Quantifying Emissions and Costs of Geologic Hydrogen: An Integrated Lifecycle Emissions and Techno-economic Approach

by
Timothy Blackford

Bachelor of Engineering (Mechanical Engineering, 2011)
University of Western Australia

Bachelor of Commerce (Management, 2011)
University of Western Australia

Submitted to the System Design and Management Program
in partial fulfillment of the requirements for the degree of
MASTER OF SCIENCE IN ENGINEERING AND MANAGEMENT
at the
MASSACHUSETTS INSTITUTE OF TECHNOLOGY

September 2024

Authored by: Timothy Blackford
MIT System Design and Management Program
August 9, 2024

Certified by: Ruaridh Macdonald
Energy Systems Research Lead, MIT Energy Initiative
Thesis Supervisor

Certified by: Joan Rubin
Executive Director, MIT System Design and Management Program
Thesis Supervisor

Accepted by: Warren Seering
Weber-Shaughness Professor of Mechanical Engineering

Quantifying Emissions and Costs of Geologic Hydrogen: An Integrated Lifecycle Emissions and Techno-economic Approach

by

Timothy Blackford

Submitted to the MIT System Design and Management Program
on August 9, 2024 in partial fulfilment of the requirements for the degree of

MASTER OF SCIENCE IN ENGINEERING AND MANAGEMENT

ABSTRACT

In the pursuit of sustainable energy solutions, this thesis explores the lifecycle emissions and economic feasibility of geologic hydrogen production. This research extends Brandt's 2023 study of 'prospective' lifecycle assessment (LCA), enhancing the underlying open-source LCA model used in this work and adding a preliminary techno-economic analysis (TEA). The findings demonstrate that geologic hydrogen developments should have emissions intensities that compare favourably to all other hydrogen production pathways. The value of lifetime emissions intensity for Brandt's Baseline case is estimated at 0.40 $kgCO_2e/kgH_2$, representing an increase of ~6% over Brandt's estimation. The study also highlights the potential for geologic hydrogen to achieve competitive levelized costs (estimated at $1.45/kg), making it a promising candidate in the hydrogen economy. It finds that to achieve the best possible emissions and economic results, proponents of geologic hydrogen developments should seek to maximise the productivity of each well. It also studies the impact of the United States regime of production tax credits for hydrogen, finding that the fivefold increase in the magnitude of credits for meeting employment conditions is generally more impactful than lowering emissions intensity. The thesis underscores the importance of continued refinement of LCA and TEA models to understand geologic hydrogen resources better and ensure they are developed appropriately.

Thesis Supervisor: Dr. Ruaridh Macdonald

Title: Energy Systems Research Lead, MIT Energy Initiative

Thesis Supervisor: Joan Rubin

Title: Executive Director, MIT System Design and Management Program

Acknowledgments

As with all personal accomplishments, the publication of this thesis was only possible through the support and input of others in my 'village'. I am most grateful for the support of my wife, Sarah, whose self-sacrifice and hard work allowed me the opportunity to focus on this effort and was of the utmost importance to my achievement. I could not have done it without her. I must similarly thank my parents, whose support has always been central to my successes.

My supervisor at the MIT Energy Initiative (MITEI), Ruaridh Macdonald, provided the initial inspiration for the topic and was also an excellent colleague and partner on the high-paced journey to completion. My thesis supervisor and academic advisor from the System Design and Management (SDM) program, Joan Rubin, provided much-appreciated support and guidance to ensure the sailing was as smooth as possible.

Throughout this work, I was fortunate to discuss this topic informally with various experts, whose comments, opinions, and advice were much appreciated. This includes Barry Katz of Chevron, Emily Yedinak of Koloma, Avon Macintyre of Hyterra, Guiyan Zang of MITEI, and other members of the broader MITEI research group. The support, professionalism and congeniality of the System Design and Management (SDM) program faculty and broader 'SDM family' were also all much appreciated.

I must also acknowledge my employer, Chevron, for sponsoring my participation in the SDM program. It has been a true privilege and an absolute honour.

I dedicate this thesis to my dear, dear friend, Lloyd Muir. The heights of your warmth, your dedication to your friends and your family, especially your children, and your joyfully earnest appreciation of life are but a few of your traits to which I will always aspire. I will forever regret that moving away for this year unknowingly deprived us of more catch-ups over beer or coffee to share the highs and lows. A truly good man that the world is a better place for having, and I am a better person for having known.

Table of Contents

List of Figures

List of Tables

Acronyms, Terms, and Definitions

Acronym	Expansion
AACEI	Association for the Advancement of Cost Engineering International
AGRU	Acid-gas removal unit
ANL	Argonne National Laboratory
APC	Announced Pledges Case
BBL	Barrel (of liquid)
BCF	Billion (standard) cubic feet
BIL	Bi-partisan Infrastructure Law
CAPEX	Capital expenditure
CCS	Carbon (dioxide) capture and storage
CDF	Cumulative distribution function
CEPCI	Chemical Engineering Plant Cost Index
CHPS	Clean Hydrogen Production Standard
CSD	Compression, storage and dispensing
DoE	Department of Energy
DPI	Discounted Profitability Index
EIA	Energy Information Authority
EPA	Environmental Protection Agency
EUR	Estimated Ultimate Recovery
GHG	Greenhouse gas
GREET	Greenhouse gases, Regulated Emissions, and Energy use in Technologies
GWP	Global warming potential
IEA	International Energy Agency
IPCC	Intergovernmental Panel on Climate Change
IRA	Inflation Reduction Act
IRR	Internal rate of return
ISBL	Inside battery limits
LCA	Lifecycle analysis
LCOE	Levelised cost of energy
LCOH	Levelised cost of hydrogen
MIT	Massachusetts Institute of Technology
MITEI	Massachusetts Institute of Technology Energy Initiative
MMSCF	Thousands of standard cubic feet
NPV	Net present value
NZE	Net Zero Emissions Scenario
OPEX	Operational expenditure
OPGEE	Oil Production Greenhouse Gas Emissions Estimator
OSBL	Outside battery limits
PDF	Probability density function
PSA	Pressure swing adsorption
psig	Pounds per square inch, gauge
PTC	Production tax credit
SDM	System Design and Management

