. It is also expected that PEM will soon technically outperform AEL and thus become the more dominant technology for PtG systems [6,7,30].

3.1.1.4 Solid oxide electrolysis cells (SOEC)

SOEC, also known as high temperature electrolysis, is considered a future electrolysis technology for PtG systems. It is still at an early stage of development with the investment costs yet to be distinguished. No commitment to producing MW scale units in the medium term has been made [22,25]. SOEC operates at high temperature (700-800°C) using ceramic materials for both the electrolyte and electrode materials; the high temperature reduces the electrical input required for the water to dissociate. The significant advantage of

SOEC technology is its high efficiency (typically 80 to 90%). The high temperatures also limit the systems flexibility as they are not stable against fluctuating or intermittent power [10,43]. The biggest challenge to the viability of SOEC is the fast material degradation and limited long term stability of operation [44].

Future integration with an exothermic reaction (for instance, catalytic methanation) would allow for heat recovery to produce steam for the electrolysis stack and could theoretically lead to efficiencies above 100% [43]. However, at present, SOEC is considered to be at a low TRL [16,25,45].

3.1.2 Methanation

The methanation phase for PtG refers to the reaction between carbon dioxide (CO₂) and hydrogen, in a Sabatier process as described by Equation 3.2.

$$CO_2 + 4H_2 \xrightarrow{\text{yields}} CH_4 + 2H_2O(g) - 164kJ.mol^{-1}$$
 (3.2)

A secondary reaction between carbon monoxide and hydrogen is also likely to occur due to its presence in the feed gases and the decomposition of CO₂. This reaction is described in equation 3 and will occur under the same conditions and in the presence of the same catalyst as in Equation 3.2 [46].

$$CO + 3H_2 \xrightarrow{\text{yields}} CH_4 + H_2O(g) - 206kJ.mol^{-1}$$
 (3.3)

The equilibrium of the reaction is influenced by pressure and temperature. In thermodynamic equilibrium, high pressures favour the production of CH₄ whilst high temperatures limits production.

The reaction is thermodynamically limited to 74% efficiency (LHV: CH₄ (10.494 kWh/m³) / (4 x H₂(3.543 kWh/m³)) and is highly exothermic; thus there is potential for the utilisation of waste heat.

Two established methods of methanation are possible, biological and catalytic; neither technology can be considered mature in the application to PtG. Comprehensive reviews of both can be found in literature [10] as well as details of ongoing and completed PtG projects [47]. Other innovative upgrading techniques have also been explored and show significant potential future alternatives [48].

3.1.2.1 Biological methanation

Biological methanation (BM) is a process whereby CH₄ is produced using hydrogenotrophic methanogenic archaea that consume both hydrogen and CO₂ [49]. The reaction is anaerobic and takes place in an aqueous solution, at atmospheric pressure, and at temperatures between 20 and 70 °C [25,47]. BM has the potential to be a lower cost option due to simple reactor designs, low pressures, and low temperatures [16,33]. BM can be in-situ (using the existing methanogenic archaea present in an anaerobic digester) or ex-situ (reaction takes place in an external vessel specifically inoculated with methanogenic archaea). For PtG applications the high gas flow rates, mixing requirements, required purity, and controllability make the ex-situ process more suitable [22].

However, several barriers to higher efficiencies exist for ex-situ BM. The solubility of hydrogen in the reaction medium is greatly hindered by the gasliquid interface. This is addressed by higher mixing rates which increases the parasitic energy load [10,22]. BM is also susceptible to undesirable mixing of unreacted gases with product gases in the reactor (back mixing) and dilution of the reaction medium due to the formation of water in the reaction (washout) (Eq. 2 and 3) [10].

There is no biologically dictated minimum load in terms of hydrogen throughput and immediate load change from 100 to 0% can be made without effecting the process [30]. Effective resumption of BM has been demonstrated after 560 hours of stagnant operation without harmful consequences, indicating high flexibility [30]. However, the practical minimum load (approximately 10%) occurs when the energy required of the stirrers exceeds that of the CH₄ being produced [30]. A high tolerance for impurities and gas composition variation make the coupling of biogas from anaerobic digestion with BM particularly apt [23].

3.1.2.2 Catalytic methanation

Catalytic methanation (CM) is a thermochemical process which takes place at high temperatures (200 - 700°C) and at higher pressures between 1-100 bar
[8,50]. In large-scale and continuous operations, the most common technology is the adiabatic fixed-bed reactor; smaller scale or intermittent operation (as with PtG) can be achieved with isothermal reactors [16]. The heat released must be controlled to avoid catalyst degradation and maintain a forward reaction and is also the focus of much research [10,25]. Recent experiments using a nickel catalyst have produced conversion efficiencies of 99.06% when reacting at 20 bar, 450°C, and stoichiometric CO_2/H_2 ratios [50].

Operational flexibility is a key issue with CM as load changes may induce runaway heating or cooling of the reactors, and a complete shutdown requires flushing with an inert gas or hydrogen. A minimum load of 40% or temperature of 200°C to avoid such issues is desired, to prevent the formation of catalytic poisons, and to allow for fast restarts [10,30]. CM requires a high purity feed gas and thus biogas from anaerobic digestion must be cleaned upstream prior to use [10].

Much faster rates of production are achieved with CM as compared to BM due to the favourable conditions, presence of a catalyst, and absence of a gasliquid mass transfer resistance [47,51]. CM processes also have a lower power requirement per unit of gas produced than that of BM [10]. Opportunities exist for CM to produce steam from the cooling circuit to pre-heat the feed gases, with sufficient energy left to run a steam turbine or use elsewhere, increasing the process efficiency and allowing for cost savings [8,22,50]. However, quantifying this was considered beyond the scope of this paper.

3.1.3 Hydrogen storage

As the electrolysers can be operated more dynamically than the methanation reactor there is a need for a minimum volume of hydrogen storage as a buffer. The smaller or less dynamic the methanation reactor, the larger the required hydrogen storage [7,23,29,47]. Suitable methods of storage include compressed gas tanks, cryogenic compressed liquid hydrogen tanks, and metal hydride storage [10].

The issues arising from operating a methanation plant intermittently could be lessened by optimising the hydrogen storage and methanation reactor volume to minimise the number of shutdowns. This would require having the shutdown and start-up costs of the system and a highly accurate estimation of the operation schedule of the electrolyser (weather and market dependent). Neither of these are readily available. The CAPEX of hydrogen storage is significant and depending on plant setup can outweigh the methanation CAPEX. In a study by Aicher et al. the total investment cost of a PtG plant was reduced by 8.4% through dynamic operation of the methanation system lessening the hydrogen storage requirement with similar annual productions of CH₄ achieved [52].

3.1.4 Source of carbon dioxide

The particular source of CO₂ is irrelevant in terms of the overall conversion process⁴ however BM is much more tolerant of impurities (such as H₂S) than CM. PtG could utilise the CO₂ content of biogas as a novel upgrading system, offsetting significant costs of traditional upgrading with the additional benefit of utilising the waste heat. Several industries generate relatively pure sources of CO₂ that could also potentially be used such as distilleries and wastewater treatment plants (WWTPs) [53,54]. Ideally the source of CO₂ would be biogenic (biogas plants, WWTPs, and distilleries) such that the methanation process is carbon neutral, as opposed industrial sources which increase lifecycle emissions [55].

3.1.5 Gas quality

The high selectivity of the methanation process leads to a CH₄ content of approximately 95% in the product gases. However, this still results in an energy content less than that of natural gas due to the lack of higher hydrocarbons [10]. In smaller quantities, the gas produced by PtG can be compressed and injected into the transmission grid without issue but in some

⁴ Specifying the source makes the results less easily interpreted in terms of other processes such gasification, therefore the system boundary is drawn not to include this.

instances the addition of propane may be required to meet the gas grid specifications, particularly when injecting into the distribution network [25,56]. Though it is possible for hydrogen to be injected directly into the gas grid several issues would arise since the existing natural gas grids were designed for methane [57]. Hydrogen leads to much more permeation and corrosion than methane and for safety reasons the maximum hydrogen content is limited to between 0.1 and 10% by volume; depending on the country, limits up to 20% have been discussed [57–60]. The amount that can be injected is also limited by gas quality regulations, as hydrogen has approximately one third the volumetric energy content as compared to methane (12 v. 36 MJ/m³) [56,61]. Therefore, power-to-hydrogen for grid injection requires further work to define and standardize the allowable limits and is not feasible in the short-medium term in many regions.

3.1.6 PtG modelling: system performance and costs

The model used in this study does not explicitly differentiate between technologies and instead uses input parameters such as cost, efficiency, energy consumption and lifetime of the parts⁵. As indicated, in the time periods analysed, PEM electrolysis will have superior efficiency, greater ability to facilitate VRE and have greater cost reduction potential than the AEL and SOEC systems. Thus the PEM was considered most suitable for PtG [7,10,37,45] and the model proposed herein. Preliminary analysis of the likely operation schedule of an electrolyser engaging in the electricity market (as represented by the electricity market in Ireland for this study: Appendix 3.2) showed that annual run hours would need to be high to minimise the LCOE. Thus, the high flexibility of BM would be somewhat negated, with the higher efficiency of CM being preferred (no stirring required and waste heat utilisation). At scales in excess of 5MW, CM technology was also found to be more economic [30]. Thus, the envisaged system in the model consisted of 10 MW_e PEM electrolysis coupled with CM. Ancillary components such as supply water purification, pumps, and electronics are included for in the balance of

⁵ The model referred to is the MS Excel® cash flow model and associated calculations.

plant (BoP), the operational cost (OPEX) is broken into fixed and variable components.

The requirement for hydrogen storage is largely dependent on the bid strategy of the facility, and resultant intermittency of the production of the gas. Thus, a small volume of storage is included in the contingency and BoP in order to simply regulate the flow of hydrogen to the methanation process. With the high costs associated with hydrogen storage infrastructure it is was considered best to minimise this element [61]. The envisaged system for the model can thus operate part load, experience down time, and due to its bidding strategy will not go long periods without operating. Future models may have the capacity to achieve greater cost savings by integrating more hydrogen storage despite the associated high CAPEX. Table 3.2 illustrates the average specifications of PEM electrolysis and CM found in literature and hence used in the model.

Time Period		2020	2030	2040
Electrolysis	(kWh/m ³ H ₂)	4.92	4.66	4.43
	%	72	76	80
Methanation	(kWh/m³ CH₄)	0.3 (2020	0.13 (2030	0.08 (2040
		base value)	base value)	base value)
	%	72.5	73.4	73.7
Overall	%	52.2	55.8	59.0
Efficiency				

Table 3.2:Electrolysis and methanation energy consumption and efficiency
inputs to model

The whole stack efficiency of the electrolysis process is listed together with the energy consumption of the methanation process, with their corresponding percentage efficiencies for the years 2020, 2030 and 2040. The figures in Table 3.2 attempt to account for pumping, parasitic loads, partial load inefficiencies etc. and thus may appear conservative when compared to some past literature [25,29,62]. Valorisation of waste heat is not included.

Furthermore, the technological advances have not materialised to the extent predicted in much of the literature.

The flexibility and partial load capabilities of the electrolysis and methanation processes are not included in the model, however, as the system is not set up to solely take advantage of otherwise curtailed electricity this is not of considerable concern. In reality, the run hours and energy consumed will be somewhat lower than predicted.

Table 3.3 contains the cost estimates for PtG obtained from literature on which the financial model in this study was based. Where it was deemed that insufficient data was available, the authors' own data was fitted. Where values were given in kW gas a conversion to kWe was achieved by dividing by 0.56, analogous to the 2030 figures for electrolysis and methanation combined efficiency, as suggested in Lehner [45]. In addition to those stated in Table 3.3, several other references were used to inform the estimates [6,7,10,24,42,63].

The time period costs for CAPEX, BoP and OPEX are shown in Table 3.4. These conservative cost estimates allow for project issues and other hidden costs that would arise on projects of this scale [52,64]. Much uncertainty remains regarding such investment costs and future costs.

Several costs are not explicitly included in the model, either because they were deemed to be specific to certain sites, too ambiguous, or already accounted for in BoP. Excluded costs include for compression costs in the event of grid injection, the cost of CO₂ (site specific), and taxes and fees for grid connection [40]. Planning, wages, regulatory issues, and breakdowns beyond that budgeted for are also not included. The introduction of other costs increases uncertainty without additional accuracy, the conservative BoP yielded similar results without the complexity seen in other works [26]. The model also does not account for inflation, nor substantial economies of scale as previous research has shown it not to apply with units tending to be modular [22]. In Table 3.4 the BoP and OPEX costs of electrolysis and methanation are presented as decimal fractions of their corresponding CAPEX, as are electrolyser replacement and catalyst replaced.

Electrolysis	Methanation	Project	Other (€)	Note	Ref
(€/kW _e)	(€/kW _e)	Costs (€)			
1250 (2020)	840 (2016)				[16]
1230 (2020)	280 (2030)				[10]
1000 (2020)	840 (2016)	Inclusive of	OPEX 1-2% (10MW) of	Electrolysis cost is	[25]
700 (2030)	560 (2030)	transport	CAPEX, more for smaller	turnkev	[20]
400 (2050)	390 (2050)	installation, and	units.	Maximum 10-20%	
		commissioning	Cell stack replacement	scale effect.	
		at 10-20%	50% every 40.000 hrs.		
		CAPEX.	Additional 50% BoP for		
			methanation, 5-10%		
			OPEX.		
800 – 1500	200 – 1000		500 – 800/kWe Complete		[30]
(2014)	(2014)		cost including 12hr		
			memory is future target		
			(2030)		
	160 - 280 (2014)			In agreement with	[45]
				Kinger 2012 and	
				Sterner 2009	
500 (2050)	340 (2050)		8% discount rate. OPEX		[65]
			of 3%.		
1300 (2011)	100 – 700 (2011)	10% CAPEX for	5% cost of capital	Includes for	[22]
		project,		connection and design	
		construction,		(Proton-Onsite). PEM	
		and unforeseen		has reduced	
		costs		significantly since.	
		5% Eng. And	OPEX is 2%.	5% working capital.	[66]
		design, 10%	25% of CAPEX for		
		contingency, 2%	replacement cost of		
		other.	electrolysis stack every 7		
			years.		
750 (combined f	uture costs)		6% interest rate. 4%	25-year depreciation	[62]
			OPEX,	period	
1000 (2016)	1650* (2016) 400		4% OPEX,	*Inclusive of BoP,	[64]
850 (2020)	(2020)			installation etc.	
710 (2030)					

Table 3.3: Review of literature costs for PtG systems

2490 (2011)	10%	4% OPEX, 7.5% interest	25-year depreciation	[29]
1200 (2020)	construction,	rate	period	
	delivery etc			

Year of data in brackets.

Time Period		2020		2030			2040			
		Low	Base	High	Low	Base	High	Low	Base	High
Electrolysis	CAPEX	650	850	1000	500	700	850	400	560	660
	(€/kW₀)									
	ВоР	0.1	0.15	0.2	0.1	0.15	0.2	0.1	0.15	0.2
	OPEX	0.03	0.04	0.05	0.02	0.032	0.04	0.02	0.032	0.04
Electrolyser Replacement		0.2	0.32	0.4	0.2	0.32	0.4	0.2	0.32	0.4
(Years 1	0, 17, 24)									
Methanation	CAPEX	135	160	185	110	140	170	100	125	150
	(€/kW _e)									
	ВоР	0.85	1	1.15	0.85	1	1.15	0.85	1	1.15
	OPEX	0.05	0.057	0.065	0.05	0.057	0.065	0.05	0.057	0.065
Catalyst Replacement		0.7	0.8	0.9	0.7	0.8	0.9	0.7	0.8	0.9
(Year 15)										

Table 3.4: Time period costs for CAPEX, BoP and OPEX

Figures for BoP, OPEX, and Replacement as expressed as decimal fraction of respective CAPEX

3.1.7 Model to calculate LCOE

A bespoke discounted cash flow model in Microsoft Excel® is used to calculate the LCOE of the methane produced and the other figures contained in this paper. Calculating LCOE is a standard practice and was previously outlined by Visser and Held (2014) [67] and frequently referenced in past literature [27,68– 72]. It allows for intuitive comparison with electricity generators and other storage methods⁶. In this study, the LCOE represents the breakeven selling price of the gas produced and is defined as per Equation 3.4.

$$LCOE = \frac{\sum_{i=0}^{n} \frac{Costs in year i}{(1+Discount rate)^{i}}}{\sum_{i=0}^{n} \frac{kWh of gas produced in year i}{(1+Discoun rate)^{i}}}$$
(3.4)

The timeline of the model is shown in Figure 3.2 It includes for a 3-year commissioning phase, 30 years of operation (during which the electrolysis units are replaced three times and methanation unit replaced once) and one-year decommissioning. The figures for commissioning/decommissioning are based upon industry averages for similar scale projects [73]. The component replacement intervals were calculated using specifications found in literature and assuming 6500 hours per annum run time, to give component lifetime in years. Conservatively, these worked out to be 7 and 15 years respectively for electrolyser stacks and methanation catalyst units. The replacement schedule is then optimised such that both the methanation plant and electrolysis stack will reach the end of their life in approximately the same year, avoiding shutting down the plant with relatively new components in place [74].



ESR – Electrolysis Stack Replacement MCR – Methanation Catalyst Replacement

Figure 3.2: Lifecycle of the Plant used in the Cash Flow Model

A cost to include land purchase, permits, transport, site preparation, engineering and design costs, grid connection as well as contingency was calculated according to the Equation 3.5, derived in Appendix 3.1 at the end of this chapter:

⁶ More complex analysis would be off little benefit at this stage of research, the assumptions required would mean results are more difficult to interpret or apply to different regions.

Land Capital = $\in 18.687(kW_e \text{ of Electrolysers}) + \in 331,313$ (3.5)

This would be paid in year 0. The remaining CAPEX is paid in instalments in years 0, 1, and 2 at 20%, 50%, and 30% of total CAPEX respectively. Decommissioning costs were 20% of CAPEX and paid in the final year. A discount rate of 7% was used throughout in line with much of the literature as referenced in Table 3.3; calculating the perceived risk to an investor is beyond the scope of this study.

The cost of CO₂ was not included as this paper was written to examine the financial feasibility of locating PtG next to current sources of large quantities of rejected CO₂ (distilleries, WWTPs, biogas plants etc.). The cost of water was included without consideration of recovery of water in the methanation step.

The Irish single electricity market (SEM) is a whole island grid, predominantly served by natural gas power plants and wind generation, with limited interconnection to the UK. It is similar to other European grids in that it is operated with the aims of maintaining stability, integrating VRE, and minimising cost to the consumer [75]. Reliance on imported fossil fuels mean that the average electricity cost in Ireland is at the higher end of European prices [76]. With respect to electricity price and run hours, preliminary examination of the 2016 Irish SEM indicated that a bid price of \leq 50/MWh yielded run hours of ca. 6500 and an average electricity cost of \leq 35/MWh (Appendix 3.2). Thus, these assumptions were used throughout and thought to be analogous to 2020 data.

3.2 Results and discussion

3.2.1 Levelised cost of energy of PtG

Table 3.5 contains the results of the model for the low, base, and high cost scenarios specified in Table 3.4 for the three selected time periods (2020, 2030 and 2040). Taking into account the new electricity market data, updated cost estimates, and a full plant lifecycle, the results of the generated model are consistent with many found in literature [10,24,30,31,65] but within a much smaller range. Comparison can be made to those outlined in Table 3.1.

Table 3.5: LCOE of the envisaged PtG system under different scenarios

Scenario	2020	2030	2040	
LCOE of 10MWe plant (€/MWh)	Low	107	89	81
- Average cost of electricity of €35/MW _e h exclusive of taxes/tariffs.	Base	124	105	93
- Run hours of 6500 p.a. Analogous of 2020 SEM data.	High	143	121	103

3.2.2 Breakdown of LCOE

Hypothetically, in the 2020 base scenario, if the electricity was available at zero cost for the same number of hours, the LCOE would drop to €55/MWh. At a minimum, exclusive of CAPEX and OPEX, the methane generated in PtG systems has a cost as determined in Equation 3.6, assuming positive or zero electricity costs.

$$Min. Cost of Produced Gas\left(\frac{\epsilon}{_{MWh}}\right) = \frac{Electricty Cost\left(\epsilon/_{MW_eh}\right)}{Electrolysis efficiency \times Methantauion efficiency} (3.6)$$

If the respective efficiencies of electrolysis and methanation are 72% and 72.5%, as in the 2020 scenario (Table 3.2) then the gas can be expected to be approximately double ($0.72 \times 0.725 = 0.52$) the cost of the electricity (as per

Eq. 5) plus the levelised CAPEX and OPEX costs. This illustrates the importance of sourcing low-cost electricity. Figure 3.3 shows the breakdown of the 2020 base scenario LCOE into its components and further highlights the importance of low-cost electricity in producing competitively priced methane.





As seen in Figure 3.3 the LCOE is dominated by electricity costs (56%) with the remainder consisting of electrolysis (25.5%), fixed OPEX (9.9%), methanation (7.4%), and other (1.1%). Thus, it can be seen that the conservative assumptions for system CAPEX and subsequent cost reductions (particularly in the electrolysis technology) over time do not impact the LCOE as considerably as may be expected; this is further demonstrated in section 3.2.3. Consequently, the benefits of modelling ambitious reductions are limited. Equipment being replaced/upgraded during the system's lifetime will most likely be done so at a lower cost and higher specification than when first installed, however this is unaccounted for in the model. Only in the event that efficiency improved vastly would it have a significant impact on the LCOE. As discussed in 3.1.1.3, if the PEM system has a 5% better efficiency (70 vs 75%) in 2020, for example, than the AEL system, it is justified to pay up to 46.6% more for a PEM electrolyser and still reduce the system LCOE under base conditions (Appendix 3.4). This effect is lessened with reduced annual run hours and electricity cost but exacerbated when high capacity factor and high energy costs are used.

Decommissioning is assumed to cost 20% of the CAPEX and is paid in the final year of the project; this is a conservative estimate as in reality the recyclability of the system may even command a fee.

Should PtG be used in place of traditional biogas upgrading, as suggested in literature, a portion of the capital will be offset [33,48,53]. The upgrading plant required to process an equivalent volume of CO₂ as the 2020 base scenario, in the form of raw biogas (assumed 60:40 CH₄ to CO₂), would cost ca. €2.45 million [77]. The model in this paper calculates a 10MW_e PtG system would cost ca. €13m in 2020, and €9m in 2040 but with a better efficiency. This equates to an investment cost of €3,018/Nm³CH4/h for traditional pressure swing adsorption (PSA) upgrading versus €10,236/Nm³_{CH4}/h (2020) and €6,383/Nm³CH4/h (2040) for a PtG system (Appendix 3.3). Therefore, the increased production of biomethane from PtG upgrading would seem to justify the additional expense when compared to PSA. The profitability of this configuration will be determined by the value of the additional biomethane produced in PtG versus PSA upgrading (762 vs. 1270 Nm³_{CH4}/h in 2020), and the plant's ability to extract value from the electrolysers. The energetic expense of such a configuration, compared to consuming raw biogas, is then justified by the ability to inject low carbon gas into the grid, as well as other potential secondary benefits such as those identified in the introduction [48].

3.2.3 Sensitivity analysis

Figure 3.4 illustrates the effect of varying the five most sensitive model parameters by +/-25% on the LCOE⁷. The five parameters were electricity cost, run hours, total CAPEX, discount rate, and fixed OPEX.

⁷ Monte Carlo simulation was considered but there is insufficient data available to develop the probability distributions required. Therefore, inclusion of such analysis at this stage would introduce more uncertainty than benefits to the body of knowledge.



Figure 3.4: Sensitivity Analysis of the 2020 base scenario

Like Figure 3.3, Figure 3.4 illustrates that the electricity cost has the most significant effect on the LCOE, followed by run hours. Run hours are a function of the bid price and electricity market, and hence are closely related to the electricity cost. Results show that a lower capacity factor (lower run hours) coinciding with cheap electricity increases the LCOE. It was previously proposed that an increased bid price associated with longer run hours may reduce LCOE [13,14], and this was found to be true in this case. The benefits of paying more for the electricity and the associated increase in capacity factor outweigh the additional costs, as high run hours are required to produce sufficient quantities of gas to amortise the project cost. Thus, there is potential scope to optimise the bid strategy of PtG systems to increase the run hours and reduce the LCOE (non-linear relationship), as suggested by Vandewalle et al. [24].

It is proposed that a business model based upon the sole consumption of otherwise curtailed energy may not be viable due to the low capacity factor, even in high VRE scenarios. Considerable value would need to be placed on the grid stability function provided with the energy supplied at near zero cost. Similar conclusions were found in studies by Gotz et al. [10] and de Bucy [8]. Reductions in CAPEX and OPEX will make future projects more attractive but without considerably affecting the LCOE. Further analysis reveals that for the LCOE to fall by 20%, the total CAPEX of the system would need to drop by 76.2%, or the cost of electricity would need to fall by 35.9%.

3.2.4 Potential for incentivisation

The LCOE of renewable gas produced from a PtG system, as shown in Table 3.5, is higher than fossil fuel alternatives such as diesel transport fuel (it would be more correct to compare to other advanced biofuels but few are at a sufficient TRL to do so). Diesel retails at €105/MWh excluding value added tax (VAT) in Ireland (47.3% of which consists of other taxes) [78]. To reduce GHG emissions in the transport sector, many countries may look to introduce subsidies to incentivise advanced biofuels such as gaseous fuel from nonbiological origin from PtG. In this study, the LCOE of the 2020 base scenario was calculated at €124/MWh. This would imply that an incentive of €19/MWh is required for PtG to reach price parity with diesel (if not subject to similar excise duty type taxes). This incentive can be considered modest although it is likely that the product gas will be subject to some taxes or other charges and as such the required gas sale price or incentive will be higher than quoted. However, scope exists for a modest incentive to make gaseous fuel from non-biological origin competitive with diesel. Given the low TRL of other advanced biofuels this is encouraging. In the longer term, it is highly likely that diesel will not be the competition as its use will be prohibited in many cities. Mexico, Paris and, Athens have prohibited diesel use by 2025. In essence, the end product of PtG will only be in competition with advance biofuels and electricity as a source of propulsion.

Utilising the by-products of PtG can add financial competitiveness. For example, if valorisation of the oxygen (from electrolysis) can be achieved, this could provide a significant additional income [24]. Given that there is an established demand for pure oxygen, especially within the medical industry, and with the opportunity for it to be marketed as "green" oxygen, this is not unfeasible. In Breyer et al. a value of 8c/kg O₂ (11.43c/Nm₃) was suggested

[27]. In this study, if a 10c/Nm₃ profit can be achieved through the sale of oxygen, the LCOE would fall from €124 to €105/MWh (2020 base scenario).

Modern electrolysers have been shown to have the technical capacity to provide ancillary services to the grid delivering benefits to its operation [7,27,79]. In previous literature it has been suggested that a fee could potentially be paid by the TSO for the availability to consume energy or provide power balancing services through PtG; such a fee would again reduce the LCOE of the system [4,6,73,79,80]. In the short term, no great precedence exists for the collection of fees for these grid services however future potential has been highlighted and discussed by policymakers [4,5,81,82]. Several works have shown that it is essential in order for PtG to become competitive [5,79]. In Breyer et al. [27] a grid service payment of €35/MW_e was assumed, ultimately making the plant profitable in that scenario. This was considered a highly optimistic target given the advantages of interconnection and potential increases in the allowable limit of non-synchronous generation (VRE). A payment of €15/MWe was chosen as a more conservative estimate for the calculations in this study. Assuming 8500 hrs availability per annum (€15/MWe x 8500 hrs/a x 10 MW_e = €1,275,000 pa), the payment lowered the LCOE to €87/MWh.



Figure 3.5:Effect of incentives and supplementary income on effective 2020 base systemLCOE with market prices of diesel and household natural gas ex. VAT for reference

Figure 3.5 demonstrates how the competitiveness of gaseous fuel from nonbiological origins increases with respect to diesel and household natural gas as incentives and supplementary incomes are applied. It can be seen that a combination of incentives and valorisations could potentially make the gas cheaper than its competitors, again given a favourable tax status.

3.3 Conclusion

PtG is considered a technology of the future with much debate on the actual cost of the energy provided; the literature suggests LCOE in the range \in 75 to \in 600/MWh of CH₄ (Table 3.1). This paper applied a commercial perspective on the lifetime of a PtG system including for the maintenance schedule and associated costs, commissioning/decommissioning, fixed and variable operational expenditure and maintenance (OPEX) and real-world electricity market data. This process yielded the LCOE of a PtG system for low, base, and high cost scenarios for 2020 (\in 107-143), 2030 (\in 89-121), and 2040 (\in 81-103).

It is also perceived that PtG can utilise cheap electricity which would otherwise be curtailed or constrained. This paper highlighted that the most important variables in the LCOE of PtG are electricity cost, run hours per annum and the total CAPEX. The cost of electricity increases with increase in run hours but CAPEX decreases with increase in run hours. Overall it is shown that an increase in run hours to a certain level reduces the LCOE.

Hypothetically, in the 2020 base scenario, if the electricity was available at zero cost for the same number of hours, the LCOE would drop to €55/MWh. However, this paper shows that operating as a wholesale agent of electricity in Ireland, a bid price of €50/MW_eh leads to an average cost of electricity of €35/MW_eh for 6500 run hours per annum.

Should PtG be used in place of traditional biogas upgrading, as suggested in literature, a portion of the capital will be offset. The profitability of this configuration will be determined by the value of the additional biomethane produced in PSA versus PtG upgrading (762 vs. 1270 Nm³_{CH4}/h in 2020), and the plant's ability to extract value from the electrolysers.

Incentives, tax exemptions, valorisation of oxygen, or exemption from grid access payments may be required in order to make PtG more financially competitive as a source of advanced transport fuel. Since PtG can facilitate additional VRE on the electricity grid it may also receive a fee for such services. Combinations of incentives and supports would make PtG potentially much more competitive than other advanced biofuels.

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3.4 Appendices: Chapter 3

Appendix 3.1: Land Capital cost (Equation 3.5)

In reviewing the literature no standard calculation for the costs of land purchase, site preparation, planning, permits, etc. was apparent [26,67]. Estimates were found to vary from 15% of total CAPEX to 30% of installed CAPEX [25] but did not account for all anticipated costs. Other literature used to inform the calculation includes [66,74,83]. A minimum of €350,000 for a 1MW plant, up to a maximum of €2.2m for a 100MW plant was identified for projects of this nature. This information was used to construct a graph and derive an approximate equation for "Land Capital" cost based upon the capacity of electrolyser being installed.



Figure 3.6: Land Capital cost as a function of installed electrolyser capacity

A straight-line relationship was assumed between the two points and the equation shown was used in the model.

Appendix 3.2: Derivation of Electricity Market Data (Section 3.1.7)

"With respect to electricity price and run hours, preliminary examination of the 2016 Irish single electricity market (SEM) indicated that a bid price of €50/MWh yielded run hours of ca. 6500 and an average electricity cost of €35/MWh. Thus, these assumptions were used throughout and thought to be analogous to 2020 data".

Data for the 2016 Irish electricity market was downloaded from

http://www.sem-o.com/

System marginal price (SMP) is the island wide price of electricity at each half hour interval.

The number of run hours at a given bid price was found using the formula below.

$$Run Hours = \frac{\sum Half hourly intervals for which SMP < Bid price}{2}$$

Average cost of the electricity was given by

 $Average \ Electric ty \ Cost = \frac{\sum SMP \ of \ Intervals \ for \ which \ SMP < Bid \ Price}{\sum Number \ of \ intervals \ for \ which \ SMP < Bid \ Price}$



Figure 3.7: Change in LCOE of a PtG system with respect to changing bid price for the 2016 Irish electricity market.

When data for run hours and average cost of electricity based upon a given bid price was fed into the model and plotted (as in Figure 3.7) it was found that a bid price of \leq 50/MWh approximately minimised LCOE. This corresponded to an average cost of electricity of approximately \leq 35/MWh and run hours of 7080. The figure used for run hours was slightly reduced to 6500 to reflect the fact an actual plant would not be perfectly flexible and have the ability to ramp up and down to take advantage of each half hour at which the SMP was less than the bid price.

Appendix 3.3: Investment cost of Upgrading versus PtG (Section 3.2.2)

10*MW* electrolyser @ 72% $\eta \rightarrow$ 7200 kWh H₂/hour

 $7200 \, kWh \, H_2 @ \, 3.54 \, kWh/m^3 \rightarrow 2033m^3 \, H_2/hour$

2033 $m^3 H_2 \xrightarrow[4:1 H_2:CO_2]{} 508 m^3 CO_2/hour$

508 $m^3 CO_2/hour \xrightarrow{Biogas @ 60:40 CH_4:CO_2} 1270m^3 Biogas/hour$

Thus, a 10MW PtG system can upgrade $1270m^3$ of biogas per hour. Traditional pressure swing absorption (PSA) upgrading costs ca. $\in 1800/m^3$ at this scale, ca. $\in 2.3m$ suitable sized plant here [77]. The model in this paper calculates a 10MW PtG system would cost ca. $\in 13m$ in 2020, and ca. $\in 9m$ in 2040 but with a better efficiency. As the PtG system will result in higher volumes of CH₄ being produced it is fairer to compare them on an investment cost per unit of gas produced basis.

Results:

PSA:	$€2.3m \div 762m^3 CH_4/hour = €3018/m^3 CH_4/hour$			
PtG:				
72% η in 2020:	€13 $m \div 1270m^3 CH_4/hour = €10236/m^3 CH_4/hour$			
80% η in 2040:	€9m ÷ 1410m ³ CH ₄ /hour = €6383/m ³ CH ₄ /hour			

Appendix 3.4: AEL vs. PEM (Section 3.1.7)

"As discussed in 3.1.1.3, if the PEM system has a 5% better efficiency (70 vs 75%) in 2020, for example, than the AEL system, it is justified to pay up to 46.6% more for a PEM electrolyser and still reduce the system LCOE under base conditions." From section 3.2.

Under 2020 base conditions:

Electrolysis η of 70% (AEL) - LCOE of €127.27 Electrolysis η of 75% (PEM) - LCOE of €119.05

Using the goal seek function of Excel we can vary the CAPEX of the electrolyser to match the LCOE of €127.27 while maintaining the 75% η of PEM. This gives a value of €1246.8/kW compared to €850/kW in the base case, 46.7% higher.

I.e. A PEM system at 75% η will produce the same LCOE as an AEL system at 70% in the event that their CAPEXs are €1246.8/kW and €850/kW respectively.

Thus, the increased η of PEM is preferred provided it is no more than 46.6% more expensive than the AEL system, when reducing the LCOE is one's goal. As the model in this paper calculates BoP as a fraction of CAPEX, should BoP remain unchanged between the two scenarios this figure would become greater still.

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4 The effect of electricity markets, and renewable electricity penetration, on the levelised cost of energy⁸

Abstract

Power-to-Gas (PtG) is a technology that converts electricity to gas and is termed gaseous fuel from non-biological origin. It has been mooted as a means of utilising low-cost or otherwise curtailed electricity to produce an advanced transport fuel, whilst facilitating intermittent renewable electricity through grid balancing measures and decentralised storage of electricity. This paper investigates the interaction of a 10MW_e PtG facility with an island electricity grid with limited interconnection, through modelling electricity purchase. Three models are tested; 2016 at 25% renewable electricity penetration and 2030 at both 40% and 60% penetration levels. The relationships between electricity bid price, average cost of electricity and run hours were established whilst the levelised cost of energy (LCOE) was evaluated for the gaseous fuel produced. Bidding for electricity above the average marginal cost of generation in the system (€35-50/MW_eh) was found to minimise the LCOE in all three scenarios. The frequency of low-cost and high-costs hours, analogous to balancing issues, increased with increasing shares of variable renewable electricity generation. However, basing PtG systems on low-cost (less than €10/MW_eh) hours alone (999 hours in 2030 at 60% renewable penetration) is not the path to financial optimisation; it is preferential to increase the run hours to a level that amortises the capital expenditure.