Acronym	Expansion
SMR	Steam methane reforming
STEPS	Stated Policy Scenario
TEA	Techno-economic analysis
UCCI	Upstream Capital Costs Index
US	United States
VFF	Venting, flaring and fugitive (emissions)
WACC	Weighted-average cost of capital
AACEI	Association for the Advancement of Cost Engineering International
AGRU	Acid-gas removal unit
ANL	Argonne National Laboratory
APC	Announced Pledges Case
BBL	Barrel (of liquid)
BCF	Billion (standard) cubic feet
BIL	Bi-partisan Infrastructure Law
CAPEX	Capital expenditure
CCS	Carbon (dioxide) capture and storage
CDF	Cumulative distribution function
CEPCI	Chemical Engineering Plant Cost Index
CHPS	Clean Hydrogen Production Standard
CSD	Compression, storage and dispensing
DoE	Department of Energy
DPI	Discounted Profitability Index
EIA	Energy Information Authority
EPA	Environmental Protection Agency
EUR	Estimated Ultimate Recovery
GHG	Greenhouse gas
GREET	Greenhouse gases, Regulated Emissions, and Energy use in Technologies
GWP	Global warming potential
IEA	International Energy Agency
IPCC	Intergovernmental Panel on Climate Change
IRA	Inflation Reduction Act
IRR	Internal rate of return
ISBL	Inside battery limits
LCA	Lifecycle analysis
LCOE	Levelised cost of energy
LCOH	Levelised cost of hydrogen
MIT	Massachusetts Institute of Technology
MITEI	Massachusetts Institute of Technology Energy Initiative
MMSCF	Thousands of standard cubic feet
NPV	Net present value
NZE	Net Zero Emissions Scenario
OPEX	Operational expenditure
OPGEE	Oil Production Greenhouse Gas Emissions Estimator
OSBL	Outside battery limits
PDF	Probability density function

Acronym	Expansion
PSA	Pressure swing adsorption
PTC	Production tax credit
SDM	System Design and Management
SMR	Steam methane reforming
STEPS	Stated Policy Scenario
TEA	Techno-economic analysis
UCCI	Upstream Capital Costs Index
US	United States
VFF	Venting, flaring and fugitive (emissions)
WACC	Weighted-average cost of capital
OPEX	Operational expenditure
OPGEE	Oil Production Greenhouse Gas Emissions Estimator
OSBL	Outside battery limits
PDF	Probability density function
PSA	Pressure swing adsorption
PTC	Production tax credit
SDM	System Design and Management
SMR	Steam methane reforming
STEPS	Stated Policy Scenario
TEA	Techno-economic analysis
UCCI	Upstream Capital Costs Index
US	United States
VFF	Venting, flaring and fugitive (emissions)
WACC	Weighted-average cost of capital

Chapter 1: Introduction

1.1. Background

The case for change

The emission of greenhouse gases (GHGs) from human activities is causing climate change. The effects of this change are already being felt across every region in the form of widespread adverse impacts, losses and damage (Calvin et al., 2023). While the need for action has been recognised by many in the global community for multiple decades, the development of the Paris Agreement has been one of the most effective means of garnering commitments and concrete actions to reduce these harmful emissions. Specifically, the Paris Agreement encouraged societal groups (nations, corporations, multi-national unions, institutions, etc.) to set 'net-zero' commitments comprising targets and timebound plans to reduce emissions and increase GHG-absorbing, or "carbon-negative" activities. These net-zero commitments see participating groups aim to cease their contribution to ongoing increases in the concentration of atmospheric carbon dioxide and other GHGs (Fankhauser et al., 2022). The commitments ultimately signal the respective groups' acknowledgement and contribution towards the Paris Agreement goal of limiting global warming to well below 2 degrees Celsius (°C) above pre-industrial levels, with a target of limiting increases to 1.5 °C (*United Nations Framework Convention on Climate Change. Paris Agreement. Article 2(a)*, 2015).

In developing models that consider potential climate outcomes, the Intergovernmental Panel on Climate Change (IPCC) has developed numerous scenarios to describe potential emissions "pathways" and enable the assessment of climate outcomes under these scenarios (Calvin et al., 2023). Related organisations have subsequently translated the IPCC work and Paris Agreement targets into industry-specific contexts. For example, the International Energy Agency (IEA) recognises that the energy sector is responsible for approximately three-quarters of GHG emissions, so it has developed a 'road map' for the global sector that acknowledges its critical role in the fight against climate change. IEA analysis considers three separate scenarios: (i) the Stated Policy Scenario (STEPS), which models the global impact of the implementation of existing and stated policies in the energy sector that have been confirmed via legislation or regulation, (ii) the Announced

Pledges Case (APC), which models the consequences if all national emissions-reduction pledges made public at the time of modelling were achieved on time and in full, and (iii), the Net Zero Emissions by 2050 Scenario (NZE), which demonstrates the requirements of the energy sector to achieve net-zero carbon dioxide emissions by 2050. The IEA analysis details the differing climate impacts in each of these scenarios. In STEPS, the global average surface temperature rise in 2100 is predicted to be approximately 2.7 °C. The predicted rise falls to 2.1 °C under APC, and only the NZE is consistent with limiting the rise to 1.5 °C without a temperature overshoot, which aligns with the Paris Agreement target. The road map is thus based on NZE and describes actions and milestones the energy sector should take to achieve 'net zero by 2050'. It is "designed to maximise technical feasibility, cost-effectiveness and social acceptance while ensuring continued economic growth and secure energy supplies" (*Net Zero by 2050 - A Roadmap for the Global Energy Sector*, 2021, p. 13).

Hydrogen's role in a 'net-zero economy'

A key finding from the modelling associated with each IEA scenario is that there is an increase in the production and use of lower-emission alternatives to fossil fuels, including hydrogen. Figure 1.1 shows the total hydrogen consumption in each IEA scenario in 2030 and 2050 against a benchmark of 2022 production levels. This indicates that hydrogen production is expected to increase by at least 3,940% by 2030 and that production will increase by four orders of magnitude by 2050 in the net zero emissions case.

Table 1-1 - Forecast total global consumption of hydrogen in 2030 and 2050 in each IEA scenario, including comparison to 2022 actual consumption (*World Energy Outlook 2023*, 2023)

Scenario	Forecast Year	Total Consumption (EJ)	Consumption Increase Over 2022 Level
2022 Actual	N/A	0.005	N/A
STEPS	2030	0.197	3,940 %
	2050	1.292	25,840 %
APC	2030	0.723	14,460 %
	2050	9.582	191,640 %
NZE	2030	2.094	41,880 %
	2050	15.898	317,960 %