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4.1 Introduction

The impact of climate change and the harmful nature of fossil fuels are well established. In response to this the European commission has set a target of at least an 80% reduction in greenhouse gases (GHGs) by 2050 relative to 1990 levels, with the ultimate goal of keeping climate change below 2°C [1,2]. It is estimated that achieving such a target will require a 75-80% share of low carbon technologies in the power sector [1]. Wind, and increasingly solar, will make up the majority of this variable renewable electricity (VRE) generation, as they are the current state of the art technologies available at the required scale. The EU have also encouraged the need for sustainably-produced third generation (advanced) biofuels, which must hold at least a 3.6% share of energy in transport by 2030 [3]. Transport is a particularly difficult sector to achieve emissions reductions in; the EU suggest anything from a potential increase of 20%, to a reduction of 9% in transport emissions by 2030 in their roadmap to a low carbon economy in 2050 [1]. However, heavy goods vehicles and captive fleets are especially suited to early adoption of renewable gaseous fuels where growing restrictions on particulate emissions, more predictable vehicle usage, stronger influence of policy, and increasing deployment of refuelling infrastructure facilitate the uptake of compressed natural gas (CNG) vehicles [4,5].

Increasing shares of VRE in the electricity mix can give rise to issues of grid balancing, stability, curtailment, and an increased need for storage, potentially affecting security of supply [6–9]. Large scale and flexible energy storage options are seen as a means of reducing these effects [10–12]. Presently deployed solutions such as pumped hydro storage are insufficient should significant dispatch down of VRE be avoided as they are limited by geography, and currently installed capacities are much less than the anticipated future requirements [13–15].

Power-to-Gas (PtG) has been proposed as a technology that can provide a storage mechanism for VRE and ultimately can produce an advanced transport fuel, that will help satisfy the EU target of 3.6%. PtG is a process whereby electricity is used to generate hydrogen (H₂) via the electrolysis of water, and

this hydrogen can then be combined with CO₂ to produce methane (CH₄) via a Sabatier reaction (CO₂ + $4H_2 \rightarrow CH_4 + 2H_2O$). Thus, PtG changes the energy vector, storing electricity in the form of methane, also known as gaseous fuel from non-biological origin. The technology does not require the favourable geography of other electricity storage options [10] and offers superior storage capacity and discharge times since the gas is of similar guality to natural gas and can be injected in to the natural gas grid, where it can access available markets [16]. It is intended that the fuel produced be used in the transport sector, and not for heating or power generation, as the availability of alternatives or low round trip efficiency of these routes make it inappropriate, especially considering the difficulties in decarbonising transport [4]. The ability of PtG to rapidly ramp up and down demand allows PtG to utilise difficult to manage electricity that may otherwise be curtailed [17-20]. Therefore, it can in theory provide ancillary grid balancing services that enable further integration of VRE into the electricity mix [4,21]. It may also receive a fee for this service, aiding its economic viability. Furthermore, PtG can be positioned as a novel biogas upgrading solution, utilising its CO₂ content, increasing the sustainability of biogas plants, potentially offsetting some of the capital required, and promoting a circular economy [18,22].

Many technology reviews and studies are available which detail the working principles, relative advantages and disadvantages, and trends in PtG technologies [18,19]. Wide scale deployment of PtG will be largely dependent on the cost of the gas produced and how it compares to competing advanced transport fuels. Previous work by the authors found the levelised cost of energy (LCOE) of a PtG system to be dominated (56%) by electricity costs and highly sensitive to changes in capacity factor (run hours) [23]. This paper aims to demonstrate that the figures for run hours and electricity cost are dependent on the market in which the PtG plant is engaged and are largely determined by the electricity at any given time (\notin /MW_eh). To test this, a PtG system will be modelled as a large flexible consumer within an electricity market, represented by the lrish grid with limited interconnection, in 2016 and simulations of the 2030 market at different penetrations of VRE.

The relationships between a PtG system, its bid price, and the resultant effect on LCOE will be examined. This work advances upon previous research where values for electricity cost and run hours were fixed or independent of one another [20,24–26]. The operational impact and effects of curtailment on PtG have been studied previously [10,13,27] but not with the intention of observing the impact on the financial viability of PtG, as in this study. In this work, the bid price, which the facility has control over, will be optimised to minimise the cost of the produced gas. To the best of the authors' knowledge this has not been done before.

The objectives of the paper are to:

- Examine electricity market data for trends that will affect PtG viability.
- Investigate the interactions between the electricity market and the LCOE of a PtG system modelled as a large flexible consumer.
- Examine the theory that PtG can be run economically off otherwise curtailed electricity, at different levels of VRE penetration on an island grid.
- Identify the optimum bid strategy that minimises the LCOE of gaseous fuel from non-biological origin.

4.2 Methodology



Figure 4.1: Inputs and outputs of the model used to calculate LCOE.

4.2.1 PtG model to calculate LCOE

In a previous study by the same authors, a model of a PtG system was built in order to calculate the LCOE (Equation 4.1) for a range of cost scenarios and time periods [23]. This process or "Model to calculate LCOE" is indicated in Figure 4.1. The LCOE, or breakeven selling price of the gas, was chosen as the key metric as it accounts for the project capital and allows for easy comparison with other fuels. It is derived using a bespoke discounted cash flow model in MS Excel®. Firstly, the most suitable technologies for electrolysis and methanation were identified; details of these calculations and explanations of rationale can be found in McDonagh et. al [23]. Secondly, the specifications of the chosen technologies (polymer electrolyte membrane (PEM) electrolysis and catalytic methanation) were fed into the model such that capital expenditure (CAPEX), balance of plant (BoP), operating expenditure (OPEX), maintenance, and other associated costs could be accounted for. The model runs for 30 years (including 3 years commissioning, 1-year decommissioning at a cost of 20% CAPEX) at a discount rate of 7%, during which time the electrolysis stack and the methanation unit are replaced three times and once respectively. Again, a more detailed description can be found in a previous paper [23], wherein the model used fixed values for average electricity cost and run hours (€35/MWeh and 6500 respectively) analogous to a PtG system operating in the 2020 Irish electricity market at a bid price of €50/MWeh. In this paper however, the electricity market data affects the LCOE as the average cost of electricity and the run hours are dependent variables fed into the model. In Equation 4.1, "Costs" then consist of the items detailed in Figure 4.1 and this paragraph.

$$LCOE = \frac{\sum_{i=0}^{n} \frac{Costs in year i}{(1+Discoun \ rate)^{i}}}{\sum_{i=0}^{n} \frac{kWh \ of \ gas \ produced \ in \ year i}{(1+Discoun \ rate)^{i}}}$$
(4.1)

The PtG system then consisted of a 10MW_e PEM electrolyser, which was considered more suitable than an alkaline electrolysis cell (AEL) and solid oxide electrolysis cell (SOEC). McDonagh et. al [23] also contains detailed analysis of the technologies and their applicability to PtG, and concluded that given the superior efficiency of PEM in the time period being assessed it would

be justified to pay up to 46.7% more in CAPEX under base conditions, and still minimise LCOE. Other factors considered were the ability to quickly ramp up and down (allowing for grid service provision), OPEX, technology readiness level, and purity of hydrogen [18,24,28,29]. Similarly, catalytic methanation (CM) was chosen over biological methanation (BM) due to faster rates of production and lower specific energy consumption, despite its higher capital cost [18,30,31]. Also included was a small volume of hydrogen storage to act as a buffer for the dynamic operation of the electrolysers and methanation reactors [19,31,32].

The effect of incentives or valorisation of the oxygen produced during electrolysis will not be considered in this paper, nor will parameters beyond the control of the PtG operator. The perspective is that a PtG plant has been built and is operating in the 2030 Irish electricity market thus, measuring the effect of changes on the LCOE is sufficient to examine the relationships and observe whether optimisation is being achieved. The 2030 base scenario identified in McDonagh et al. [23] yielded an LCOE of €105/MWh and is used as the reference scenario in this paper (Table 4.1). In the same scenario, approximately 60% of the LCOE consisted of electricity costs as reported in McDonagh et al. [23], therefore changes in the interaction with the electricity market will have a large bearing on the LCOE.

	Electrolysis	Methanation	Note
CAPEX	700	140	1 BoP OPEX and Component Replacement given
(€/kW₀)			as decimal fractions of CAPEX.
BeD	0.15	1	2. Plant runs for 30 years.
БОР	0.15		3. Electrolysis stack replaced in years 10, 17, and 24.
OPEX	0.032	0.057	4. Methanation catalyst replaced in year 15.
Component	0.32	0.8	5. "Land Capital" costs of €(18.7(kW _e of electrolysers)
replacement			+ 331313) for facilities greater than 1MW includes for
-			additional costs E.g. H ₂ storage, planning, etc [23].
Electrical	4.66	0.13 kWh/m ³	6. Figures are in 2016 euros.
demand	kWh/m ³ H ₂	CH ₄	

Table 4.1:	Economic ass	umptions in the	e model
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4.2.2 Source of carbon dioxide

The envisaged system is capable of utilising any source of CO₂ that has been sufficiently scrubbed of impurities and potential catalytic poisons such as chlorine compounds or hydrogen sulphide [18,31]. Many potentially low-cost and relatively pure sources have been identified including CO₂ from industrial processes (including biogenic sources should upgrading already be in place), or biogas (mixtures of CH₄ and CO₂ from biological processes), where direct utilisation avoids the significant cost of traditional upgrading. Previous works have investigated the possibility of utilising various sources of CO₂ such as that from distilleries, wastewater treatment plants, cement production facilities, and others, and found them to be suitable and abundant [33,34]. This means that provided the facility is appropriately located, and the electrolysers appropriately sized, producing sufficient hydrogen is the limiting factor. As PtG costs have been shown not to scale significantly above 1MW, the economics of these potentially small facilities do not differ greatly, any increases seen would be more than offset by the availability of cheap CO₂ [35].

The model does not include an explicit cost of CO₂ as this would make the LCOE site specific and does not affect the results in terms of evaluating whether optimisation is being achieved in the systems interaction with the grid,
as the paper intends. Further to this, a study from ENEA Consulting used a highly conservative figure of \in 50/ton of CO₂ transported at 10 bar and found it added a maximum of 4.5% (\in 8/MWh) to the LCOE. Sensitivity analysis showed that varying this figure between \in 20 and \in 80/ton resulted in a ±3% change to the LCOE [28].

The ideal source of CO₂ is biogenic and located close to the PtG facility such that the product gas has a lower carbon intensity, as would be the case if PtG were used as a novel biogas upgrading method for an anaerobic digestion (AD) system [36,37]. It is also relatively pure thus, avoiding the high energy penalty associated with direct air capture or capture from flue gases [33]. It is anticipated that in the time period analysed, AD systems will become much more prevalent.

4.2.2 Electricity Market Data

The system marginal price (SMP) can be considered as the hourly or halfhourly island wide wholesale price of electricity. It includes for the cost required to meet the forecast demand and additional costs associated with start-up or operating as a reserve that a generator will need to recover (costs known as uplift). In general, the SMP is low when there is more than sufficient generation capacity online to meet demand. When the amount of generation online to meet demand is scarce, the resulting SMP is higher. The SMP is set by the marginal costs of the last generator online to meet demand. In Ireland this is often gas fired generation. The SMP is also influenced by zero marginal cost VRE which tends to supress the SMP in times of high VRE production. In times of excess VRE generation, curtailment may take place. Current electricity market rules offer VRE priority dispatch on the electricity grid, therefore curtailment of VRE is often a last resort. In analysing the electricity market data, it is proposed that very low SMPs (less than €10/MWeh) can be equated with curtailment and high VRE production; strong positive correlation has been found between increased shares of VRE and the periodic availability of lowcost electricity [38]. For the purposes of this study, information for the half hourly SMP of electricity for 2016, available for download from the single

electricity market (SEM) operator [39], was collected and organised in spreadsheets.

To determine the SMP in 2030, PLEXOS models of the electricity market were developed. PLEXOS Integrated Energy Model is a power systems modelling tool used for electricity market simulations [40]. The power systems model develops an hourly SMP for the Irish electricity market based on current rules, and it has been benchmarked against historic market data and has been validated by the regulator to reproduce realistic results. The model uses deterministic mixed integer linear optimisation to minimise the costs of the electricity dispatched including for fuel costs, start-up costs, penalties for unserved energy, and a penalty cost for not meeting reserve requirements [41]. The model optimises thermal generation (fossil fuel and renewable), VRE, pumped storage, interconnection, as well as reserve classes subject to operational and technical constraints [27,42]. Also included are constraints on the unit operation of each power plant including minimum and maximum generation, minimum and maximum up and down time and the system ramp up and down rates, as well as a system level constraint consisting of an energy balance equation ensuring supply meets regional demand at each period [27]. Two PLEXOS models were tested, at 40% and 60% renewable electricity (RE) respectively. Thus, as outlined in Figure 4.2, three models in total were examined.



NG – Natural Gas, RE – Renewable Energy, VRE – Variable Renewable Energy

Figure 4.2: Details of the three electricity market models used in this study and the levels of RE and VRE in each.

Renewable energy (% RE) is calculated as delivered MW_eh of electricity from all renewable sources, as a percentage of total delivered electricity. Variable renewable energy (% VRE) then only includes intermittent sources (wind, solar, and wave), and not those that are dispatchable and therefore do not contribute to the fluctuations in supply that would affect price (CHP, co-firing of biomass, and hydropower). The "Other" portion of these charts consists mainly of peat with small volumes of heavy fuel oil, both of which are dispatchable thermal generators.

These represent the current (2020) and future (2030) targets for Ireland [43]. The vast majority of this RE will be provided by wind and other intermittent sources. The 40% RE scenario is representative of a case where the rate of new installed RE capacity does not increase drastically beyond the levels seen today. The 60% RE scenario requires the rate of additional installed capacity of RE to substantially outpace that of increasing demand. Both scenarios are feasible and therefore their implications on PtG worthy of investigation.

4.2.3 Calculating run hours and average cost of electricity from the models

In this study, the envisaged system engages in the electricity market without priority as a large consumer, a similar purchaser approach was used to model charging electric vehicles [44]. This means that the consumption of electricity is technology neutral and that PtG will compete for energy (against storage or interconnection for example) as it would in a functioning electricity market. The PtG plants are assumed to be ideally flexible and the model does not include constraints or costs for start-up and shut-down. No mechanism or widespread precedence has been set that would allow a plant to consume energy, even that which would otherwise be curtailed, without engaging in the electricity market. This also means that as of now PtG cannot directly benefit from its ability to provide grid balancing services and receive "free" electricity, with some rare exceptions [45,46], though this is the subject of much discussion [10,14,47–49]. Thus, the bid price of the plant directly informs the number of runs hours. The formulae in Equations 4.2, 4.3 and 4.4 were used to extract

figures for run hours and average cost of electricity.

$$Run Hours (2016) = \frac{\sum Half hourl intervals for which SMP < Bid price}{2}$$
(4.2)

Run Hours $(2030) = \sum$ Hourly intervals for which SMP < Bid price (4.3)

Average Electricity Cost =
$$\frac{\sum SMP \text{ of Intervals for which SMP < Bid Price}}{Resultant Annual Run Hours}$$
(4.4)

4.3 Results and discussion

4.3.1 Electricity market data relevant to PtG

Figure 3 illustrates for how many hours in the year (2016 or 2030) electricity was available at a given price (\notin /MW_eh). As expected, there is a significant jump between \notin 30/MW_eh and \notin 45/MW_eh in all three datasets, the approximate range of the marginal cost of the large generators in the system. This implies that generation and demand are relatively matched for the majority (>5500 hours) of the year, limiting the opportunities for PtG to take advantage of system imbalances. At certain times, the SMP was also greater than \notin 300/MW_eh (typically less than 0.5% of the year) but this data was excluded in order to avoid skewness of the graph. An SMP of over \notin 300/MW_eh corresponds to times when demand significantly exceeded production.



Figure 4.3: Cumulative number of hours for which electricity is available at a given SM

Table 4.2:	The average SMP throughout the year for each of the electricity markets tested

2016 (25%)	2030 (40%)	2030 (60%)
41.83	58.91	56.08
	2016 (25%) 41.83	2016 (25%) 2030 (40%) 41.83 58.91

Table 4.2 gives the average system marginal price in each of the scenarios tested. For a number of reasons, the costs in 2016 are lower than those of the 2030 models. Within the 2030 models some of the increased electricity costs can be attributed to a projected increase in the use and price of natural gas, carbon taxes, and increased uplift costs. Natural gas traded at an unusually low average of \in 2.27/GJ plus shipping and charges in 2016 [50] and is included in the model at \in 3.84/GJ. It accounts for 43% of generation in 2016, 54% in 2030 (40% renewable penetration scenario), and 38% in 2030 (60% penetration scenario) [43]. The cost of coal falls from \in 2.77/GJ [51] to \in 1.58/GJ but accounts for only 3% of generation in 2030 compared to 17% in 2016 [43]. The carbon tax increases from \in 5.34/tonne [52] to \in 33/tonne whilst the uplift costs increase substantially from \in 3/MW_eh to approximately \in 56/MW_eh. These costs are reflected in the SMP, and as the LCOE of a PtG facility is a function

of the electricity market as a whole, it will also increase. It must also be noted that the average SMP is an incomplete measure of whether PtG LCOE will increase as the bid price methodology (outlined in section 2.4) aims to take advantage of periods of lower cost electricity, and switch off during high cost periods. It is not possible to accurately infer the LCOE from an average SMP, hence the need for further examination of the electricity market.



Figure 4.4: Change in average cost of electricity with increasing bid price

Figure 4.4 shows that the average price paid for electricity does not vary linearly with increasing bid price. At low bid prices there are very few run hours available, consisting of mostly near zero cost energy associated with difficulties in balancing the network. This is seen as the low, almost flat parts of the graph between €0-20/MW_eh. As the bid price is increased the number of hours during which the plant will now run increases rapidly. As higher price electricity is incorporated, the average cost increases. The large increase is then simply due to the plant moving from consuming a few hours of low-cost energy, to a much greater number of hours of energy at a significantly higher cost. The sharp rise at ca. €30/MW_eh corresponds to the jump in cumulative run hours around the average marginal cost of generation, noted in Figure 4.3. However, above ca. €50/MW_eh the numbers of additional units of electricity purchased now make up a less significant portion of the total and thus, despite their high cost do not affect the average to the same extent.

The exception being the 2016 data whose hourly prices were not so concentrated around the average marginal cost of production and where the lower levels of VRE penetration did not lead to these periods of low-cost energy resulting from grid imbalances. This leads to a more gradual increase in average cost versus bid price.

Similarly, Figure 4.5 shows that increasing the system bid price increases the run hours non-linearly. Again, a sharp rise occurs at ca. €30/MWeh corresponding to the large increase in cumulative run hours seen in Figure 4.3. The available run hours are greater in 2016 (25%) despite the smaller share of VRE as the cost of electricity is lower, therefore the bid price will be above the SMP for more of the time. Hours with SMP greater than €100/MWeh also occur much less frequently in 2016 (25%) than in either 2030 model. Only at bid prices less than €25/MWeh are there notably more run hours in the 2030 (60%) model than in either of the others. This implies that penetration levels of 60% RE are required in order to see substantial periods of low-cost energy due to difficulties in integrating VRE [8]. This also suggests that the existence of such low-cost periods (as seen in the 2030 (60%) model) does not necessarily increase the total hours a system will run for; an overall lower average cost of electricity does this to a greater extent.



Figure 4.5: Change in run hours with increasing bid price

This paper attempts to investigate the interactions between the bid price of a PtG system and its LCOE by looking at the effect on both run hours and electricity cost (inputs for the discounted cash flow model). Previous studies have shown that the electricity cost and run hours are highly sensitive parameters in determining the LCOE of PtG system [24,28,53–55]. The author's previous work explicitly identifies them as the two most sensitive process inputs [23]. This leads to the possibility of optimising the bid price (the parameter a PtG facility operator ultimately has control over and the one under investigation) to minimise the LCOE of a system. Other parameters such as curtailment, interconnection, and market rules are reflected in changes in the SMP, and hence the average cost of electricity and run hours. Thus, run hours and average price of electricity are sufficient to ascertain whether optimisation is occurring with respect to bid price. To the best of the authors' knowledge this has not been examined previously.

4.3.2 PtG interactions with the electricity market and effect on LCOE

Figure 4.6 outlines the increase in LCOE with the increase in average cost of electricity. For instance, increasing the average cost of electricity from ≤ 10 /MW_eh to ≤ 40 /MW_eh, a 300% increase, produces a 90% increase in the LCOE (from ≤ 60 /MWh to ≤ 114 /MWh). This increase in electricity cost is considerable and can be equated to an increase in electricity bid price from ≤ 28 to ≤ 60 /MW_eh, beyond the average marginal cost of generation.

In Figure 4.7 a non-linear relationship between run hours and LCOE is illustrated. Increasing the run hours from 2000 to 8000, again a 300% increase, produces a 51% decrease in LCOE (from €200/MWh to €98/MWh). This jump in run hours is not unrealistic and could be observed with modest increases in electricity bid price. Consequently, in many cases, the drop in LCOE associated with increasing run hours may potentially outweigh the rise due to increases in the average cost of electricity.



Figure 4.6: Change in LCOE with increasing cost of electricity and fixed run hours of 6500 per year



Figure 4.7: Change in LCOE with increasing run hours and a fixed cost of electricity of €35/ MW_eh

4.3.2.1 Combined effects on the LCOE of PtG

The combined effects of the parameters investigated in (Figures 4.4 to 4.7) culminate in the sharp drop in LCOE seen in Figure 4.8. This is a result of the dramatic increase in cumulative run hours between \in 30 and \notin 45MW_eh (seen in Figure 4.3) relative to increasing SMP. Thus, it is proposed that it is far more economical, in terms of minimising LCOE, to increase the system bid price and

hence its capacity factor. The drop in LCOE with increasing bid price implies that lower capacity factors will not be sufficient to amortise the project debt given the smaller quantities of gas produced. At bid prices greater than €50/MW_eh the majority of affordable energy has been captured, and so the cost is no longer compensated for by additional run hours. At these higher bid prices, the LCOE remains steady or begins to rise slightly. The bid price that minimises the LCOE is found to be approximately €50/MW_eh in this case.



Figure 4.8:Change in LCOE with increasing bid price including for associated variation in
run hours and average cost of electricity

Table 4.3:The LCOE of a PtG system bidding €50/MWeh in each of the three electricity
markets including its market interactions

Electricity market		2016 (25%)	2030 (40%)	2030 (60%)
Resultant	Run hours	7080	5714	5756
€50/MW _e h	Average cost of electricity (€/MW _e h)	34.41	38.16	32.39
LCOE (€/MWh)		100.90	116.85	106.08

The LCOE was 5% higher when using the market data of the 2030 (60%)

model, and 16% higher when using the 2030 (40%) model as compared to the recorded data for 2016 (25%). As Table 4.3 indicates, the 2016 (25%) average cost of electricity was higher than in 2030 (60%), but the run hours were much greater, compensating for this. As stated previously this is partially due to the lower prices of natural gas, carbon, and uplift compared to the 2030 models, leading to more sustained periods of electricity under the bid price.

Also contributing to this is the volatility of the SMP in the models. As well as increasing shares of VRE resulting in more hours of low-cost energy, hours of high-cost energy also become more prevalent. The SMP decreases when generation exceeds demand, and increases when demand exceeds supply. The frequency of both of these scenarios increases with additional VRE [6]. Defining high-cost as greater than €100/MW_eh, it is evident from Figure 4.3 that in 2016 (25%) this occurs for 180 hours, 1065 hours in 2030 (40%), and 1152 hours in 2030 (60%).



Figure 4.9: LCOE breakdown of a PtG system bidding €50/MW_eh in three electricity markets including for annual gaseous fuel output

In Figure 4.9 the variable OPEX, which dominates the LCOE, consists almost entirely of electricity costs. At higher production levels of gas, the LCOE falls and the contribution of capital expenditure (methanation, electrolysis, and other) diminishes. This again demonstrates that the increased capacity factor associated with a higher bid price leads to a more economical system. As capital costs fall the economic viability of PtG will still be largely dependent on affordable electricity. Access to electricity at a final purchase price of close to €25/MWeh for more than 6,000 hours appears unlikely in the Irish electricity market by 2030. Thus, it will be difficult for gaseous fuel from non-biological origins to achieve further cost reductions. Charges additional to the SMP (such as grid connection and taxes) will add to costs, however, incentives to produce an advanced renewable fuel may well more than offset these costs. Biomass sources such as wood chips are already close to competing with heating oil on a cost basis and so the environmental credentials can justify the switch; however, the same cannot be said for PtG derived gas as a transport fuel. The low market value of natural gas hampers the development of PtG, and carbon is not sufficiently priced to create an economic impetus for change. However, legislation requiring decarbonised bus fleets, directives mandating advanced transport fuels, and the requirement to reduce carbon intensity by 2050 to 20% of present levels will lead to gaseous fuel from non-biological origin competing with advanced biofuels (which at present are not as commercial) and electricity as a source of propulsion, which is not expected to be practicable for heavy goods vehicles and inter-city bus fleets [56].

The strategy identified here, bidding above the marginal cost of generation, has been shown to minimise LCOE by optimising run hours and electricity costs. It has the advantage of also producing larger volumes of gas than strategies predicated upon low-cost energy analogous to curtailment. In the event that increased gas production becomes more valuable, such as in the event incentives per unit of renewable fuel produced become available, this advantage becomes more significant. Scope would then exist to further increase the bid price, producing more gas, without considerable increases being made to the LCOE. This is true for all three models tested.

4.3.2.2 Running solely on low-cost or otherwise curtailed electricity

Previous literature has often assumed that PtG may only operate at times of excess or low-cost electricity (defined in this paper as less than €10/MW_eh), capitalising on market fluctuations largely due to the feed in priority of RE [25].

However, this work has shown that opportunities for PtG to take advantage of balancing issues and hence low-cost energy are limited. In the 2030 (60%) model 999 hours at an average cost of €0.28/MWeh are available, the most of all three models, due largely to the increased mismatch between VRE production and demand. This would still result in an uncompetitive LCOE of €273/MWh due to the low volume of gas produced (5.62 GWh/a). In the 2030 (40%) and 2016 (25%) scenarios only 58 and 12 hours of low-cost energy are available at average costs of €0.37/MWeh and €3.77/MWeh respectively, making running solely on low-cost energy entirely unfeasible in these markets. This highlights that increasing the share of RE to 60% increases the availability of low-cost energy (from 58 hours to 999 hours between the 35% and 55% VRE penetration scenarios in 2030), but not to the levels required to produce competitive PtG derived gas. PtG then can be said to be an increasingly attractive solution as the share of VRE grows, but only consuming in times of surplus VRE is not proposed to be a viable business model. The availability of large quantities of surplus electricity is symptomatic of an inefficient electricity network and thus is a resource that one aims to minimise.

Real world data may provide somewhat higher quantities than those modelled, as demand and generation will not be so well forecast, but not to the point where sufficient quantities become available [42]. Operating the plant only during these periods would not allow for amortisation of the capital expenditure. Consequently, a compromise must be found between amortisation and running the plant only during the cheapest hours. This phenomenon is essentially independent of the size of the system. The volume of gas a larger system would produce, in attempting to capitalise on the low-cost electricity, would be proportional to the increased capital cost of the system. The economies of scale associated with PtG are not sufficient for this to be economically viable due in part to their modular nature [24].

4.4 Conclusion

The effect on the LCOE of a PtG system when it interacts with the electricity market was examined. Three electricity markets at different shares of RE (25,

40, and 60%) consisting mostly of VRE were analysed for their interactions with a 10MW_e PtG facility. It was noted that the available run hours and average cost of electricity do not increase proportionally. Thus, it was found that increasing the bid price to beyond the average marginal cost of generation, approximately €35-50/MW_eh here, minimised the LCOE. Increased shares of VRE led to more hours of both high-cost (greater than €100/MW_eh) and low-cost (less than €10/MW_eh) electricity, but the number of low-cost run hours resulting from this was found to be insufficient to sustain a PtG facility alone. The bid strategy that minimised LCOE also produced the highest volumes of gas, ideally placing it to take advantage of incentives should they become available. Overall it was established that the viability of PtG relies on the availability of affordable energy for long periods of time and not positioning itself to take advantage of periods of low-cost energy.

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 5 Are electrofuels a sustainable transport fuel?
 Analysis of the effect of controls on carbon, curtailment, and cost of hydrogen⁹



Graphical abstract

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Abstract

Variable renewable electricity (VRE) decarbonises the electricity grid, but its intermittency leads to variations in price, carbon intensity, and curtailment over time. This has led to interest in utilising difficult to manage electricity to produce electrofuels (such as hydrogen via water electrolysis) for transport. The vast majority of the environmental impact of electrofuels is contained in the electricity they consume however, only consuming otherwise curtailed electricity (produced when supply exceeds demand) leads to prohibitively expensive hydrogen due to low run hours.

Using a model which bids for wholesale electricity, two operational strategies (controls) aimed at increasing sustainability without requiring policy changes were tested in electricity system models of 40% to 60% renewable electricity penetration. (1) Bid price control set a maximum price the plant will pay for electricity. (2) Wind forecast control dictated that the plant may only run when a minimum forecast VRE production is met.

It was shown that sourcing electricity at times of low cost or high forecast wind power can lead to more decarbonised hydrogen production (up to 56% more) at a lower cost (up to 57% less). When economically optimised (minimising levelised costs) the bid price control reduced the carbon intensity of the electrofuel produced by 5% to 25%, and the wind forecast control by 14% to 38%, compared to the grid average. Both controls demonstrated a high proclivity to utilising otherwise curtailed electricity and can be said to aid grid balancing. The bid price control also greatly reduced the average cost of electricity to the plant. The positive impacts increased with renewables penetration, and significant synergies between economic and environmentally conscious operation of the plants were noted.

The operational strategies tested in this paper allow for transport fuels to be produced from grid electricity, without exacerbating the mismatch of supply and demand. Future decentralised quasi-storage using these operating strategies may economically produce transport fuel, and aid grid balancing.

5.1 Introduction

In response to climate targets, high levels of Variable Renewable Electricity (VRE), in particular wind and increasingly solar, are being integrated into the electricity grid; with increasing shares of VRE come issues of grid balancing, stability, curtailment, and storage needs, potentially affecting security of supply [1,2]. It also leads to price volatility [3] and reduced system marginal prices [4,5], and as this paper aims to explore, fluctuations in the carbon intensity of the electricity generated, defined as the units of carbon dioxide emitted per unit of electricity generated, and later as units of carbon dioxide embodied per unit of fuel produced. Large scale and flexible energy storage options [6,7] as well as Demand Side Management (DSM) [8,9] and price controls [10] are seen as a means of reducing these effects with presently deployed solutions such as pumped hydro storage [11] insufficient to avoid significant dispatch down of VRE [12,13].

Electrofuels have been proposed as an advanced transport fuel, DSM of electricity, and a flexible storage mechanism for VRE. Power-to-Gas (PtG) is one such electrofuel whereby electricity is stored as hydrogen (H₂) via electrolysis of water. Thus, PtG changes the energy vector to a gaseous fuel from non-biological origin. PtG is gaining attention as a highly scalable flexible consumer [14], offering quick response for storing excess electricity and adding stability to the electricity grid [15], while producing an advanced renewable transport fuel [16,17]. The ability of PtG to rapidly ramp up and down demand allows it to utilise difficult to manage electricity [18,19] that may otherwise be curtailed [12,20]. Operating ideally, PtG offsets the need for energy imports and abates GHG emissions [21,22] by providing ancillary grid balancing services that enable further integration of VRE [15,20]. Converting electrical energy into chemical energy allows for large-scale storage through injection into existing gas grid infrastructure (subject to constraints [23]) or establishment of hydrogen fuelling stations, where it offers high storage capacity and discharge times [24]. It may also receive a fee for this service, aiding its economic viability. Many technology reviews and studies are available which detail the working principles, relative advantages and

disadvantages, and trends in PtG technologies [18,25]. Besides PtG other electrofuels (PtX) include methane, ammonia, dimethyl ether, and methanol all of which rely upon the electrolysis of water as the key enabling technology; therefore insights from this work are applicable to all PtX technologies [26].

Much of the focus of electrofuel research has focused on utilising surplus [27] or otherwise curtailed VRE [28,29], or as an alternative to network expansion [20,30]. However, previous work by the authors has shown that higher run hours are required for an economical system and therefore, surplus VRE alone is insufficient even at very high penetration levels [31,32]. The intermittency too would mean that large hydrogen buffers and storage would be required, and the actual volumes of gas produced would be limited, rendering the system prohibitively expensive. Yet, as we aim for higher levels of renewable energy in power systems the production of renewable synthetic fuels, as an alternative to fossil fuel products, is a path which demands more attention [33].

Furthermore, PtG can be positioned as a novel biogas upgrading solution, utilising its CO_2 content to produce renewable methane (CH₄) via a Sabatier reaction ($CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$). This could increase the sustainability of biogas plants, practically doubling methane output, potentially offsetting some of the capital required, and promoting a circular economy [17,18,27,34].

The EU have outlined that Renewable Energy Sources in Transport (RES-T) must hold at least a 14% share of energy in transport by 2030 [35]. PtG is promoted within the EU framework due to its low indirect land use change, potentially low carbon intensity, and waste to energy/circular economy characteristics. It is expected that the hydrogen produced will be used in the transport sector as this sector has low levels of decarbonisation and there are limited alternatives for advanced renewable transport fuel production [22,36]. As electric vehicles are likely to dominate the private passenger fleet, the best route for PtG is to displace diesel in heavy commercial long distance vehicles [22]. This is due to its superior energy to mass/volume compared to batteries, growing restrictions on particulate emissions, and associated proposed bans on diesel powered engines [22,37].

It is critical to maximise the sustainability of PtG from grid electricity for use as a renewable transport fuel. Several studies have concluded that the majority of the climate impact of PtG can be attributed to the electricity consumed in the electrolysis step [38–40]. Parra et al [41] indicated that electrolysis and its associated energy consumption contribute more than 90% of the potential environmental impacts (climate change, particulate matter, ozone depletion, eutrophication) of PtG with the electricity generation method being the most sensitive parameter. Similar results were found by Collet et al. and Reiter et al. who determined low carbon electricity was mandatory to achieve a sustainable production of PtG [42,43]. As such, reductions in the carbon intensity of the electricity consumed are analogous to reductions in the environmental impact of PtG. This concept is central to the paper.

The gap in the research identified is the use of static or average values for the carbon intensity of the electricity consumed [38–44]. This is inconsistent with the complexity of the interaction with the electricity grid of such systems [12,30], and challenges the prevalent simplified assumption that PtG is sustainable as it operates on curtailed renewable electricity alone [16,27]. Potential changes in the carbon intensity of the electricity consumed dictate the carbon intensity of the gas produced and understanding this is critical to fully understand the sustainability of PtG/electrofuel systems.

To test this, a PtG system will be modelled as a large flexible consumer within an electricity market with limited interconnection at renewable electricity penetrations of 40%, 50%, and 60%. Parameters the PtG plant operator can control, herein referred to as the "plant", will be varied to assess changes to carbon intensity of the hydrogen produced, cost of electricity consumed, and potential effects on curtailment.

In line with configurations found in the latest EU Renewable Energy Directive [35] that aim for PtG to consume low carbon and/or difficult to manage electricity, two methods are proposed. One, the plant will only run when the system marginal price (SMP) is below a threshold figure (Box 2), as drops in the SMP are indicative of balancing issues [3–5]. And two, a wind forecast control, will allow the PtG plant to run only at times when forecast wind

generation is above a threshold figure (Box 3). See Section 2.4 for further explanation. Within these two controls, Optimum high and Optimum low are defined. Optimum high is the application of the controls that would allow for 6000 run hours, Optimum low allows for 4200 run hours, identified in previous research as the upper and lower ends of a range that was found to minimise the levelised cost of energy (LCOE) of a PtG system [31,32].

This work advances upon previous research by the authors [31,32] in the relationship between a PtG system, the electricity grid, the running schedule, and the levelised cost of energy. To the best of the authors' knowledge this has not been done before. The objectives of the paper are to:

- Examine the effect manageable controls (operational strategies), bid price and wind forecast, have on the sustainability of an electrofuel system;
- Investigate the proclivity to utilise otherwise curtailed electricity and hence, the effect on demand for fossil fuel-based electricity generation when applying these controls;
- Compare and contrast these results to the grid average carbon intensity;
- Investigate the trends and change in sustainability of electrofuels with increasing shares of VRE.

5.2 Methodology

5.2.1 Power to Gas/Electrofuel system

The system modelled consists of electrolysis to produce hydrogen and auxiliary processes such as pumping, cooling, and compression to a minimum of 25 bar (Figure 5.1). It is assumed that when the controls have been met the electrolysers consume energy, without technical constraints such as ramp-up or buffer capacity. The current commercial state of the art electrolysis technology, polymer electrolyte membrane (PEM) has demonstrated the required operational flexibility [45,46]. Thorough descriptions of electrolysis can be found in past literature [47].