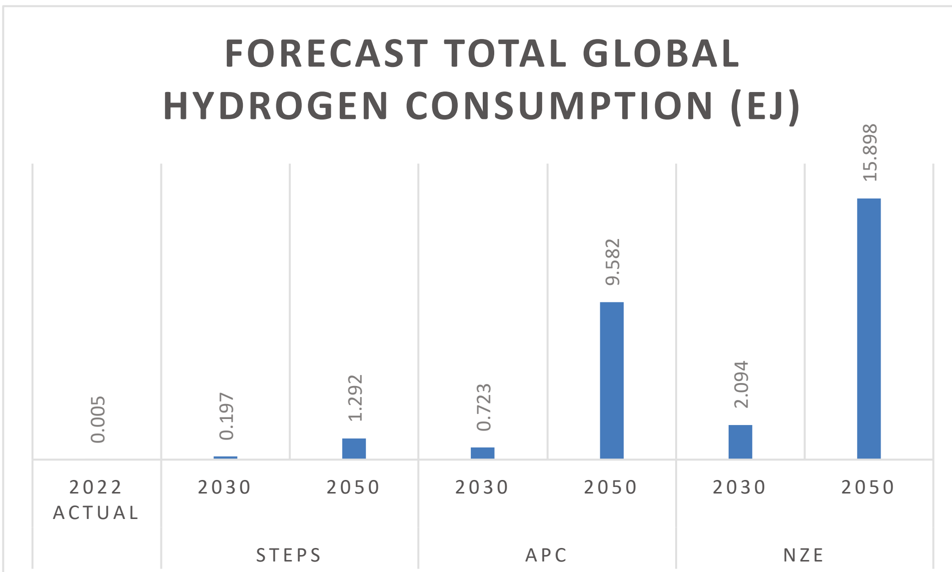


Figure 1.1: Visualisation of forecast total global consumption of hydrogen in 2030 and 2050 in each IEA scenario (*World Energy Outlook 2023*, 2023)

Chapter 2 examines the 'tailwinds' driving the dramatic increase in forecast hydrogen demand and the 'headwinds' that challenge hydrogen's contribution to the transition away from a fossil fuel-based economy. It points out that there are numerous production pathways for hydrogen, but none of these pathways is a 'clear winner', with no single pathway expected to dominate the industry. It further points out that there is a nascent and novel production pathway for hydrogen that is worthy of careful consideration: geologic hydrogen. This thesis aims to contribute to the burgeoning body of knowledge regarding geologic hydrogen and its potential contribution to the fight against climate change.

1.2. Research Objectives

As will become apparent in Chapter 2, geologic hydrogen may significantly benefit society, but along with its high potential benefit comes similarly high uncertainty in many key characteristics. Of these uncertain characteristics, the most notable are the expected emissions intensity and levelised cost of production. Accordingly, this research aims to extend the state-of-the-art understanding of these areas.

1.3. Research Questions

Put more specifically, this thesis addresses the following research questions:

1. How can the state-of-the-art understanding of geologic hydrogen emissions intensity be improved?
2. Is the development of geologic hydrogen resources appealing from a techno-economic perspective? To this end:
    a. What are the estimated development costs?
    b. Will geologic hydrogen developments be attractive investments if market forces dictate modest prices for hydrogen supply? If so, at what price?

1.4. Research Approach

This thesis considers Brandt's (2023) paper as the state-of-the-art publication on the potential lifecycle emissions intensity of geologic hydrogen. Accordingly, the approach taken here is to review this work in detail by first recreating the relevant components of the lifecycle analysis (LCA) model that form the basis for the conclusions drawn in the paper. This thesis will then identify and implement potential improvements to the original modelling approach and examine their significance to the overall conclusions drawn from the model. Finally, this work extends Brandt's work on lifecycle emissions by adding a preliminary consideration of levelised cost and techno-economics. By maintaining a consistent set of assumptions and scenarios between the lifecycle analysis and cost analysis, this thesis enables consideration of potential synergies or tensions that may exist between low-emissions developments and low-cost developments.

1.4.1. Included in research scope

More specifically, the scope of this research includes:

- Replication of Brandt's mature, existing physics-based LCA model that was used to assess the emissions intensity of geologic hydrogen. In doing so, Brandt's model is used as a reference to build a new modelling tool that facilitates third parties' interpretation and verification of the model.

- Correct any errors or omissions from the reference model.
- Extend upon the reference model to generate additional useful outputs. Specifically:
    - Examine the impact of uncertainty associated with key assumptions used in the model;
    - Develop preliminary (i.e. coarse) cost estimates for the baseline and key sensitivity cases and;
    - Estimate the price of hydrogen that would be necessary to make the development of a geologic hydrogen resource a compelling investment proposition.

1.4.2.Excluded from research scope

Considering the time and resources available to complete this work, the following items are expressly excluded from consideration:

- Components of techno-economic analysis that rely on proprietary data (e.g. cost databases) and price forecasts
- Assessment of stimulated geologic hydrogen production (so-called 'orange hydrogen')

1.4.3.Note on the use of Artificial Intelligence tools

The work in this thesis is the author's and responsibility is taken for all content. Noting this, the author did use artificial intelligence tools to assist in some aspects of the research. Specifically, ChatGPT 4, ChatGPT 4o, and GitHub Copilot were used to improve the efficiency and productivity of code generation during modelling work. The written portion of this thesis does not use content generated by artificial intelligence tools.

1.5. Thesis Structure

This document is structured in chapters that allow sequential development of interim findings. This structure is as follows:

- Chapter 1: Introduction
- Chapter 2: Literature review
- Chapter 3: Review of state-of-the-art LCA

- Chapter 4: Improvements and Extensions to State-of-the-Art LCA
- Chapter 5: Extension of state-of-the-art LCA to include analysis of uncertainty
- Chapter 6: Extension of LCA via preliminary TEA: Extension of LCA via preliminary TEA
- Chapter 7: Conclusions and Future Research

Chapter 2: Literature review

Chapter 1 established that there is an urgent need to act to limit the harmful effects of climate change caused by anthropogenic GHG emissions. It further highlighted the role that hydrogen is expected to play in the adapted global energy system. This chapter reviews the relevant literature to establish the advantages and challenges faced by the nascent transition to a global 'hydrogen economy'. It then presents the potential posed by the discovery, extraction, and use of naturally-occurring, geologic hydrogen to assist the transition and contribute to minimising the harmful effects of climate change.

Factors driving increased hydrogen demand

There are several reasons for the forecast of increased consumption of hydrogen discussed in Chapter 1. From an 'end use' perspective, hydrogen has several characteristics that render it attractive over other energy sources or industrial feedstocks.

First, its use does not typically result in the emission of any GHGs. Efficient combustion or oxidation of hydrogen produces only water vapour as a by-product. Thus, emissions associated with the 'hydrogen value chain' (from production through to consumption) are limited to those emissions associated with the various hydrogen production pathways and those associated with transportation and storage. Eliminating end-use emissions would be a step-change improvement over the 'fossil fuel value chain', which also has emissions associated with transportation and storage. So, while hydrogen is more likely to be 'low emissions' than 'no emissions', it is expected to contribute significantly to the world's 'net-zero' ambitions.

Second, hydrogen's primary advantage over alternative 'zero-emissions' energy sources is its specific energy (otherwise known as 'energy per unit mass', or gravimetric energy density). When processed appropriately (i.e. compressed, liquified, or attached to 'carrier' molecules), the volumetric energy density (i.e. energy per unit volume) is also sufficiently high to be competitive with alternative energy storage vectors. The most prevalent and relevant comparison technology is energy storage provided via battery-electric means. This is particularly important in use cases where self-weight of fuel can be a performance-limiting factor, such as aviation.