Figure 5.1: Graphical representation of the model

Electrolysis stack efficiency at NTP is estimated at 4.4kWh/Nm³ [31,48,49], compression energy consumption of 0.2kWh/Nm³ [48,50,51], and auxiliary power consumption of 0.1kWh/Nm³ [31]. This gives an overall efficiency of converting electricity to compressed hydrogen of 4.7kWh/Nm₃ or 75% (H₂ HHV of 3.54kWh/Nm³) for 2030, the period analysed. The carbon intensity of the compressed hydrogen (CO₂ embodied per unit) is then equal to the carbon intensity of the electricity (CO₂ emitted per unit) multiplied by the reciprocal of the conversion efficiency expressed as a decimal (see Box 1).

Box 1: Example of relationship between carbon intensity of electricity and that of hydrogen

An electricity carbon intensity of $200gCO_2/kWh$ will lead to a compressed hydrogen carbon intensity of $200/75\% = 266.6gCO_2/kWh$.

Inversely, a compressed hydrogen carbon intensity of $350gCO_2/kWh$ is indicative of an electricity carbon intensity of $350 \times 75\% = 262.5gCO_2/kWh$.

Results can be converted from g/kWh to g/MJ by dividing by 3.6.

Use 39.4kWh/kgH₂ to convert to kgCO₂/kgH₂ if desired.

Previous work concludes that relying on curtailed energy alone is uneconomical due to the small and intermittent volume of hydrogen that would be produced [31,52]. Therefore, grid connection and market engagement are essential for PtG systems. The electricity consumed constitutes the vast majority of PtG life cycle carbon emissions and wider environmental impacts [38–43]. This allows us to equate reductions in the carbon intensity of the energy consumed, with increases in the sustainability of the process. The results of applying the operational strategies (controls) detailed in this paper will be compared to the grid average and economically optimised PtG systems in terms of overall sustainability.

5.2.2 The power system models

The envisaged system engages in the Irish Single Electricity Market (ISEM) without priority as a large flexible consumer, a market similar to those around the world. Therefore, consumption of electricity is technology neutral and PtG will compete for energy against demand/storage/interconnection as it would in a functioning electricity market. The PtG plants are assumed to be ideally flexible and the model does not include constraints or costs for start-up and shut-down, ramp-up, or buffer capacity. No mechanism or widespread precedence has been set that would allow a plant to consume energy, even that which would otherwise be curtailed, without engaging with an electricity market. PtG does not directly benefit from its ability to provide grid balancing services and receive "free" electricity, with some rare exceptions [53,54], though this is the subject of much discussion [6,13]. Thus, the amount the plant is willing to pay for electricity (its bid price) directly informs the number of runs hours and when these hours occur unless the plant operates according to schedule (as may be informed by wind generation forecast). The bid price and up/down times of the plant are two parameters that a plant operator would control when interacting with the electricity market and therefore, using them to manipulate the sustainability and cost of the end product is worth investigating.

To determine the running schedule of the electrolysers, PLEXOS models of the ISEM in 2030 were developed. PLEXOS Integrated Energy Model is a power systems modelling tool used for electricity market simulations [55]. The power systems model develops an hourly System Marginal Price (SMP) for the ISEM based on current rules, and it has been benchmarked against historic market data and has been validated by the regulator to reproduce realistic results [56]. The SMP can be considered as the hourly island wide wholesale price of electricity. The model uses deterministic mixed integer linear optimisation to

minimise the costs of the electricity dispatched including for fuel costs, start-up costs, penalties for unserved energy, and a penalty cost for not meeting reserve requirements [57]. In general, the SMP is low when there is more than sufficient generation capacity online to meet demand, such as when wind power is being curtailed. When the amount of generation online to meet demand is scarce, the resulting SMP is higher. The SMP is set by the marginal costs of the last generator online to meet demand. In Ireland this is often gas fired generation. The SMP is also influenced by zero-marginal cost VRE which tends to supress the SMP in times of high VRE production. In times of excess VRE generation, curtailment may take place. Current electricity market rules offer VRE priority dispatch on the electricity grid, therefore curtailment of VRE is often a last resort. The model optimises thermal generation (fossil fuel and renewable), VRE, pumped storage, interconnection, as well as reserve classes subject to operational and technical constraints [16,58]. Also included are constraints on the unit operation of each power plant including minimum and maximum generation, minimum and maximum up and down time and the system ramp up and down rates, as well as a system level constraint consisting of an energy balance equation ensuring supply meets regional demand at each period [16]. The combination of these constraints, and the objective function of minimising production cost leads to the merit order, or the sequence in which the generators will be dispatched. Due to zero-marginal cost generation and/or renewables priority dispatch, wind energy and other renewables are first in the merit order meaning they run most consistently. The deficit is then made up of traditional generators. More detail on how ISEM operates can be found online [59,60].

Three PLEXOS models were tested at 40%, 50%, and 60% renewable electricity (RE) respectively with projected planned interconnection outside the island. Thus, as outlined in Figure 5.2, three energy mixes were tested.



RE – Renewable Energy, FF – Fossil Fuel



Renewable energy (RE) is calculated as delivered MW_eh of electricity from all renewable sources, as a percentage of total delivered electricity. VRE then only includes intermittent sources (wind, solar, and wave), and not those that are dispatchable (combined heat and power, co-firing of biomass, and hydropower) and therefore do not contribute to the fluctuations in supply that would affect price. The other Fossil Fuel (FF) portion of these charts consists mainly of coal, peat (co-fired with biomass), and small volumes of heavy fuel oil, all of which are dispatchable thermal generators.

These mixes represent potential future (2030) targets for Ireland [61]. The vast majority of this RE will be provided by wind and other intermittent sources. The 40% RE scenario is representative of a case where the rate of new installed RE capacity does not increase drastically beyond the levels seen today. The 60% RE scenario requires the rate of additional installed capacity of RE to substantially outpace that of increasing demand. The 50% RE scenario is an intermediate. Each of these is feasible and therefore their implications for PtG worthy of investigation. Table 5.1 outlines the various levels of VRE production in each scenario, data was obtained by analysing the output of the power systems model described above.

VRE production	40% RE	50% RE	60% RE
(MW)*			
Min	140	169	196
Average	2079	2540	3048
Мах	5931	6510	7370

Table 5.1: Characteristics of VRE production in each of the %RE scenarios

*Refers to the MW of VRE generated in a given hour.

5.2.3 Calculation of carbon intensity of electricity consumed

Should the control criteria be met for a given hour, the plant will consume electricity. As PLEXOS gives hourly data this calculation can be ran for each interval and hence a total number of run hours in a year established (Equations 5.1 and 5.3). Similar methods give us the average cost of electricity for said run hours (Equations 5.2 and 5.4). As well as SMP, the model also calculates the volume of CO₂ produced from electricity generation during each hour. By dividing the CO₂ emissions by the energy generated we calculate the carbon intensity in gCO₂/kWh in each hour (Equation 5.5).

Equations for bid price control:

$$Run Hours = \sum Hourly intervals for which SMP < Bid price$$
(5.1)

Average Electricity Cost =
$$\frac{\sum SMP \text{ of Intervals for which SMP < Bid Price}}{Resultant Annual Run Hours}$$
(5.2)

Equations for wind forecast control:

Run Hours = \sum Hourly intervals for which VRE forecast > Threshold (5.3)

Average Electricity Cost =
$$\frac{\sum SMP \text{ of Intervals for which VRE for cast > Threshold}}{Resultant Annual Run Hours}$$
(5.4)

Carbon intensity equation is applicable to both controls:

$$Carbon intenisty per interval = \frac{Hourly CO_2 Emissions}{Hourly System Generation}$$
(5.5)

5.2.4 Derivation and explanation of controls

5.2.4.1 Bid price control

Due to the effects of market interactions, merit order, the priority dispatch of renewables, zero-marginal cost VRE generators, and curtailment on the SMP, the authors hypothesised that low-cost electricity should be analogous to more sustainable electricity, as would be reflected in its lower carbon intensity. As the relationships between SMP, VRE production, and carbon intensity are complex, a direct correlation does not exist (as exemplified by an R² value, statistical measure of how close the data is to the fitted regression line, of 0.08 for VRE versus SMP in the 50% RE scenario). Export of electricity, pumped hydro storage, imports, priority dispatch, and the mixed portfolio of efficiencies and costs for generators make the relationship difficult to define and would require information beyond that available to those participating in the market. However, the bid price is controllable and if a PtG facility's bid price is below the marginal cost of generation of fossil fuel plants (Coal, Oil, Peat, and Gas) then the likelihood of it operating at times of high carbon intensity is much lessened, allowing operation on a majority VRE through market forces alone.

When generators are placed in descending order of capacity factor (ratio of actual output to maximum output) it is roughly equivalent to the merit order and hence, we can see how carbon intensity will change as demand increases and more generators are brought online. Market effects dictate that the low-cost and renewable generators tend to run first therefore, they have the highest capacity factors on the system. The same would not be true for an electricity market where coal was the ubiquitous low-cost baseload generator, however it is expected that an effective Emission Trading Scheme (ETS) price will be in place to act against this. Figure 5.3 shows that the plants with the highest capacity factor typically also have the lowest emissions; the first ten plants in Figure 5.3 are modern combined cycle gas turbines (CCGT).



Figure 5.3: Capacity factor and carbon intensity of electricity produced by large dispatchable thermal generators on the ISEM for 50% RE scenario. Each bar represents a single generator/plant.

In Figure 5.4 a marked increase in carbon intensity can be seen once cumulative capacity exceeds approximately 4500MW. It is at this point that additional older, more expensive, and less efficient generators will be dispatched beyond those already generating for power quality or network stability reasons, this will then be reflected in the SMP. This is due to the fact that the lowest marginal cost generators also tend to be the cleanest as seen in Figure 5.3.



Figure 5.4:Cumulative generation capacity and moving average carbon intensity of
electricity produced by large dispatchable thermal generators on the ISEM for
50% RE scenario. Each dot corresponds to a single generator/plant along the X-
axis.

In analysing the electricity market data, it is proposed that lower SMPs can be equated with lower emissions and higher VRE production; positive correlation has been found between increased shares of VRE and the periodic availability of low-cost electricity in other studies too, but this has not then been linked to carbon intensity [3–5,10,33]. For the analysis, the plant was only to run when the SMP was below a fixed value (Box 2).

Box 2: Bid price control, example of operation

Should the plant bid price be €50/MWh, and the current system marginal price (SMP) be €30/MWh, the plant will run. Once the SMP exceeds €50/MWh, the plant will turn off until such a time as the SMP falls below €50/MWh again. This applies to the results in Figure 5.9, Tables 5.5 and 5.6, and throughout.

5.2.4.2 Wind forecast control

Should the PtG plant only run at times when the levels of VRE in the energy mix are sufficiently high, the authors theorise that the likelihood of consuming high carbon electricity is lessened. In the case of the ISEM, VRE is almost entirely wind energy, thus, it is proposed that the PtG plant only run when predicted wind energy is above a certain level, referred to as the minimum wind forecast. Wind and solar energy forecast methodologies for the ISEM can be found online [62].

Information was collected to examine if forecast and actual wind generation closely matched, to verify the applicability of this operational strategy. The relationship between wind energy (99% of VRE in the ISEM) and the carbon intensity of the electricity was examined for similar reasons. Three separate approximately 30-day periods were tested, one of which included extreme weather events in order to fully test the robustness of the correlation. Data was downloaded from the EirGrid website as referenced; Table 5.2 outlines the information collected [63]. The periods examined are representative of an average wind energy (VRE) penetration of 34% and thus, overall RE penetration of 36% when including hydropower and other existing RE sources.

Table 5.2:	Data downloaded from EirGrid to test correlations
Table 5.2:	Data downloaded from EirGrid to test correlation

Period/Data	Forecast Wind	Actual Wind	Carbon	Extreme
	Generation	Generation	Intensity	Weather
	(MW)	(MW)	(gCO₂/kWh)	
1. 20/9/17 – 19/10/17	✓	✓	~	~
2. 28/1/18 – 26/2/18	\checkmark	✓	\checkmark	×
3. 27/2/18 – 28/3/18	\checkmark	✓	~	×

Figure 5.5 is graphical representation of the clear positive correlation between the forecast and actual wind generation for period 2. Regression analysis was carried out to quantify the relationship between the variables. The three periods were found to have very high levels of correlation (R-squared values of 0.83, 0.91, and 0.90 respectively). It can be concluded that forecasts provide sufficiently accurate data for the method to hold up to scrutiny at this stage.





Figure 5.6 indicates a clear negative correlation between actual wind generation and the carbon intensity of the electricity for period 2. Again, this is true for all three periods which have R-squared values of 0.81, 0.89, and 0.92 respectively.



Figure 5.6: Actual wind generation and carbon intensity of electricity for period 2.

The same regression analysis was carried out on the data from the PLEXOS models in an effort to further validate the models and ensure that correlations seen in real world data still applied (Figure 5.7). The 40%, 50%, and 60% RE models produced R-squared values of 0.91, 0.92, and 0.88 respectively across one complete year, confirming the relationships.



Figure 5.7: Carbon intensity of electricity and VRE generation for a thirty-day period of the 50% RE model, illustrative of the correlation.

In conclusion, if a PtG plant is to base its operating schedule on forecast wind generation it will lead to consuming energy in times of reduced carbon intensity electricity. For the analysis, the plant was only to run when certain levels of wind were predicted, expressed as a percentage of the average wind generated; this will be known as the wind forecast control (Box 3).

Box 3: Wind forecast control, defining a "150% wind" operational strategy

If average wind generation is 2500 MW, and the Wind forecast control dictates a 150% minimum for the PtG to run, therefore, PtG will "turn on" only when the forecast wind generation is above 3750 MW (2500 x 150%).

This applies to the results in Figure 5.10, Tables 5.7 and 5.8, and throughout.

5.2.4.3 Grid average and economically optimised PtG system

To assess whether positive carbon effects are seen and ensure that the controls do not sacrifice economic viability in an attempt to improve environmental sustainability, the results are compared to the carbon intensity of hydrogen from the grid average and of the economically optimised system. Too low run hours of the PtG plant may maximise environmental benefits but will not allow for project amortisation. Too high run hours and the system may be unnecessarily consuming energy, increasing its environmental impact without
reducing the Levelised Cost of Energy (LCOE) [32]. Optimisation was defined as minimising the LCOE by adjusting the bid price until the rise in average electricity cost was no longer compensated for by the subsequent increase in run hours under base 2030 cost assumptions, as per McDonagh et al. [31]. More details on this rationale and methodology can be found in McDonagh et al. [32].

As can be seen in Figure 5.8 sharp rises in LCOE are observed as PtG plant run hours fall below approximately 3800 p.a. with the plant no longer producing enough hydrogen to effectively pay back the capital cost. The optimum number of run hours was found to be between 4200 and 6000 p.a across all three %RE scenarios. In this case increasing run hours further will not reduce the levelised cost of the product hydrogen (LCOE) as the electricity during these additional hours is more expensive, and more emissive [32]. Thus, for the plant to remain economical two strategies to be tested were conceived: Optimum low is the required minimum wind forecast/bid price to allow 4200 run hours p.a.; Optimum high allows for 6000 run hours p.a.





Figure 5.8:Change in LCOE and run hours of a PtG system with increasing bid price for the
50% RE scenario. Equivalents for the 40% and 60% scenarios can be found in
supplementary data.

Table 5.3 contains the results for each scenario in terms of the carbon intensity of the compressed hydrogen produced.

Table 5.3:The carbon intensity of compressed hydrogen when consuming grid electricity
assuming 75% conversion efficiency (box 1) and the average SMP in each of the
%RE scenarios.

Hydrogen carbon intensity (gCO ₂ /kWh)	40% RE	50% RE	60% RE
Min	104	81	75
Average	324	295	303
Мах	720	641	711
Econ. optimised	308	274	269
Average SMP (€/MWh)	59	57	56

For reference Fossil Fuel comparator from the EU RED for transport is 338.4gCO₂/kWh.

The total emissions from the electricity grid are greater at 60% RE than at 50% RE due to increased (5.5 times) exports to the UK via an interconnector in the 60% RE scenario, and increased use of pumped hydro storage, indicative of the difficulties in facilitating very high VRE penetration. This is reflected in the increase in hydrogen carbon intensity between the 50% and 60% scenarios. The 40% RE scenario is a net importer via the interconnector and does not show such issues. The carbon intensity results of each of the economically optimised hydrogen systems is less than it would be from production from the respective grid average.

5.2.4.3.1 Measuring effects on curtailment

Ultimately the installed capacity of PtG is what determines the effect on curtailment, larger systems will capture more potentially curtailed electricity. However, should the plants have a tendency to consume at times of curtailment above that which could be attributed to randomness then the presence of PtG can be said to have a positive externality on the grid. By consuming during curtailment, PtG acts as a surrogate storage mechanism and reduces the peaks and troughs of the supply/demand curve. The consumption profiles that result from each control will be compared to Table 5.4, data which was collected by analysing the output of the power systems model.

Scenario	40% RE	50% RE	60% RE
Hours of curtailment	70	422	1213
Proportion of year	0.8%	4.8%	13.8%
Highest curtailment	823 MW	2131 MW	3686 MW
Typical curtailment*	300 MW	654 MW	1132 MW

 Table 5.4:
 Occurrence of curtailment in each scenario calculated over each one-hour period

*Typical curtailment calculated as the average of the non-zero hourly curtailment values thus, is the average value of curtailment when it occurs.

5.3 Results and Discussion

5.3.1 Bid price method

5.3.1.1 Bid price method optimises low cost hydrogen

Both the carbon intensity and run hours experience large increases at bid prices of approximately \leq 32-35/MWh (Figure 5.9). Below this the carbon intensity is significantly lower, showing a correlation between lower cost and lower carbon intensity electricity. A bid price of \leq 30/MWh leads to a 55-58% reduction in carbon intensity but only allows for 150, 557, and 1264 run hours in the 40%, 50%, and 60% scenarios respectively which even at the resultant low average costs of electricity will not make a viable system. However, the resource of low cost/low carbon electricity is shown to increase with increasing VRE penetration.



Note: 40%, 50%, and 60% relate to the percentage renewable electricity penetration. Therefore, "C intensity 50%" is the carbon intensity of hydrogen in the 50% renewable electricity penetration scenario, "Run hours 50%" is similarly defined. "RED FF Comparator" (334.8 gCO2/MJ) is the standard emissions value for fossil fuel transport, against which renewables are compared [35].