Third, the fluid nature of energy stored in hydrogen means that it can be easily distributed from central storage to end-users. Hydrogen technologies are expected to be particularly advantageous in 'hard to abate' sectors of the energy economy, such as heavy land-based transportation and shipping. In these sectors, battery-electric solutions require either long-duration recharge times or battery change-out arrangements, which require duplication of the costly components (*U.S. National Clean Hydrogen Strategy and Roadmap*, 2023).

Fourth, hydrogen can be produced by numerous 'production pathways'. Several of these pathways are mature, well-understood, can be scaled rapidly and include 'low or no' emissions alternatives. Other pathways are nascent or more novel. Each pathway has advantages and disadvantages, and there is, at present, no single 'winner takes all' pathway or associated technology. The range of potential hydrogen production sources and processes are often described using a system of colour-coding, the extent of which now spans a veritable rainbow. Table 2-1 provides an overview of the most typical production pathways. The range of available technologies implies that proponents of hydrogen-producing systems can select a technology that most aligns with their particular circumstances, including their resources, expertise and specific needs.

Fifth, current sources of demand for hydrogen as a feedstock (rather than an energy source) are expected to grow and be supplemented by additional demand from industrial processes that transition to using hydrogen as a feedstock (*U.S. National Clean Hydrogen Strategy and Roadmap*, 2023). Currently, the manufacture of ammonia for fertilisers is a leading source of demand for hydrogen. In line with global population growth and agricultural intensification, global fertiliser demand is expected to increase, directly increasing hydrogen demand (*Fertilizer Market Size & Share | Growth Forecast Report – 2032*, 2024). Similarly, emissions-intensive industrial processes such as steelmaking may achieve decarbonisation by transitioning to hydrogen as both a feedstock and a source of energy and/or heat (Liu et al., 2021). Accordingly, fertiliser manufacturing and steel-making stand alongside electricity generation as examples of major potential sources of future demand for hydrogen.

Factors mitigating increased hydrogen demand

Despite the reasons that explain the forecasted drastic increase in hydrogen demand, it is important to acknowledge the risks and other potential downsides associated with this shift in the energy system. One of these critical caveats is the global warming potential (GWP) of molecular hydrogen released into the atmosphere. Recent work has demonstrated that, while hydrogen does not directly contribute to the greenhouse effect, it interferes with the natural decay of other, 'direct' GHGs like methane. The delayed decay increases the global warming effect associated with the direct gases. Accordingly, hydrogen is considered an 'indirect' GHG. The severity of the indirect greenhouse effect is under investigation, with an early study determining a GWP of 5 (i.e. 1 tonne of hydrogen has the equivalent global warming effect of 5 tonnes of carbon dioxide), with more recent studies determining GWPs of 10.9 and 11.6 (R. Derwent et al., 2006; R. G. Derwent et al., 2020; Sand et al., 2023; Warwick et al., 2022). These estimates are all significantly less damaging than methane (which has a GWP of 29.8 for 'fossil' sources (Intergovernmental Panel On Climate Change (Ipcc), 2023). However, it highlights that minimising the emissions intensity associated with the entire hydrogen value chain will require close attention to be paid to its storage and transportation. Venting (i.e. deliberate releases to the atmosphere) and fugitive emissions (i.e. inadvertent releases to the atmosphere) are thus a key consideration for LCA of any hydrogen development. While a hydrogen economy is generally expected to be responsible for fewer climate impacts than our 'fossil-fuelled' economy, minimising these emission sources is still necessary to minimise residual climate impacts (Ocko & Hamburg, 2022).

Table 2-1 - Summary of hydrogen production pathways.

Production Technology	'Colour-Code' Designation	Estimated Emissions Intensity ($gCO_2e/MJ\ H_2$)[1]	ANL Intensity ($kgCO_2e/kgH_2$)[2]
Gasification of organic compounds (e.g. coal)	Black	246.1	20[3]
Gasification of organic compounds with CCS	N/A	72.5	2.9
Gasification of biomass	N/A	177.9	1.7
Gasification of biomass with CCS	N/A	-28.6	N/A
Splitting of hydrocarbons (methane), typically via steam methane reforming (SMR) and venting by-product CO_2	Grey	114.4	9.4
Water electrolysis powered by zero-emission, renewable sources of electricity	Green	23.1	0.0
Splitting of hydrocarbons (methane), typically via steam methane reforming (SMR) with capture and sequestration of by-product CO_2	Blue	46.6	3.4
Methane pyrolysis	Turquoise	N/A	3.6 (with US 2023 grid mix) 0.32 (renewable power)[4]
Water electrolysis powered by nuclear power plants	Pink	9.6	N/A
Water electrolysis powered by local grid electricity	N/A	211.3	N/A
Exploitation of naturally-occurring geologic hydrogen	White/Gold	N/A	N/A
Induced geologic formation and production of hydrogen via injection of reagents	Orange	N/A	N/A

Note: Argonne National Laboratory (ANL) emissions are estimated using the GREET LCA model, which does not include embodied emissions.

1: (Busch et al., 2023)

2: (Elgowainy et al., 2022)

3: (Lewis et al., 2022)

4: (Vyawahare et al., 2023)

The hydrogen-production technologies described in Table 2-1 each face barriers to widespread adoption. Some of these barriers are as follows:

- The conventional technologies (i.e. SMR of methane and gasification of coal) with vented CO_2 emissions have high emissions intensity. Scaling these technologies to meet future demand is counter to the need to simultaneously reduce global emissions to zero.
- The technologies that reduce their emissions intensity via CO_2 capture and sequestration or disposal systems will be inherently limited by their access to such systems. These will not necessarily be widely available and, where they are available, may not have sufficiently attractive techno-economics to justify use for hydrogen production.
- Technologies that rely on access to suitable and sufficient low-emissions electricity (i.e., electrolysis processes) will be constrained by the availability of low-emissions electricity production. To enable continuous production, facilities may be required to install excess intermittent renewables generation capacity coupled with sufficient energy storage capacity. Alternatively, they may require access to local grid electricity (if available), which is often unlikely to be low-emissions. The United States hydrogen roadmap indicates that, in most regions of that country, electrolysers using electricity from the current grid will have higher emissions than hydrogen produced from SMR (*U.S. National Clean Hydrogen Strategy and Roadmap*, 2023). If the grid is already completely 'green', then there may be little incentive to build dedicated, local renewable electricity generation capacity. In this case, coupling industrial-scale hydrogen production to a local electricity grid may have undesirable consequences, such as increased prices or additional emissions if new renewable electricity generation capacity is diverted to hydrogen production (Giovanniello et al., 2024).
- Electrolysis technologies typically require access to clean water. In general, clean water sources are valuable resources to their surrounding communities. 'Creating' clean water (e.g. via reverse osmosis of seawater requires significant amounts of additional energy, which increases the emissions intensity and decreases the economic viability of these facilities.