Figure 5.9: Change in carbon intensity of hydrogen produced and run hours of the PtG system with increasing bid price.

The trends in the lines for run hours are largely explained by the availability of less than $\leq 1/MWh$ electricity in the 60% scenario (962 hours), symptomatic of balancing issues, and the relative lack thereof in the 40% scenario (56 hours). Above bid prices of $\leq 30/MWh$ the lines begin to converge as the average costs are similar (Table 5.3) however, the maximum SMP is largest in the 60% scenario. Therefore, the number of run hours achieved at the highest end of the bid price range will be greater in the 40% scenario. The 50% scenario represents intermediate values.

Low (€35/MWh) and High (€70/MWh) bid prices were chosen as values that lay either side of the large increase in run hours observed in Figure 5.9. In all bid price controls the carbon intensity was reduced with the greatest effect seen at the lowest bid prices, confirming the hypothesis that lower cost electricity would be more sustainable in the ISEM. This effect was more pronounced as VRE penetration increased.

From Table 5.3 we see that a bid price of €35/MWh reduces the carbon intensity of the electricity consumed by 20-36% scenarios, but the system operates for sub-optimal run hours in all scenarios. A €70/MWh bid price allows for 3-7% reduction and can in fact run for longer than is necessary to minimise the LCOE while still producing positive carbon effects. In the economically optimised range we see a 5% (optimum high 40% RE) to 25% (optimum low 60% RE) reduction in carbon intensity. The synergies between economic and environmental operation are striking with reductions of 34-50% in the cost of electricity compared to the grid average within the optimised range. All scenarios see large drops in electricity cost, by far the largest contributor to PtG LCOE.

In Tables 5.5 and 5.6 "Optimum low" and Optimum high" refer to the required minimum bid price to achieve 4200 and 6000 run hours per annum respectively, see Box 1 and 2.4.3 for further details. "Low" and "High" are bid prices that lie either side of the large increase in run hours seen in Figure 5.9.

	40%	RE pene	tration		50%	RE pene		60% RE penetration				
	BP	RH	H ₂	DGA	BP	RH	H ₂	DGA	BP	RH	H ₂	DGA
		(AC)	CO ₂			(AC)	CO ₂			(AC)	CO ₂	
Low	35	1967	260	-20%	35	2543	219	-26%	35	3057	195	-36%
		(32)		(-46%)		(29)		(-49%)		(24)		(-57%)
Optimum	43	4200	289	-11%	41	4200	251	-15%	39	4200	228	-25%
low		(36)		(-39%)		(32)		(-44%)		(28)		(-50%)
Optimum	55	6000	309	-5%	54	6000	276	-6%	55	6000	273	-10%
high		(39)		(-34%)		(36)		(-37%)		(33)		(-41%)
High	70	6702	313	-3%	70	6757	283	-4%	70	6622	281	-7%
		(41)		(-31%)		(39)		(-32%)		(36)		(-36%)

Table 5.5: Results for carbon intensity and cost of bid price method

RE = Renewable Electricity, BP = Bid Price in €/MWh, RH = Run Hours, AC = Average Cost of electricity in €/MWh, $H_2 CO_2$ = Carbon intensity of hydrogen produced in gCO₂/kWh, DGA = Difference from Grid Average, the % difference between the resultant value and the average carbon intensity or average cost of electricity from that scenario

Example interpretation of Table 5.5:

We can see that in a 60% RE scenario bidding "Low" for electricity at €35/MWh will lead to run hours of 3057, an actual electricity cost of €24/MWh, and a hydrogen carbon intensity of 195 gCO2/kWh. These are 36% less emissive and 57% cheaper respectively than the grid average.

5.3.1.2 Bid price method enhances demand side management reducing curtailed electricity

The PtG system runs the vast majority of times during which VRE is being dispatched down as the bid price control disproportionally consumes otherwise curtailed electricity, likely due to curtailment being reflected in the SMP. The percentage of run hours that coincide with curtailment is greater than the average in all scenarios. Again, this has the effect of acting as both DSM and storage with the effect increasing with VRE penetration.

Table 5.6: Results for effect on curtailment of bid price control

	40%	RE pe	enetratio	n	50% RE penetration					60% RE penetration				
BP control	RH	HC	RH% (0.8%) ¹	C% (70) ²	RH	НС	RH% (4.8%) ¹	C% (422) ²		RH	HC	RH% (13.8%) ¹	C% (1213) ²	
Low	1967	61	3.1%	87.1%	2543	359	14.1%	85.1%		3012	974	32.4%	80.3%	
Optimum Iow	4200	66	1.6%	94.3%	4200	373	9.0%	88.4%		4200	986	24.3%	81.3%	
Optimum high	6000	70	1.2%	100%	6000	395	6.6%	93.6%		6000	1050	17.5%	86.6%	
High	6702	70	1.0%	100%	6757	400	5.9%	94.8%		6622	1100	16.6%	90.7%	

RE = Renewable Electricity, RH = Run Hours, HC = Hours where consumption coincides with Curtailment, RH% = % of Run Hours during which curtailment occurs, C% = % of total number of hours during which curtailment occurs that have been captured.

¹% of the year during which curtailment occurs in the given scenario from Table 5.4.

² Number of hours per year during which curtailment occurs in the given scenario from Table 5.4.

Example interpretation of Table 5.6:

We can see that in a 50% RE scenario bidding "Optimum high" in order to achieve 6000 run hours, the plant will run for 395 hours during which curtailment is occurring. This represents 6.6% of the system run time and a 93.6% match to times when curtailment is occurring, significantly greater than the grid average.

5.3.2 Wind forecast method

5.3.2.1 Wind forecast method allows synergies between decarbonisation and cost of PtG

If we recall Box 3 and the wind forecast control, the minimum wind forecast is the minimum volume of wind generation forecast in order for the PtG plant to run under this strategy. The plant will produce hydrogen if the forecast is greater than or equal to this set point.

From Figure 5.10, we see that the carbon intensity of hydrogen decreases as the minimum wind forecast for the plant to run increases however, associated run hours decline faster. This means the most environmentally beneficial system is unlikely to be economical without large incentives, as exemplified by the sub 3000 run hours above 120% minimum wind forecast.



Note: 40%, 50%, and 60% relate to the percentage renewable electricity penetration. Therefore, "C intensity 50%" is the carbon intensity of hydrogen in the 50% renewable electricity penetration scenario, "Run hours 50%" is similarly defined. "RED FF Comparator" is the standard emissions value for fossil fuel transport, against which renewables are compared [35].

Figure 5.10:Change in carbon intensity of the hydrogen produced and run hours of the PtG
system with increasing minimum forecast wind energy required to run,
expressed as a percentage of average wind generation.

From Table 5.7 we see that dictating for a minimum forecast of 150% wind reduces the carbon intensity of the electricity consumed by 39-56%, but as with the bid price control the system operates for sub-optimal run hours in all. A 50% wind threshold allows for an 8-14% carbon intensity reduction and again similarly to the bid price control means the system can in fact run for longer than is deemed optimal. In the economically optimised range we see a 14% (optimised high 40% RE) to 38% (optimised low 60% RE) reduction in carbon intensity. This implies there are synergies between economically and environmentally conscious driven operation of the PtG system, with all scenarios producing an average cost of electricity less than the grid average. The positive carbon effects of the wind forecast control are enhanced as the level of VRE penetration increases.

In Tables 5.7 and 5.8 "Optimum low" and Optimum high" refer to the required wind forecast to achieve 4200 and 6000 run hours per annum respectively, see Box 2 and 2.4.3 for further details. "150% wind" is used as an example of an operational strategy focused on producing low carbon fuel, and "50% wind" is a compromise of economic and environmentally conscious operation. These tables can be interpreted similarly to Tables 5.7 and 5.6.

	40% RE penetration)% F	RE pene	tration	1	60% RE penetration					
	MW	RH	H ₂	DGA	M	W	RH	H ₂	DGA	MW	RH	H ₂	DGA		
		(AC)	CO ₂				(AC)	CO ₂			(AC)	CO ₂			
150%	3118	1706	197	-39%	38	810	1781	157	-47%	4573	1713	132	-56%		
wind		(45)		(-24%)			(45)		(-21%)		(46)		(-18%)		
Optim	1909	4200	250	-23%	23	52	4200	210	-29%	2922	4200	187	-38%		
um		(50)		(-15%)			(50)		(-12%)		(50)		(-11%)		
low															
Optim	1364	6000	280	-14%	16	56	6000	245	-17%	2029	6000	233	-23%		
um		(54)		(-8%)			(54)		(59/)		(54)		(-4%)		
high									(-5%)						
50%	1039	7097	299	-8%	12	270	7075	264	-10%	1524	7127	261	-14%		
wind		(56)		(-5%)			(56)		(-2%)		(56)		(-		
													0.2%)		

Table 5.7:	Results for carbon intensity and cost of wind forecast method.
	······································

RE = Renewable Electricity, MW = Minimum Wind forecast in MW, RH = Run Hours, AC = Average Cost of Electricity in €/MWh, H₂ CO₂ = Carbon intensity of hydrogen produced in gCO₂/kWh, DGA = Difference from Grid Average, the % difference between the resultant value and the average carbon intensity or average cost of electricity from that scenario

5.3.2.2 Wind forecast method prioritises consumption of curtailed electricity

Table 5.8 shows that the wind forecast control could have a significant effect on curtailment. In all scenarios the percentage of run hours that contain curtailment are above average, meaning that they disproportionally consume otherwise wasted electricity. This effect is increased with increasing penetration of VRE and is somewhat intuitive as high levels of wind energy in the mix generally lead to some dispatch down of VRE. The wind forecast control inherently prioritises the consumption of potentially lost electricity generation acting as a form of DSM/storage.

	40% RE penetration					50% RE penetration					60% RE penetration					
WF	RH	HC	RH%	C%		RH	HC	RH%	C%		RH	HC	RH%	C%		
control			(0.8%) ¹	(70) ²				(4.8%) ¹	(422) ²				(13.8%) ¹	(1213) ²		
150%	1706	70	4.1%	100%		1781	403	22.6%	95.5%		1713	887	51.8%	73.1%		
Wind																
Optimum	4200	70	1.7%	100%		4200	422	10.0%	100%		4200	1213	28.9%	100%		
low																
Optimum	6000	70	1.2%	100%		6000	422	7.0%	100%		6000	1213	20.2%	100%		
high																
50%	7097	70	1.0%	100%		7075	422	6.0%	100%		7127	1213	17.0%	100%		
Wind																

Table 5.8: Results for effect on curtailment of wind forecast control

RE = Renewable Electricity, RH = Run Hours, HC = Hours where consumption coincides with Curtailment, RH% = % of Run Hours during which curtailment occurs, C% = % of total number of hours during which curtailment occurs that have been captured. ¹ % of the year during which curtailment occurs in the given scenario.

² Number of hours per year during which curtailment occurs in the given scenario.

5.3.3 PtG systems generate advanced transport fuels without irregular charging associated with electric vehicles

In purely carbon emissions terms all scenarios outperform the Renewable Energy Directive (RED) Fossil Fuel Comparator (FFC) within the energy mixes examined when producing hydrogen at 75% efficiency [35]. Electrofuels may have significant positive externalities before a fixed reduction target is met and there are advantages in terms of air quality, indigenous low input fuel production, facilitation of additional VRE, leveraging VRE in transport, and grid stability. The results in this work add weight to the argument that regulations should be adapted in relation to electrofuels as present regulations hinder their development, with special consideration paid to preventing a situation where grid electricity is consumed and substituted elsewhere with fossil generation [39]. The latest RED is an attempt at this [35]. Electrofuel contributions to renewable targets are complex but at a minimum are based upon the average share of RE in the country; for example, in a country with 70% RE, 70% of the hydrogen is counted as renewable [35]. When renewable generation can be matched with consumption and guarantees of origin given, or when the installation is used to relieve grid congestion the fuel may be counted as 100% renewable but may require a premium on the electricity cost [35]. These are significant as the volume of energy required to meet the RES-T targets is large, sufficient alternatives for advanced transport fuels are in short supply, and there is a proposed cap on first generation biofuels [35]. Electrofuels then contribute to a country's RES-T targets in much the same way as Electric Vehicles (EVs).

A possible criticism of electrofuels is their possible support of inflexible fossil fuel thermal generators. The operational strategies proposed in this paper largely avoid such issues as these same generators tend to have higher marginal costs and thus, in the presence of market forces, overarching RE targets, and increasing carbon taxes, will play a decreasing role in the future energy system. The load shifting characteristics mean PtG at various scales does not create additional peak load demand, may lessen the frequency of CCGT start-up/shut down, and act as DSM reducing need for less efficient generators to come online [10]. Employing these operational controls in PtG overcome disadvantages of EVs where charging is decentralised and erratic and may exacerbate the peaks and troughs that produce difficulty in balancing supply and demand.

5.3.4 Operational strategies reduce carbon intensity and cost of hydrogen produced

Both operational strategies reduced the carbon intensity of the hydrogen produced and disproportionately consumed otherwise curtailed energy, largely avoiding consumption in times of excess demand, with the wind forecast control doing both to a greater extent. The controls also allowed for reduced electricity costs aiding financial sustainability. By providing demand during times of curtailment the facility reduces the need to dispatch down VRE boosting its economic viability [16]. However, operating the plant only during periods of greatest environmental benefit would not allow for amortisation of the capital expenditure without significant grid services payments/incentives for either control [31,32]. Sufficiently monetising the services offered to the electrical grid could negate the need to consume unsustainable electricity; this is independent of the size of the system. What is most promising is that economically optimised systems showed GHG savings and this effect increased with increasing VRE penetration.

Across all scenarios the wind forecast control had greater environmental benefits, and more effectively captured curtailment than the bid price control. Periods of reduced carbon intensity and curtailment aligned well with high forecast generation delivering GHG savings. Wind forecast controls would be most applicable when the primary concern is maximising the use of VRE in electrofuels (positive carbon effects) and a sufficient incentive to produce electrofuels exists.

Dictating a maximum bid price for the system resulted in GHG savings too, though not as significantly as the wind forecast control. The mixed portfolio of marginal costs, efficiencies, and ramp capabilities mean that the point at which the electricity mix moves from VRE supported by CCGT, to more emissive generators (such as coal fired) is difficult to define. However, the bid price control also delivers large savings in electricity costs. Bid price controls are most applicable in a free market where PtG plant aims to minimise costs, and carbon savings are coincidental and synergistic.

5.3.5 Comparing electrolytic hydrogen from our scenarios to steam methane reforming

Hydrogen is a valuable input to many chemical processes, and the potential to produce low carbon hydrogen has also generated interest in its use as a transport fuel. It can be combined with carbon dioxide to create methane in the power to gas process [18] or used directly in fuel cells where compressed hydrogen offers superior charging times and energy density to batteries. Figure 5.10 provides a direct comparison between the electrolytic hydrogen produced in the scenarios tested and that derived via Steam Methane Reforming (SMR). Values of 8.9 to 12.9kgCO_{2-eq}/kgH₂ were found in literature representing the upper and lower limits of carbon intensity for SMR [40]. A value of 11.5kgCO_{2-eq}/kgH₂ is used in Figure 5.10 to allow for reduced fugitive emissions and the

use of partially decarbonised energy in the process. No fugitive methane is produced during electrolysis and so kgCO₂/kgH₂ to kgCO_{2-eq}/kgH₂ provides a fair comparison.



Note: Section 2.4.3, Table 5.5, and Table 5.7 provide brief explanations of the derivation of "Low", Optimum Low", "Optimum High", and "High"

Figure 5.10:Carbon intensity of the hydrogen produced from electrolysis using the Bid Price
and Wind Forecast methods in each RE penetration scenario, the carbon
intensity of SMR is shown for reference.

From Figure 5.10 it can be seen that at least 50% RE penetration is required to outperform SMR under all bid strategies in terms of carbon emissions. At penetrations of 50% and above significant reductions are noted implying that when aiming to displace fossil derived hydrogen, electrolytic hydrogen is suitable under these controls. These results are also of importance to those attempting to reduce the environmental impact of processes that consume hydrogen such as oil refining and fertiliser production.

5.3.6 Potential to displace fossil fuels in heavy goods transport

It is the author's opinion that the thermodynamic inefficiencies of hydrogen production and use, combined with the vast improvement in passenger Electric Vehicle (EV) technology make hydrogen passenger transport unattractive in the short to medium term. The figures below do not account for the difficulties the grid faces when charging a large number of electric vehicles, or the advantages of decentralised hydrogen production but they do illustrate the unsuitability of hydrogen to passenger transport in this context. From Box 5 it is clear that passenger EVs are far less emissive than Fuel Cell Vehicles (FCVs) and this unlikely to change significantly by 2030.

Box 5: Passenger electric vehicle (EV) versus fuel cell vehicle (FCV) emissions per 100km

Taking the 50% RE penetration scenario and assuming the EV charges at the grid average.

Hyundai Ioniq (EV) [64]: 15.5kWh/100km

 $\frac{15.5kWh/100km}{90\%\eta \ charging} \times \frac{221gCO_2}{kWh} = 3.8kgCO_2/100km$

Toyota Mirai (FCV) [65]: 67MPG_e ≈ 1kgH₂/100 km

From "150%" Wind forecast to "High" Bid price = $6.2 - 11.1 kgCO_2/100 km$

However, unlike passenger vehicles a clear alternative to fossil fuels suitable for Heavy Goods Vehicles (HGVs) has not arisen largely due to their energy density requirements, policy constraining first generation liquid biofuels (such as 3.6% cap for 2030 in RED), and prohibitive costs [66]. Hydrogen fuel cells are a promising technology for HGVs offering zero PM, NO_x, and SO_x emissions, and a route to low carbon transport. Box 6: Diesel versus hydrogen fuel cell heavy goods vehicle (HGV) emissions per 100km

Taking the 50% RE penetration scenario and a standard diesel truck in 2030.

Diesel HGV allowing for η improvements to 2030 [67]: 37I/100km

$$\frac{37l}{100km} \times \frac{2827gCO_2}{l_{diesel}} = 104.6kgCO_2/100km$$

Fuel cell HGV combined n of 55% [68]: 282kWh/100km

From "150%" Wind forecast to "High" Bid price = 44.3 – 79.8kgCO₂/100km

HGV operating on EU RED liquid biofuel [35]: Minimum 65% savings versus FFC of 94gCO_{2-eq}/MJ

Combusted in diesel engine assuming equal $\eta = 47 kg CO_2 / 100 km$

References and calculations can be found in the supplemental data.