In combination, these barriers effectively impose a limit on the rate at which hydrogen production can be increased or 'scaled'.

Economic and policy factors affecting hydrogen adoption

In almost all cases, the barriers described above do not render hydrogen developments technically infeasible. Rather, the cost required to overcome the barriers challenge the economics and 'business case' of any prospective development. These costs can be estimated with reasonable confidence. Revenue, on the other hand, is significantly more uncertain. As discussed previously, global hydrogen demand is forecast to rise dramatically but present demand levels are being met by existing supply capacity. In the absence of policy settings that consider the emissions intensity associated with hydrogen production ('carbon pricing', for example), then it is difficult to see how new, low-emissions sources of hydrogen will be able to compete on cost with existing suppliers. To this end, several jurisdictions worldwide have implemented policies that either directly or indirectly incentivise low-emissions hydrogen developments. Further, the United States Inflation Reduction Act (IRA), Bi-partisan Infrastructure Law (BIL), and the associated Production Tax Credits (PTCs) for low-emission hydrogen production provide direct incentives (*U.S. National Clean Hydrogen Strategy and Roadmap*, 2023).

The discussion above outlines the societal and economic/business justifications for pursuing hydrogen developments. Specifically, there is an urgent need for action to reduce emissions and reduce the harmful effects of climate change. Hydrogen has several significant technological advantages that explain dramatic increases in forecasts of demand growth, and governments are implementing policies to acknowledge emissions intensity and directly incentivise investment in hydrogen developments. Noting these drivers, it is unsurprising that significant activity is being dedicated both in academia and business to solving the critical challenges of supplying the world with low-emissions hydrogen. Much of the effort is being directed at solving the challenges with the means of production outlined in Table 2-1 and discussed above. Other efforts are considering entirely more novel ideas, including novel sources.

Geologic hydrogen: An ideal solution?

One such novel potential source of hydrogen supply is that which occurs naturally in geologic formations. Zgonnik (2020) completed a comprehensive review of the evidence and supporting literature for the occurrence and geoscience of “natural hydrogen”. The review argues that molecular hydrogen is widespread within geologic structures around the world and estimates that 23 teragrams (Tg, 10^{12} grams) of hydrogen flows from geologic sources to the atmosphere each year.

Zgonnik’s review reveals that the literature on geologic hydrogen focuses almost exclusively on ‘subsurface’ or geologic considerations. It considers hypotheses regarding formation mechanisms and diffusion and accumulation mechanics. These hypotheses inform implications about where geologic hydrogen is most likely to exist and the exploration techniques likely to be suitable to deploy when attempting to locate accumulations of it (including, for example, the work of Truche and Bazarinka (2019)).

The hypothesis regarding the potential existence of geologic hydrogen accumulations that may be exploited for societal benefit is most powerfully supported by the inadvertent discovery of a high-purity source of hydrogen in an intended water well near the village of Bourakebougou, in Mali. While it was discovered inadvertently (while drilling a water well), subsequent drilling activities have further characterised the reservoir (Prinzhofer et al., 2018). The gases produced from the original well were characterised as 98% hydrogen, with the remainder a mix of nitrogen and carbon dioxide. Hydrogen from this well has been powering a small internal combustion engine-driven electricity generator from approximately 2011 to the present day (i.e. for 13 years), over which time pressure in the reservoir is reported to have increased from 4.5 to 5 bars. This suggests a possibility that the hydrogen in the reservoir may be being regenerated at a rate faster than it is consumed via the well (Maiga et al., 2023).

There have been several other significant discoveries of hydrogen of geologic origin, including in Albania, France, and Australia (McDonald, 2024; Pironon & Donato, 2023; Truche et al., 2024). Accordingly, the occurrence of geologic hydrogen accumulations and seepage has been proven. What remains to be proven is the ability to harness geologic hydrogen as a natural resource that is useful at regional or global scales. Despite the uncertain viability, the potential commercial benefit of a successful geologic hydrogen development is attracting significant private-sector activity to the industry. It has been reported that the number of companies actively undergoing exploration activities increased from 10 in 2020 to 40 in late 2023, and these activities are globally dispersed between Australia, the United States, Spain, France, Albania, Colombia, South Korea and Canada (*The White Gold Rush and the Pursuit of Natural Hydrogen*, 2024).

Several key presumptions drive the interest in geologic hydrogen. The primary presumption is that geologic hydrogen should be able to be developed by applying well-established technologies developed and proven within the oil and gas industry. Much of the existing research on this topic has focused on repurposing exploration and reservoir characterisation techniques and workflows from the oil and gas industry to be useful in the geologic hydrogen industry (Dugamin et al., 2019; Lefeuvre et al., 2021; Lévy et al., 2023; Truche & Bazarkina, 2019). This is a non-trivial task because the differences in formation mechanisms between geologic hydrocarbons and molecular hydrogen are thought to typically occur in regions with significantly differing geologic characteristics (i.e. hydrogen is not expected to be found in areas that have already been well-explored and exploited for hydrocarbon production) (Zgonnik, 2020).

The existing geologic hydrogen literature pays scant attention to the requirements of surface processing facilities. This is likely a result of the design maturity for hydrogen processing equipment in existing facilities (e.g. SMR plants within oil refineries). Hydrogen molecules from geologic sources should behave identically to those from other sources. So, there is little reason to expect significant technical challenges when applying proven equipment designs in new, geologic hydrogen applications.

Further, the assumed potential for the repurposing of existing development technologies, such as those required to drill and complete wells, surface processing equipment, and transportation equipment (particularly pipelines), means that it is expected that the cost of production will be low, the carbon-intensity of production will be similarly low, and there could be a short lead time to scaled production. In addition, it is considered possible that an abundance of valuable resources are prevalent across geographies (Ellis & Gelman, 2022). Finally, there is a possibility that resources will regenerate, leading to a genuinely sustainable (i.e. non-depleting) resource (as suggested by the lack of observed pressure decline during operation of the Bourakebougou well).

Hydrogen as an industry platform

Fuel markets and their supply chains can be viewed as ‘industry platforms’, as they enable third parties to exchange goods and develop complementary products and services, and they involve obvious network effects, where their value increases proportionally with the number of users or customers (Gawer & Cusumano, 2014). Industry platforms must have at least two 'sides', which in this case can simply be considered as hydrogen producers and hydrogen consumers. Thus, findings from research on industry platforms can be informative when considering the establishment of the hydrogen market. The three key stages in creating an industry platform are (i) coring, (ii) seeding, and (iii) tipping (Gawer & Cusumano, 2008).