Box 6 demonstrates a clear carbon saving in utilising hydrogen in FC HGVs well in advance of a fully decarbonised electricity system when utilising the controls tested. The FC HGV can deliver carbon emissions reductions comparable to that of an EU approved transport biofuel at 50% RE penetration while avoiding issues of air pollution. It is hypothesised that with the continued decarbonisation of the electricity system and the superior efficiency of FC HGVs, they will significantly outperform renewable liquid biofuels in the future.

5.4 Conclusion

This work examined the effect that two operational strategies (controls) which do not require changes in policy would have on sustainability: (1) dictating a plant maximum bid price for electricity and (2) a minimum forecast VRE production. Sustainability was measured through: changes in the carbon intensity of the hydrogen produced in a PtG (electrofuel) system; the effect on curtailment; and the cost of electricity consumed. Both controls were found to produce significant benefits in terms of reducing the carbon intensity. Also shown was the increased proclivity to consuming otherwise curtailed energy and to act as a quasi-storage mechanism, especially for the wind forecast control. Notably, synergistic effects between operating an electrofuel system to minimise levelised costs and environmental impacts were demonstrated, particularly for the bid price control. However, when greater environmental benefits were sought this was at the sacrifice of an economically optimised system. The carbon intensity of the hydrogen was found to be less than the fossil fuel comparator of the EU Renewable Energy Directive (RED) in all scenarios tested (40-60% renewable electricity generation) and particularly suitable for use in fuel cell heavy goods vehicles. Environmental and cost benefits were found to increase with increasing renewable penetration. Applying these operational strategies is in line with the visions of the RED and would make electrofuel production more sustainable in advance of a fully decarbonised electricity system, and at a time when increased options for decarbonised transport are required.

The results in this paper are applicable to power-to-X, cooperative charging, or any grid interaction when engaging as a wholesale consumer/agent in an electricity market.

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Please note that Chapter 6 (pp. 150-187) is unavailable due to a restriction requested by the author.

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7 Insights from co-authored work

The following sections briefly summarise observations and results from coauthored work that influenced the direction of Chapters 3 to 6 and added to the author's understanding of PtG. These are included to demonstrate the additional knowledge required to make the detailed conclusions found in Chapter 8.

7.1 The potential of power to gas to provide green gas utilising existing CO₂ sources from industries, distilleries and wastewater treatment facilities¹¹ Abstract

The suitability of existing sources of CO₂ in a region (Ireland) for use in power to gas systems was determined using multi criteria decision analysis. The main sources of CO₂ were from the combustion of fossil fuels, cement production, alcohol production, and wastewater treatment plants. The criteria used to assess the suitability of CO_2 sources were: annual quantity of CO_2 emitted; concentration of CO_2 in the gas; CO_2 source; distance to the electricity network; and distance to the gas network. The most suitable sources of CO₂ were found to be distilleries, and wastewater treatment plants with anaerobic digesters. The most suitable source of CO₂, a large distillery, could be used to convert 461 GWh/a of electricity into 258 GWh/a of methane. The total electricity requirement of this system is larger than the 348 GWh of renewable electricity dispatched down in Ireland in 2015. This could allow for the conversion of electricity that would be curtailed into a valuable energy vector. The resulting methane could fuel 729 compressed natural gas fuelled buses per annum. Synergies in integrating power to gas at a wastewater treatment plant include use of oxygen in the wastewater treatment process.

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7.1.1.1 Relevance to this thesis

PtG (methane) is capable of utilising any sufficiently scrubbed source of CO₂. In this paper the suitability of a source of CO₂ was assumed to then be a function of the concentration, quantity, origin, and distance to the electricity and gas networks. In reality, the weighting of each criterion differs with system envisaged. For example, should the renewable gas produced be used on site then distance to the gas network becomes irrelevant. Differentiating between biogenic and fossil CO₂ is important only if this process is intended for use in a larger bioenergy with carbon capture and storage (BECCS) chain [1], where emissions will be permanently sequestered, or the EU member state in which it is deployed has opted to not include recycled carbon fuels from fossil sources in its renewable energy targets [2]. CO₂ sources (gas streams) considered included power stations, various large industries, alcohol production, and wastewater treatment plants (WWTPs) all of which emit CO₂. Biogas production is in its infancy in Ireland and so a WWTP can be considered analogous.

The paper clearly demonstrated that CO₂ was available in excess and that the electricity required to generate stoichiometric H₂ will be the limiting factor. As one might expect, the results also show that the concentration of CO₂ in the gas stream considered impacts the process viability immensely. Alcohol production and WWTPs stood out as the most suitable sources at 99% CO₂ in flue gas and 40% CO₂ in biogas respectively. The energy penalty associated with their use was negligible as both could be used in a methanation process, biological or catalytic, with only minor gas cleaning [3,4]. The suitability of distilleries and breweries who produce large volumes of highly concentrated biogenic CO₂ is clear, especially for the catalytic methanation (CM) process. WWTPs also produce large amounts of CO₂ suitable for PtG and have an onsite demand for oxygen. Combined with biological methanation (BM) WWTPs could provide highly flexible decentralised small-scale electricity storage whilst improving plant efficiency [5].

From this one could conclude that although technically feasible combining PtG with dilute sources of CO_2 (direct air capture, flue gases from fossil fuel power plants, cement production exhaust) is undesirable. To make this route

preferable severe restrictions or penalties much beyond what is expected would have to apply to CO₂ emissions. Therefore, PtG should first be implemented at the most suitable sites to maximise environmental benefits, identified here as alcohol production facilities and WWTPs, particularly if incentivisation is under consideration.

This result can be applied to all forms of carbon capture and storage, when aiming to sequester CO₂ the flue gases of a power station are an inferior source both technically and economically. This an area of much research and debate, perhaps due to the policy landscape that exists and the characteristics of the power they supply [6].

7.2 Cascading biomethane energy systems for sustainable green gas production in a circular economy¹²



Graphical abstract

Abstract

Biomethane is a flexible energy vector that can be used as a renewable fuel for both the heat and transport sectors. Recent EU legislation encourages the production and use of advanced, third generation biofuels with improved sustainability for future energy systems. The integration of technologies such as anaerobic digestion, gasification, and power to gas, along with advanced feedstocks such as algae will be at the forefront in meeting future sustainability criteria and achieving a green gas supply for the gas grid. This paper explores the relevant pathways in which an integrated biomethane industry could potentially materialise and identifies and discusses the latest biotechnological

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advances in the production of renewable gas. Three scenarios of cascading biomethane systems are developed.

7.2.1.1 Relevance to this thesis

This review paper examines biomethane production from waste, second generation (no competition with food), and third generation (no land use) feedstocks. The technical feasibility of integrating processes is explored and possible future scenarios are developed. As expanded upon in the literature review, PtG sits at the juncture of gas, electricity, and renewables policy. In creating and examining the scenarios, a number of roles for PtG emerged, not just as a hydrogen production facility, but as part of a wider renewable gas system. In this paper PtG is seen as a provider of ancillary electricity grid services, a form of biogas upgrading [4], and a source of oxygen for gasification plants improving the quality of syngas produced [7]. PtG also increases biomethane resource in regions with large VRE potential [8]. In this model PtG offers services and the hydrogen produced is no longer the sole valuable product. This combination is somewhat idealistic, but it illustrates the potential of integrated systems.

The falling costs of electrolysers will mean they can operate less frequently, lowering the likelihood that they operate on high cost or high carbon electricity. This intermittency is more suited to biological systems and may be \serendipitous. For example, micro-algae may be used in photosynthetic biogas upgrading. Photo-autotrophic micro-algae require light and as such grow best by day in open ponds, absorbing the CO₂ content of the biogas and upgrading biogas to biomethane [9]. By night as demand for electricity decreases, surplus renewable electricity may be available for hydrogen production, which can be combined with the CO₂ in the biogas to produce high quality biomethane . Overall, this paper serves to show that PtG can offer flexibility to the electricity grid, and simultaneously increase the flexibility of future integrated renewable gas systems.

7.3 Modelling power-to-X applications in the Nord Pool electricity market: Effects of different bidding strategies on plant performance¹³

Graphical abstract



Abstract

The operation of power-to-X systems requires measures to control the cost and the carbon intensity of electricity purchased from the spot market. This study investigated different bidding strategies for the Nord Pool power exchange dayahead market, with a special focus on Sweden. A price independent order (PIO) strategy was developed assisted by forecasting electricity prices with an artificial neural network. For comparison, a price dependent order (PDO) with fixed bid price was used. The bidding strategies were used to simulate H2 production with both alkaline and proton exchange membrane electrolysers in different years (2016, 2017 and 2018) and technological scenarios (2020, 2030 and 2040). Results showed that using PIO to control H2 production helped to

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avoid the purchase of expensive electricity during peak loads, but it also reduced the total number of operating hours compared to PDO. For this reason, under optimal conditions for both bidding strategies, PDO resulted in an average of 10.9% lower levelised cost of H2, and more attractive net cash flows and net present values than PIO. Nevertheless, PIO showed to be a useful strategy to control costs in years with unexpected hourly price behaviour such as 2018. It also demonstrated an ability to avoid electricity consumption during peak loads, often associated with fossil-based electricity in many regions. Furthermore, PIO could be successfully demonstrated in a practical case study to fulfil the on-demand requirement of an industrial captive customer. It was also demonstrated that given current and future estimates of cost and performance, proton exchange membrane electrolysis will likely outperform alkaline electrolysis before 2025 on a lifecycle basis.

7.3.1.1 Relevance to this thesis

Electricity markets and energy mixes vary by region [10]. Thus far the work has focused on the Irish electricity system. This work focuses on the Nord Pool electricity market in order to gain new insights, and test theories developed in previous papers. The Nord Pool (SE4) is dominated by hydropower with some VRE, which in many respects may be well suited to PtG. This work was also used to apply new tools to PtG studies and further examine electrolysis technology choice.

Two strategies are tested; (1) optimising the bid price of a PtG facility in order to minimise the levelised cost of hydrogen (LCOH), and (2) purchasing electricity predominately to satisfy local hydrogen demand. Strategy (1) is similar to that found in Chapter 4 and is used for reference, producing as much hydrogen as is required to minimise the LCOH. Strategy (2) uses a feedforward Neural Network to predict hourly day ahead electricity prices. The PtG system is then ran during the predicted lowest cost hours of electricity, and surplus hydrogen is injected into the natural gas grid. The rationale is that hydrogen storage is expensive and hydrogen's value as a transport fuel is much higher than its value in the natural gas grid [11]. The paper also considers the effect of technology (AEL vs PEM electrolysis) on the system performance, and the utilisation of waste heat in local district heating.

Both strategies avoided the purchase of high cost electricity, analogous to system imbalance in the region and can be said to have a positive effect on the electricity grid [12]. Producing hydrogen to demand resulted in a ca. 11% higher LCOH than when aiming to minimise LCOH alone, but optimisation could reduce this. Although more expensive per unit of gas, the lower capacity factor of the electrolyser meant that the gas was produced as required and could be used as a higher value transport fuel, potentially improving plant economics by avoiding storage and minimising low value grid injection. Selling waste heat to a local district is environmentally beneficial but a low heat value means plant economics are not greatly affected, reducing LCOH by only 4.2%.

The dynamics of electrolyser operation were investigated and showed that the energy penalties for cold/warm standby mode and for bringing the system into service did not significantly impact plant economics at 1.5% of electricity purchase costs. Again, it was shown that overall electricity purchase and the number of run hours are the main cost drivers. Through further analysis it was revealed that PEM electrolysis will outcompete AEL electrolysis no later than 2025, possibly as early as 2021, due to the higher efficiencies and falling costs.

In conclusion, this paper found that Neural Networks¹⁴ are not optimal to reduce electricity cost to a PtG plant but will help reduce costs when producing hydrogen according to the delivery requirements of a consumer. Hydrogen demand will soon be better served by PEM electrolysis and valorising waste heat does not affect plant income greatly. Finally, defining hydrogen storage costs are vital to future optimisation.

¹⁴ Much of the code used is available as part of MATLAB's machine learning toolbox detailed at the following link: <u>https://www.mathworks.com/matlabcentral/fileexchange/28684-electricity-load-and-price-forecasting-webinar-case-study</u>

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8 Conclusions and Recommendations

The costs and environmental impact of PtG are dominated by the electricity it consumes. This is the case now and into the future. Early concepts of converting "free" or otherwise curtailed electricity to hydrogen were misleading, but by engaging in the electricity market the significant potential of PtG as a source of low carbon advanced fuels can be realised. In advance of a fully renewable electricity network, strategies that reduce the cost and carbon intensity of the hydrogen or subsequent methane produced can be employed. PtG may also perform biogas upgrading, energy storage, and electricity grid system stabilisation, displaying a unique ability to integrate the bioenergy, electricity, gas, and transport sectors. Given the right policy and incentives, PtG can leverage the success of renewable electricity to offset fossil fuel use, balance the electricity grid, and overall accelerate the energy transition.

8.1 Contributions of this thesis

This work began at a time when detailed PtG research was in its infancy. Difficulty in finding reliable figures for component costs and a means of comparing PtG with other advanced fuels led to a desire to calculate a LCOE. Chapter 3 describes the first paper to provide a referenceable table of PtG costs over time, which were used to build a cash flow model. At the time of publication this was novel and provided a necessary base for further research. Chapter 4 then shows that contrary to much of the contemporaneous literature, basing PtG on otherwise curtailed energy is not financially viable. It also shows that electricity purchasing strategy will achieve greater cost reductions than the anticipated technological improvements, taking advantage of the peaks and troughs of the wholesale market. This is again contrary to much of the literature which instead focused on efficiency improvements and combining processes. The sustainability of PtG was uncertain however a specific contribution of Chapter 5 was to demonstrate that markets forces mean that PtG does not in fact support inflexible fossil fuel generation and is sustainable in advanced of a fully decarbonised system. Chapter 6 highlights again that curtailment will not

be the main driver of PtG investment, and it is the achievable price for the hydrogen produced that dictates investor interest. PtG does not sufficiently internalise the positive externalities which needs to be addressed if it is to play a significant role in the energy transition, a novel insight.

8.2 Addressing the high-level objectives of the thesis

At the start of this thesis a number of issues with PtG were identified including: uncertainty in cost modelling; identifying sustainable applications; and a lack of guiding literature for industry and policymakers. From these, four high-level thesis objectives were set out and addressed in each of the chapters.

Develop a model of PtG costs and the breakdown of such (Chapters 3 and 4)

- An optimised PtG lifecycle was developed including for component replacement.
- A bespoke cashflow model was created, which assessed income and expenditure over the lifetime of the PtG system.
- Levelised costs including sensitivity analysis were calculated.
- The contribution to levelised costs of each component was calculated.

Identify and address areas where improvements would be most beneficial (Chapters 3 and 4)

- Electricity purchase was identified as the largest contributor to levelised costs.
- A model of an electricity system was used to optimise electricity purchase.
- The relationships between levelised cost and plant parameters were defined.
- A strategy to minimise levelised cost without requiring policy changes or information not available to PtG operators was developed.
Develop optimisation strategies for cost and sustainability

(Chapter 5 and 6)

- Both cost and sustainability are driven by electricity consumption.
- High cost and carbon intense electricity were found to correlate.
- Controls allow PtG to operate during times of high wind forecast, or lowcost electricity.
- Large synergies exist between economic and sustainable operation.

Evaluate interest in, and potential applications for, deployment of the technology (Chapter 6 and 7.3)

- Pairing PtG with offshore wind is a promising solution.
- Interactions and conditions required for investment in PtG were described.
- PtG for local hydrogen demand and waste heat utilisation was explored.
- Beneficial policy and incentive solutions are considered.

8.3 Chapter highlights

Chapter 3 – Modelling levelised costs

- Base LCOEs of €124/MWh in 2020, €105/MWh in 2030, and €93/MWh in 2040 were found for PtG (methane).
- Electricity is by far the largest contributor to the LCOE of a PtG system.
- Zero cost electricity for 6500hrs/annum leads to a LCOE of €55/MWh.
- A 20% fall in LCOE requires a drop of 76.2% in CAPEX or a 35.9% decrease in electricity costs.
- Integration, secondary incomes, and incentives or tax exemptions are essential for competitive PtG.

Chapter 4 – Optimising electricity purchase

• The viability of PtG depends on the electricity market in which it operates.

- Solely consuming cheap or otherwise curtailed energy is not economically viable as the resultant LCOE is too high.
- Low bid prices lead to lower run hours and insufficient capacity factor.
 Higher bid price leads to a more economical system, producing more gas at a lower LCOE.
- Bidding above the average marginal cost of generation minimises the LCOE.

Chapter 5 – Electrofuel sustainability

- The carbon intensity of hydrogen produced from grid electricity is reduced with both wind forecast and price controls.
- Controls allow for preferential use of otherwise curtailed energy, and aid grid balancing of VRE.
- Significant reductions in the average cost of electricity are also noted when using the controls.
- Positive effects of both controls increase with increasing share of renewables and allow sustainable PtG in advance of a fully decarbonised electricity grid.

Chapter 6 – Hydrogen from wind

- A LCOE of €42.3/MWh_e for the wind farm gives a LCOH of €96/MWh_{H2} (€3.77/kg) should all of the electricity be coverted to hydrogen.
- The viability of the hybrid (PtG) business case lies more with with hydrogen value, as opposed to curtailment abatment.
- At €102/MWh_{H2} (€4/kg), 17% curtailment is required for hybrid system NPV to exceed that of a wind farm alone.
- A 30% fall in PtG costs would allow all electricity to be converted to hydrogen and to be as profitable as a wind farm selling electricity alone.
- Incentivisation should be considered and could be recovered from system benefits.

Chapter 7 – Co-authored work

- PtG at a biogas plant offsets some of the traditional upgrading costs.
- At WWTPs the oxygen can be economically and readily utilised.
- The alcohol industry produces CO₂ streams highly suited to PtG.

- PtG may feature in future integrated renewable gas systems as an upgrading solution, as an oxygen supply to gasification, and as an electricity grid balancing mechanism.
- Producing hydrogen on demand is more expensive but can allow access to better markets at lower costs.
- PEM electrolysis outperforms AEL, but the flexibility it offers is not the primary cause, rather increased efficiency and greater cost reduction potential.

8.4 Detailed conclusions

Several of the results from this thesis can be used to draw conclusions on different aspects of PtG. Insights from the chapters are contextualised below with respect to what the author considers key debates within PtG, helping to define its potential future role. As the electricity used in the process is central to the cost, environmental impact, and positive externalities, it is examined here from several perspectives.

8.4.1 System configuration

Investigating the likely running schedule of a PtG plant facilitated choosing the optimal technology configuration. Key considerations include: when the plant will be built; the source of carbon dioxide if any (none required for PtG (hydrogen); the intermittency of the electricity and hydrogen supplies; and cost.

8.4.1.1 Electrolysis

AEL is a mature technology and currently outperforms PEM over the lifetime of a PtG system due to its lower upfront costs. However, the continued development of PEM means that between 2021 and 2025 it will be preferred as the increased efficiency will outweigh the higher investment costs. It is justified to pay up to 46% more in CAPEX for PEM and still reduce the LCOE should the efficiency of PEM be 5% greater than AEL. The higher start up and nonoperating hours (NOH) costs of the less flexible AEL do not affect plant finances greatly, but higher PEM flexibility mean it can offer ancillary grid services which may form an important part of the business model of future PtG projects.

8.4.1.2 Methanation

Economies of scale and the carbon dioxide source influence the choice of technology here. Above 10MW_e catalytic methanation is preferred due to its lower costs per unit of gas upgraded. The potential for waste heat utilisation is also significant, but dependent on local conditions. Below 10MW_e the higher flexibility and tolerance of impurities of biological methanation may make it more suitable. Biological methanation offers great potential in decentralised systems with application to existing biogas facilities, due to the relative simplicity and comparability to the anaerobic digestion system. Only catalytic methanation is considered mature with respect to PtG applications due to its previous applications in the petrochemical industry.

8.4.2 Electricity purchase

Procuring electricity proved to be the largest cost to the system and strategies aiming to reduce this were developed in this thesis. These strategies were tested in electricity markets of various shares of VRE.

8.4.2.1 Minimising levelised costs in a given market

In order to minimise the levelised cost of the gas produced it is necessary to run for a considerable number of hours in a year such that sufficient gas is produced to amortise project debt. Depending on the specifics of the market this is approximately 4200 to 6000 hours p.a. It was noted that the run hours and average cost of electricity do not increase proportionally. Thus, increasing the bid price to beyond the average marginal cost of generation (approximately €35-50/MW_eh in Ireland) minimised the LCOE. Beyond 6000 hours p.a. the

plant begins to consume more expensive electricity, producing more gas but without a reduction in levelised costs. Eventually the levelised costs will increase as the most expensive electricity is consumed. Optimisation in terms of plant profitability is dependent on the value of the gas produced and the size of the market.

8.4.2.2 Satisfying a local demand

It was shown that forecasting electricity prices can allow a PtG facility to choose the lowest cost hours to operate in to meet consumer demand. This minimises the LCOH without producing excess hydrogen that may prove costly to store. It also proved beneficial in dealing with fluctuations in cost due to the effects of VRE or unusual weather, as in the case of a drought affecting hydropower reserves.

8.4.3 Electricity network and market interactions

PtG is promoted in part due to the potential benefits its presence has on the electricity grid. It if were the case that PtG negatively impacted the operation of the grid, it would be difficult to justify its presence in light of storage alternatives. However, this thesis has shown that the externalities of PtG are positive.

8.4.3.1 Increase shares of VRE

By effectively turning on and off to accommodate VRE through either price signals or forecasting, PtG acts to decrease the system non-synchronous penetration (SNSP) and allows more instantaneous VRE on the grid. The controls tested were shown to largely avoid operation during high demand (analogous to high cost) and provide a consumer in times of low demand. This was true even when economically optimised with synergistic effects increasing with increasing VRE penetration. A grid with flexible demand such as PtG would be able to accommodate more VRE by virtue of PtG engaging in the market.

In markets with inflexible capital-intensive base load plants, this can mean that PtG reduces the requirement to ramp down generation in times of high VRE,

reducing system balancing costs. For nuclear or hydropower this is also environmentally beneficial, though for fossil fuel plants this can be deemed undesirable.

8.4.3.2 Running on curtailment alone

Improvements in grid management have meant that curtailment (generally reflected in low prices) has not increased dramatically, nor is it expected to. Increased shares of VRE increase the availability of both high and low-cost electricity but only in an inefficient electricity network would surplus electricity be consistently available at low cost. The number of low-cost run hours is insufficient for an economic PtG facility. Even in a 60% renewable electricity system with limited interconnection only 999 hours p.a of electricity at less than €10/MWh are available. Thus, engagement in the market is necessary and provides a route to utilising these low-cost hours. Positioning PtG to take advantage of periods of curtailment alone is not viable.

8.4.3.3 Ancillary electricity grid services

PtG can offer services to the electricity grid beyond simple storage. Electrolysis, specifically PEM, can adjust power consumption in order to provide demand side management and frequency control. A reduced rate for electricity in lieu of such flexibility may constitute a significant part of PtG business models in the future, or the service may indeed command a fee. Markets currently value flexible generation though, and any such arrangements are speculative.

8.4.4 Cost of PtG

Reductions in the cost of PtG will prove to make projects more attractive. The effects of these anticipated cost reductions on levelised costs were investigated to identify areas where improvements would be most beneficial.

8.4.4.1 Levelised costs

Besides electricity purchase (56%) the majority of the remaining levelised costs were found to be made up of capital expenditure and operating costs. Electrolysis accounts for 25% of levelised costs, fixed operating expenditure 10%, and methanation just 7.5%; this means even large reductions in their costs will produce only modest improvements in the LCOE. The LCOE though is sensitive to the discount rate and reduced project risk or favourable debt to equity ratios may decrease this.

8.4.4.2 Incentivisation of PtG

By nature, PtG leads to a higher Gross Domestic Product (GDP), higher levels of quality employment, and fewer energy imports (should indigenous renewables be used). There are system wide benefits in PtG systems converting difficult to manage energy, reducing balancing costs and increasing the profitability of generators. Therefore, an incentivise should be offered cognisant of said benefits. Should system savings fund an incentive it would make PtG potentially much more competitive than other advanced fuels, catalysing further adoption.

8.4.4.3 Valorising waste heat and oxygen

The utility of waste heat is specific to the configuration and technology. Should a local demand exist electrolyser waste heat may provide a relatively small additional income; there is greater potential for catalytic methanation. Selling the oxygen produced could also provide additional income, but this market may quickly reach saturation. These supplementary incomes would be advantageous to individual projects, as demonstrated in chapter 3 and 7.3, but are unlikely to significantly contribute to the future success of PtG on a large scale.

8.4.5 Environmental impact

The GHG emissions and environmental impact of PtG are a function of the electricity utilised. The conversion inefficiencies mean that should PtG use electricity at 250gCO_{2eq}/kWh_e and 70% efficiency, the resulting hydrogen has a carbon intensity of 357gCO_{2eq}/kWh_{H2}. Therefore, reducing the carbon intensity of the electricity utilised is of great benefit to the process.

8.4.5.1 Source of electricity

As PtG has been demonstrated to utilise low value and fluctuating electricity well, its use is suited to grids with high shares of wind and/or solar energy. It would also be suited to low carbon nuclear or hydropower base load grids.

Significant GHG savings are seen in the scenarios tested and PtG has a proclivity to consume otherwise curtailed energy, thus PtG should be installed even in advance of a fully decarbonised grid if a demand for fossil hydrogen or methane can be displaced.

PtG should not be implemented in carbon intense grids. As hydrogen, PtG may improve upon the recast Renewable Energy Directive (RED) fossil fuel comparator (FFC) in grids with greater than 40% renewable electricity. As methane, it may do so at greater than 60% renewable electricity, provided controls are used. Besides renewable electricity should coal (and not natural gas or another lower carbon alternative) make up a high proportion of the remainder of the electricity mix these figures would be significantly higher.

Notably, synergistic effects between minimising costs and environmental impacts were observed however, when further environmental benefits (reduced carbon intensity) were sought, levelised costs increased due to lower run hours.

8.4.5.2 As a transport fuel

Transport is a particularly difficult sector to achieve emissions reductions in and offers the most likely entry into the market for PtG. The market value of transport fuels is higher than for heat and electricity making competitiveness more likely. Restrictions on air pollution also favour the uptake of PtG. Finally, the predictable demand, influence of policy, and lack of alternatives for heavy goods vehicles make it a promising route.

In the form of methane PtG is technically attractive as natural gas vehicles are already gaining market share with additional refuelling infrastructure built and more being deployed. The hydrogen path is much less mature but offers zero carbon exhaust emissions and vehicle running costs that are potentially lower than their diesel or methane equivalent. PtG can deliver GHG savings in much the same way as electric vehicles, moving energy demand away from liquid fossil fuels into the increasingly decarbonised electricity system.

8.4.6 Choice of energy vector

In this thesis the use of both hydrogen and methane was considered. The efficiency of first converting electricity to hydrogen and then to methane leads to an increase in the levelised cost and carbon intensity in inverse proportion to the respective efficiency. Thus, the conversion to methane should be carefully considered. For example, even at no additional expense conversion from hydrogen at €100/MWh would result in a methane cost of €133/MWh at 75% efficiency.

The lower costs, more dynamic process, and relative simplicity of hydrogen production is somewhat negated by the lack of infrastructure. Should that become available the author believes hydrogen will be a superior vector to methane.

Until then methanation may be a useful or indeed a necessary step that allows relatively unrestricted access to existing infrastructure where methane is more easily stored and transported. The ability to trade "green gas certificates" through the gas network similar to the electricity guarantees of origin may also justify the additional step.

8.4.7 Potential applications of PtG

Unless generous incentives are introduced PtG competitiveness is dependent on taking advantage of multiple potential revenue streams. The various services offered must be capable of being combined and monetised. Different elements of likely future PtG business models are commented upon below with respect to the results of this thesis.

8.4.7.1 Grid injection

Access to the gas network can connect PtG to industrial demand for low carbon energy without the large infrastructural changes associated with electrification or biomass. In gas grids where only methane can be injected the additional cost may be justified by access to industrial customers, earning a premium through the sale of "green gas certificates". This thesis demonstrated that where grid injection of hydrogen is permissible it is a more attractive option, negating the requirement for additional handling or upgrading and substantially reducing costs and carbon intensity.

8.4.7.2 Pairing directly with VRE

This thesis shows that curtailment alone will not drive investment in PtG. The system wide benefits of PtG (increasing average off peak prices by operating when demand is low) are felt by all generators but the costs are borne only by the PtG investor. Profitability drives implementation, and in many cases, curtailment may be more cost effective than PtG. Electrolysis is a large investment and so only if a combination of sale price and incentive are sufficiently high does PtG increase project value.

Therefore, an individual wind or solar farm investing in PtG is not financially advisable unless capital grants and incentives/rewards exist.

8.4.7.3 Biogas upgrading

Using PtG in place of traditional biogas upgrading offsets a portion of the capital required. However, the profitability of this configuration is still determined by the difference in value between the electricity used and the additional gas produced. The plant's ability to extract value from the electrolysers or valorise waste heat is unlikely to be sufficient for PtG upgrading to outperform traditional upgrading unless specific incentives or credits for utilising the CO₂ are introduced. These may be in the form of high carbon taxes, defined sustainability criteria for advanced fuels or minimum targets for gaseous fuels from non-biological origin in future iterations of the RED.

A future fully decarbonised grid with high shares of VRE may create surpluses that would be suitable to PtG biogas upgrading. In that case the income from offering decentralised quasi-storage could offset the cost of electricity.

8.4.7.4 Isolated community

PtG may find a role in the unique energy landscapes of remote communities. The hybrid concept is most suited to areas with high VRE resources but where grid infrastructure may hinder deployment. Here a hybrid system that engages in the electricity market and converts excess or low value electricity to hydrogen for local use might be suitable. By using the hydrogen locally, such as in a ferry or a local hydrogen grid for electricity and or heat, the goals of selfsufficiency and decarbonisation can be met.

8.5 Brief summary for policymakers

The energy transition is being driven by top down strategic decisions. When formulating policy, we should be cognisant not just of our Paris Agreement commitments but the energy transition as a whole. The persistently low cost of fossil fuels means that regulations and subsidies are required where market forces will not create the desired result. PtG is particularly reliant on coherent policy as it touches upon many sectors. The benefits of PtG are difficult to monetise and so the author believes an incentive should be introduced for gaseous fuels from non-biological origin for use as an advanced transport fuel. This could be supported by more ambitious targets in future iterations of the recast RED. This vector is ideally suited for difficult to decarbonise sectors such as haulage (ideally in a fuel cell powered truck) and aviation (necessary to hydrogenate biofuels for aviation). The technology is more mature than competing third generation biofuels (such as Fischer-Tropsch diesel) and would require fewer subsidies.

This thesis has shown that PtG leads to more stable and profitable electricity grid operation and particularly benefits VRE generators. An innovative VRE tariff regime could be used to fund the required incentive and should not be seen as a penalty. The increasing difficulty and costs of operating the electricity network are an externality of the intermittency of VRE. And as such the increased revenue of VRE generators due to additional interconnection, battery storage, or PtG capacity is a fair place from which to seek to raise funds for an incentive scheme. Comparing VRE and dispatchable electricity (such as from biogas) in terms of LCOE is not a like for like comparison, and so differentiating them here is fair. Alternatively, discounted electricity purchase could be offered in return for PtG demand side management.

8.6 Brief summary for industry

As the levelised costs of PtG are dominated by electricity, developments that focus on reducing capital costs will not greatly improve the competitiveness of the gas produced. Advancements in hydrogen storage are more likely to improve plant finances by allowing greater flexibility and decoupling electricity use from hydrogen supply. As an investor, the future viability of PtG depends on its ability to extract additional value from the capital-intensive electrolysers.

PtG is a promising solution to grid instability however, it is not as of yet a profitable solution to curtailment. Once favourable incentives are in place, future cooperative investment in PtG could allow firms to spread the cost and risk, running PtG at a loss but increasing profits on their VRE assets by a greater amount.

8.7 Recommendations

The cross-sectoral nature of PtG can make analysis of its benefits difficult but waiting for PtG to reach certain target capital costs or GHG savings shows a lack of appreciation for the role it could play in future energy systems. Although comparisons to diesel and natural gas are made in this thesis, the reality is that should we wish to meet our climate change targets PtG will be competing with other low carbon options. As of now diesel, natural gas, and other fossil fuels are not sufficiently priced to include the externalities associated with their production and use. Waiting for PtG to approach price parity with conventional fossil fuels reduces energy to a single criterion is not advised, it ignores the increasing interconnectedness and positive externalities.

PtG is at a relatively high technology readiness level (TRL) and can realise GHG savings in many applications. The author recommends increasing the allowable limits of hydrogen in the natural gas grid as it is technically feasible and would circumvent many of the issues that face PtG. By injecting renewable energy into the gas grid via PtG we overcome much of the inertia associated with industry or other natural gas users implementing large infrastructural changes, like the electrification of heat.

VRE is at the vanguard of energy system decarbonisation, but brings with it many issues, each of which can be dealt with to some degree by introducing PtG. Electrification is an increasing and important component in low carbon roadmaps, also seen as lessening these issues, but is not yet viable in all sectors however, PtG can perform electrification by proxy. Realising the full potential of VRE will lead to periods of over production and production during low demand, the author believes PtG is a technology well suited to utilising such energy, especially in light of falling revenues due to an inability to accommodate the electricity generated. For VRE to continue to provide GHG savings, PtG simultaneously balancing generation and converting the energy to a vector that can be used in other areas is desirable.

In light of overarching targets for renewable electricity penetration, PtG should be promoted in much the same way electric vehicles (EVs). EVs have been promoted prior to a wholly renewable electricity system or the introduction of smart charging (grid optimised EV charging), as they are rightly seen as a better alternative to fossil fuels. PtG could essentially act as the electrification of heavy goods vehicles (HGVs), but without the erratic electricity consumption currently seen with EVs. The author also believes that, again like EVs, PtG should not be subject to minimum GHG savings targets, rather PtG should only be implemented in regions with high shares of VRE (40% in the case of Ireland) or low carbon base load generation (such as Sweden or France). Purchasing guarantees of origin for the electricity used would make PtG prohibitively expensive and delay its implementation beyond what is necessary.

Niche applications of PtG are promising. Where GHG emissions reductions are sought, areas with local district heating and high shares of renewable electricity are ideal candidates for PtG. With or without methanation the waste heat of an electrolyser could provide a base heating load, with the stored hydrogen/methane providing peak demand, either directly or from the gas grid. As discussed, the author also believes pairing PtG with WWTPs is an avenue deserving of further research.

Identifying a suitable investor for PtG is challenging as the risks are centralised, whereas the benefits are felt across the system. Direct connection to VRE leads to underutilisation of the working capital (electrolysers operate at reduced capacity factors) and is not an attractive investment unless substantial incentives are introduced. Purchasing electricity to supplement times of low VRE generation may then be counterproductive and create demand for fossilbased energy. With this in mind the author suggests that transmission system operators (TSOs) are best placed to provide the investment. By controlling the operation of PtG they could maximise the balancing effect and distribute the cost among generators, perhaps designing the new tariff/fee to target nonsynchronous and difficult to accommodate electricity generators.

8.7.1 Future work

 Evaluate the effectiveness and cost of installing a wind and PtG hybrid energy system to provide renewable energy for isolated communities.

Isolated communities suffer from high energy costs, a lack of infrastructure, and fossil fuel reliance and therefore may be ideal candidates for such a system. Building upon previous models the potential can be investigated.

 Quantify and qualify the effect PtG has on electricity generator profits and hence, calculate the potential for net zero cost incentivisation.

Chapter 6 shows that PtG will most likely need to be incentivised, but it also provides significant positive externalities. Monetising these externalities may allow for a fair system of raising funds for PtG investment.

- Investigate the combination PtG and a WWTP to provide electricity grid flexibility including for economic utilisation of the oxygen

produced.

A through literature review will be undertaken along with modelling decentralised PtG for grid stability and improved WWTP performance. As much of the infrastructure exists and is owned by the state there may be little resistance to such a proposal.

- Compare options for heavy goods vehicle decarbonisation in a detailed multi criteria analysis for a number of scenarios.

This is an often-overlooked part of energy policy. Comparing PtG with other available options will provide much needed evidence to inform policy decisions, fuel options include hydrogen, hydrotreated vegetable oil, biogas, and biodiesel, also considering infrastructural solutions such as electric roads. Similarly, investigate the role of hydrogen in decarbonising aviation.