"Coring" a platform involves creating a new platform where none existed before. This can mean solving a key business problem for significant parts of industry or society. For a hydrogen market, the coring premise is clear: it will form a vital part of the suite of solutions required to move to a 'net zero' emissions society.

"Seeding" a platform involves attracting 'users' such that the platform can begin to operate, these users can realise direct benefits, and network benefits can take shape. The essential calculus for seeding a platform is that the benefits of using it (both stand-alone and network benefits) must outweigh the 'cost of affiliation' or the cost of using it. This is a major challenge for a fuel or industrial feedstock commodity platform, where starting production requires 'users' (i.e. supply firms) to make large capital investments, and starting consumption requires similar investment in new technology or equipment, as well as confidence that a sufficiently attractive and sustainable source of supply will exist. This is the classic 'chicken and egg' problem of platforms. In this case, attracting investment in hydrogen production is stalled by the potential lack of consumers and installation of consumption capacity does not make economic sense before there is adequate supply.

Key stakeholders have identified the challenge of seeding the 'hydrogen economy' and some have taken action to address it. Notably, some governments have taken action by implementing policies to incentivise investment in this area. For example, the BIL required the United States Department of Energy to develop a Clean Hydrogen Production Standard (CHPS). Coupled with the United States Inflation Reduction Act (IRA), this provides incentives to produce low-carbon intensity hydrogen via the Clean Hydrogen Production Tax Credit (PTC), known as "45V". As part of these laws and regulations, incentives exist for hydrogen production with "a lifecycle GHG emissions rate of not greater than 4 kilograms of CO_2e per kilogram of hydrogen" (*U.S. Department of*

Energy Clean Hydrogen Production Standard (CHPS) Guidance, n.d., p. 2). In the CHPS, the United States Department of Energy (DoE) acknowledges that other countries have established more stringent definitions of 'clean hydrogen', stating that "The European Taxonomy classifies clean hydrogen as that which achieves lifecycle emissions of <3.0 $kgCO_2e/kgH_2$ and the European Renewable Energy Directive sets a lifecycle target of approximately 3.4 $kgCO_2e/kgH_2$. As another example, the United Kingdom set a standard of 2.4 $kgCO_2e/kgH_2$" (*U.S. Department of Energy Clean Hydrogen Production Standard (CHPS) Guidance*, n.d., p. 6). Importantly, as shown in Table 2-2, the 45V PTC provides increasing benefits with decreasing emissions intensity, thus incentivising low emissions-intensity production. With these incentives, the US government has reduced the 'cost of affiliation' for prospective hydrogen producers by legislating to effectively provide them with ten years of revenue for the hydrogen they produce, regardless of the price uncertainty associated with selling into the market. It is also noted that the fivefold increase in PTC benefits for satisfying requirements associated with local employment conditions will likely be a strong motivator for firms.

Finally, "tipping" is "the set of activities or strategic moves that companies can use to shape market dynamics and win a platform war when at least two platform candidates compete" (Gawer & Cusumano, 2008). A platform has 'tipped' when it gains critical mass, achieving widespread adoption and market dominance. This is where network effects magnify, and a platform can become a defacto standard. The light vehicle market is a pertinent example. Here, it appears that the war between battery-electric and hydrogen fuel cell vehicles has been won by battery-electric technology, as evidenced by the ever-increasing sales figures and associated investments in infrastructure like charging stations. In other parts of the global economy, hydrogen is still in the fuel platform 'wars' with alternatives such as biofuels. Favourable techno-economics will be central to determining if hydrogen wins or loses these wars.

Table 2-2: Production Tax Credit benefit tiers.

'Well to Gate' Emissions Intensity ($kgCO_2e/kgH_2$)[(a)]	PTC Benefit ($US/$kgH_2$)[(b)]	PTC Benefit if Satisfying Employment Conditions ($US/$kgH_2$)[(c)]
2.5 to < 4.0	0.12	0.60
1.5 to < 2.5	0.15	0.75
0.45 to < 1.5	0.20	1.00
< 0.45	0.60	3.00

Notes: (a) 45V PTC emissions intensity is calculated using the Argonne National Labs 'GREET' LCA model, which does not consider embodied emissions. (b) These values are in 2022 dollars and are subject to annual inflation adjustments. (c) The 45V legislation allows for a fivefold increase in the value of PTCs if domestic origin, wage, and apprenticeship conditions are met (*26 USC 45V: Credit for Production of Clean Hydrogen*, n.d.).

Geologic hydrogen: A potential solution to the 'chicken or egg' problem

While the USA's PTC regime is appealing, Table 2-1 shows few production pathways with sufficiently low emissions intensity to avail themselves of the top tier of PTC benefits. Yedinak (2022) outlines both the potential for geologic hydrogen to be produced close to the US$1/kg benchmark of current production (via SMR without CCS) as well as the significant sources of uncertainty associated with achieving this benchmark, including the cost of exploration, development, and compression, storage, and dispensing (CSD). If, however, a geologic hydrogen development can achieve an emissions intensity of < 0.45 $kgCO_2e/kgH_2$, the value of the PTCs will mean that – from the producer's perspective, for ten years of operation – the benchmark can be considered effectively achieved at $1.60/kg. This equivalent benchmark cost rises to $4/kg if the emissions intensity is below 0.45 $kgCO_2e/kgH_2$ and the requisite employment conditions are satisfied.

If the presumptions of attractive emissions intensity and potential for parity in cost of production are realised, then geologic hydrogen may become an irresistible source of low-emission energy or chemical feedstock. This should spur accelerated investment in consumption technologies and supporting infrastructure like pipelines, shipping capacity and efficient market mechanisms. Even if the prevalence of low-cost geologic hydrogen resources (i.e. those that are shallow, located conveniently (to customers or transportation and storage infrastructure), sufficiently productive, and with desirable reservoir gas compositions) is limited, the exploitation of these resources may be sufficient to 'tip' the energy system platform in hydrogen's direction. Put another way, the discovery of low-cost, low emissions, readily scalable hydrogen resources may disincentivise investment in other solutions to problems that hydrogen may solve. Put yet another way, geologic hydrogen may guarantee that hydrogen is not one of many 'alternative fuels' but instead that it becomes the new 'default' fuel.

Putting the potential of geologic hydrogen under the microscope

Simply presuming that geologic hydrogen will be appealing is insufficient. It must be demonstrably so. As shown in Zgonnik's (Zgonnik, 2020) review, the existing literature has focused almost exclusively on proving the existence of geologic hydrogen and developing techniques that may potentially be used to locate valuable accumulations or sources beneath the surface of the Earth. Brandt's (2023) work is the first to examine the validity of the presumption that geologic hydrogen will have low emissions intensity. Brandt estimates that the mean lifecycle emissions intensity of a hypothetical geologic hydrogen resource, including embodied emissions, is 0.37 $kgCO_2e/kgH_2$. Excluding embodied emissions reduces this figure to approximately 0.2 $kgCO_2e/kgH_2$. At face value, these results indicate emissions intensity that is among the most attractive of any hydrogen production pathway. Brandt's paper will be discussed at length in subsequent sections of this work.

While emissions intensity is an important environmental factor, this is never the sole consideration when investing in developing a natural resource. Factors such as the 'social licence to operate' are also important, but it is inescapable that private-sector developments in market economies must also be economically viable. That is, there must be sufficient return (or potential for return) to justify the initial investment. For the prospective development of new technologies, the standard tool for assessing this risk/return trade-off is techno-economic analysis (TEA) (P. Kobos et al., 2020).

To this author's knowledge, no literature in the public domain attempts a techno-economic analysis (TEA) of geologic hydrogen development. As mentioned previously, Yedinak (2022, p. 504) refers to "an independent and preliminary analysis using the publicly reported hydrogen production rates, gas composition (100% hydrogen), and shallow well depth (100 m) for the Mali well… [finding] that it may be possible to produce hydrogen at $1/kg with a 20% internal rate of return (IRR). However, the economics for achieving an aggressive $1/$kgH_2$ production target will necessarily change if deeper wells must be drilled to access additional hydrogen accumulations. In these instances, drilling costs will be several orders of magnitude larger ($5-10 million) than those seen for water well depths ($100,000)." No further details of this analysis are made available.

Ideally, a TEA for geologic hydrogen will align with best practice methods. This includes consideration of concepts such as the levelised cost of energy (LCOE) methodology, which considers the capital cost, financing costs, taxes, operations and maintenance expenses, and fuel costs, typically normalised by the amount of energy produced in kWh to express a final value in the units of $/kWh (typically US dollars) (Aldersey-Williams & Rubert, 2019; P. H. Kobos et al., 2020). Given the increasing importance of hydrogen in the global economy, the LCOE principles have been extended to communicate the same considerations but in units specific to hydrogen production (and consumption). This manifests as the levelized cost of hydrogen (LCOH), typically expressed in $/kg of hydrogen (Ramsden et al., 2013). Developing a comprehensive cost model is not straightforward. It requires access to meaningful historical and forecast cost data, typically not in the public domain. Specialised consultants are often engaged, who may have access to proprietary, outside-the-public-domain cost databases that form the basis of their projections (Lewis et al., 2022). Accordingly, a comprehensive TEA for geologic hydrogen will be a non-trivial exercise.

Gaps in the collective knowledge regarding geologic hydrogen

As alluded to above, the high level of promise or potential of geologic hydrogen is presently matched by the amount of associated uncertainty. Fundamental knowledge that has not yet been reliably determined includes:

- Exploration and appraisal techniques to find and characterise potential geologic hydrogen resources
- Understanding of effective and efficient/optimal means of drilling, completing and operating wells into discovered geologic hydrogen resources
- The simple technical and economic viability of developing and operating a geologic hydrogen resource, either in the presence or absence of government stimulus or incentives
- The existence or prevalence of self-renewing reservoirs and – assuming their existence – the optimal way to manage the operation of these reservoirs to maximise their productivity and benefit to the operator and broader society

Stimulated geologic ('orange') hydrogen: The next frontier?

The preceding discussion of geologic hydrogen should more precisely be described as a discussion of *naturally occurring* geologic hydrogen. That distinction is necessary due to the hypothetical potential for the development of 'stimulated' geologic hydrogen resources. This thesis is not focused on stimulated geologic hydrogen. However, it is introduced briefly here to clarify both the similarities and differences between the two concepts.

Whereas naturally occurring geologic hydrogen reservoirs result from the coincidence of both suitable conditions for generation and accumulation of hydrogen in the subsurface, stimulated geologic hydrogen production proposes to locate only geology that is suitable for the formation of hydrogen. When a suitable geologic resource has been identified, it is proposed that a reagent (typically water) is injected into the rock via injection wells to a force reaction that results in the evolution of molecular hydrogen. The resultant hydrogen is then expected to be produced via production wells to the surface for potential processing and, eventually, provision to users or sale to customers.

Stimulated geologic hydrogen production may be advantageous as it is reasonable to expect that favourable geologies will be more prevalent than the coincidence of conditions necessary for the formation **and** accumulation of naturally occurring geologic hydrogen (i.e. locations where favourable reactant geology, suitable reagents, and favourable accumulation geology are all present). While geologies suitable for stimulated hydrogen production may prove prevalent, there are a range of other techno-economic hurdles that must also be cleared for this to be a viable production pathway. These include proving that the reactions that evolve hydrogen occur on timescales that are sufficiently short, understanding requirements for hydraulic fracturing of the target geology, understanding the technical requirements for injected reagents (e.g. water purity), and understanding and characterising the geotechnical risk of both deliberate and induced rock fracturing. Presently, stimulated geologic hydrogen production has not been proven possible at the field trial level (Zhang & Li, 2024).

Chapter 3: Review of state-of-the-art LCA

Noting the interest in the potential of geologic hydrogen to form an important part of the hydrogen economy, Brandt's (2023, p. 2) paper is self-described as a "prospective LCA" of a hypothetical geologic hydrogen development, which is intended "to use early information about a fundamentally new technology to make a first assessment of environmental impacts or benefits to guide further investment and development." Despite its prospective nature, Brandt's work is the first to be published on the topic, automatically rendering it state-of-the-art. As described in Chapter 1, Brandt estimates that the emissions intensity of his Baseline case is 0.37 $kgCO_2e/kgH_2$ (inclusive of embodied emissions). This indicates that such a development would qualify for the most valuable tier of United States production tax credits and be competitive with all other hydrogen production pathways. This work reviews, replicates, and critiques Brandt's LCA modelling to provide estimates of emissions intensity with increased transparency and improved logic. The observations below were made during a detailed, 'line by line' replication of Brandt's spreadsheet-based model in a 'Jupyter' notebook (Granger & Pérez, 2021). This alternative modelling software was selected with the intention of improving the visibility and interpretability of the calculations relative to Brandt's reference model. Refer to Appendix A for more specifics on the replicated model.

3.1. Overview of Brandt's approach

The fundamental assumption of Brandt's work is that the development of a geologic hydrogen resource is likely to be analogous to the development of a conventional natural gas (i.e. methane) resource. Accordingly, Brandt's prospective LCA is undertaken using an adapted version of an open-source GHG emissions calculation tool developed for application to the oil and gas industry. The Oil Production Greenhouse Gas Emissions Estimator v3.0a (OPGEE) model is well-established, having been under development for approximately 12 years and formed the basis for many published papers (*OPGEE*, n.d.). The standard OPGEE model was adapted for the work on geologic hydrogen to include allowances for hydrogen separation via a Pressure Swing Adsorption (PSA) unit and to compensate for the presence of bulk quantities of hydrogen rather than the trace quantities that may be expected in the oil and gas reservoirs that OPGEE was built to assess.

The OPGEE model uses the principle of conservation of mass to trace flows of fluids from a reservoir to either a delivery point or to a point of loss, such as via venting, flaring, fugitive (VFF) emission, or combustion in the service of providing energy to the processing equipment. It allows for preliminary engineering and sizing of processing equipment and comprehensively considers factors that contribute to the lifecycle emissions of a development. These factors include the importation of grid electricity and the combustion of hydrocarbon fuels during exploration, development, operation, and abandonment (Brandt et al., n.d.).

3.2. Key observations

The headline results of Brandt's paper indicate that, from the perspective of emissions intensity, geologic hydrogen is highly competitive with all other hydrogen production pathways,. However, any enthusiasm generated by these results should be tempered by the paucity of reliable, specific information about geologic hydrogen available to inform their calculation. It is essential, therefore, to be mindful of several key observations.

First, Brandt openly acknowledges that the nascent nature of the geologic hydrogen industry means that there is a lack of meaningful data regarding the subsurface characteristics of geologic hydrogen reservoirs. Accordingly, Brandt assumes that the hypothetical development for his 'Baseline' case will be represented by an 'average' natural gas well in North America. He consults a database of North American well characteristics and performs simple statistical analysis to generate analogous values for the following key characteristics of the hypothetical geologic hydrogen resource:

- Well depth
- Total expected productivity of a reservoir (referred to as Estimated Ultimate Recovery, EUR)
- Production decline rates

Second, Brandt assumes values for other key variables necessary to complete analysis with OPGEE without justifying the basis for these assumptions. These include

- Field life – This is assumed to be 30 years, without clear justification.
- Number of wells – The hypothetical development is assumed to involve 50 production wells, with an additional 13 gas injection wells (where one injection well is assumed necessary for every four production wells).

Third, Brandt assumes that historical fugitive emission rates from oil and gas developments appropriately represent fugitive emission rates of a hydrogen development.

Fourth, Brand assumes a 'slippage rate' (or the inverse of the separation efficiency) for the PSA unit equal to 10% of the quantity of hydrogen entering the PSA unit. This rate governs the quantity of useful hydrogen lost to the waste stream during PSA separation. The supplemental data to the paper explains that literature for gas separation of hydrogen streams via PSA reports slippage rates varying from 5% to 20%. It adds the caveat that this literature primarily considers gas compositions typically seen in industrial hydrogen production facilities, which involve gas compositions significantly different from those assumed in this geologic hydrogen analysis. The selection of a 10% slippage rate appears to have resulted from judgement applied to the range reported in the literature.

Fifth, Brandt's 'well to gate' analysis does not consider the transportation of the hydrogen from the production facility to the consumer. It does, however, assume that the small proportion of crude oil co-produced with the hydrogen is transported via the network of crude transportation pipelines within the United States.

3.2.1. Brandt's approach to uncertainty analysis

Brandt discusses his approach to uncertainty analysis directly, noting that "the nascent nature of the industry precludes assigning realistic empirical distributions to the underlying parameters" (Brandt, 2023, p. 3). Accordingly, the paper adopts a straightforward parametric sensitivity analysis approach. Here, a range of cases are thoughtfully selected to assess the impact of key assumptions deterministically. Specifically, the sensitivity cases consider the assumptions regarding:

- Gas composition
- Productivity
- Depth

Similarly, the sensitivity cases consider design decisions relating to:

- Waste gas re-injection vs flaring
- Disposal vs exploitation of reservoir methane content
- Local power generation vs grid power imports

3.2.2. Discussion of key findings

The key metric discussed in Brandt's paper is "production-weighted mean emissions" (also referred to in this document as 'lifetime emissions intensity'). However, the paper does not include a specific definition, calculation method or justification for this metric. Examining the supplementary material reveals that this value is determined by simply calculating the total mass of 'CO_2-equivalent' emissions throughout the field's life (including the entire lifecycle, from exploration to abandonment) by the total mass of useful hydrogen product that is exported from the facility over its life.

Importantly, this definition of production-weighted mean emissions differs from calculating emissions intensity for each year of field life (where production flow rates are assumed to be constant for the duration of each year). In this situation, annual emissions are divided by annual hydrogen exports to give a value for 'production-weighted emissions' for each year of operation. While calculating the mean of these annual values is not statistically valuable (because this makes low-production, low-emission years equally significant to the result as high-production, high-emission years), the annual results themselves may be meaningful. They could be used, for example, to calculate eligibility for PTCs (see Section 6.5. for a more detailed discussion of this topic). In this context, it may be most useful to report on the number or proportion of years that fall below a chosen threshold (e.g. 0.45 kg CO_2e/kgH_2) to indicate the tax-attractiveness of a potential development.

In general, Brandt's "prospective LCA" work ultimately shows sufficiently encouraging results to justify ongoing research and entrepreneurial efforts in the field of geologic hydrogen. This thesis is intended to contribute to the body of ongoing research and improve the shared understanding of geologic hydrogen's place in the energy transition.

3.3. Replication of key findings from Brandt's paper

As mentioned previously, this work bases a review of Brandt's findings on a detailed recreation of the relevant components of the OPGEE model. Brandt's key findings are replicated to validate the recreation's accuracy. Figure 3.1 shows both Brandt's key results for the Baseline case and the replicated results generated in the recreated model. Note that the 'error bars' in the original plot can be considered somewhat misleading because they do not represent statistical uncertainty, as is conventionally implied by a 'box and whisker plot'. Instead, they represent the minimum and maximum annual emissions intensity results observed over the field life. This is made more explicit in the bar chart presentation of the replicated results.

3.3.1. OPGEE calculations excluded from the replica model

Due to resource constraints and to slightly reduce the complicatedness of the replicated model, certain calculations were excluded. These are summarised below:

- Consideration of fuel gas demand from the ‘booster compressors’ that are assumed to be installed upstream of the inlet separator. These compressors are assumed only to be required once the pressure of gases leaving the reservoir drops below the 500 psi assumed operating pressure of the processing equipment (plus an allowance for pressure losses between the wellhead and the separation unit). Further, in the peak demand scenario for the Baseline case (i.e. the last year of field life, when reservoir pressure is assumed to be at its lowest), the fuel gas demand for the separation compressors is only ~1% of the demand from the waste gas reinjection compressors (in year 30). This quantity is thus assumed to be negligible.
- Reinjection compressor compressibility factor (‘Z factor’) calculations. In the module that calculates the required power demand for the waste gas reinjection compressors, the Z factors for all gas mixes have been set equal to 1 (i.e. ideal gas assumption) for simplicity.

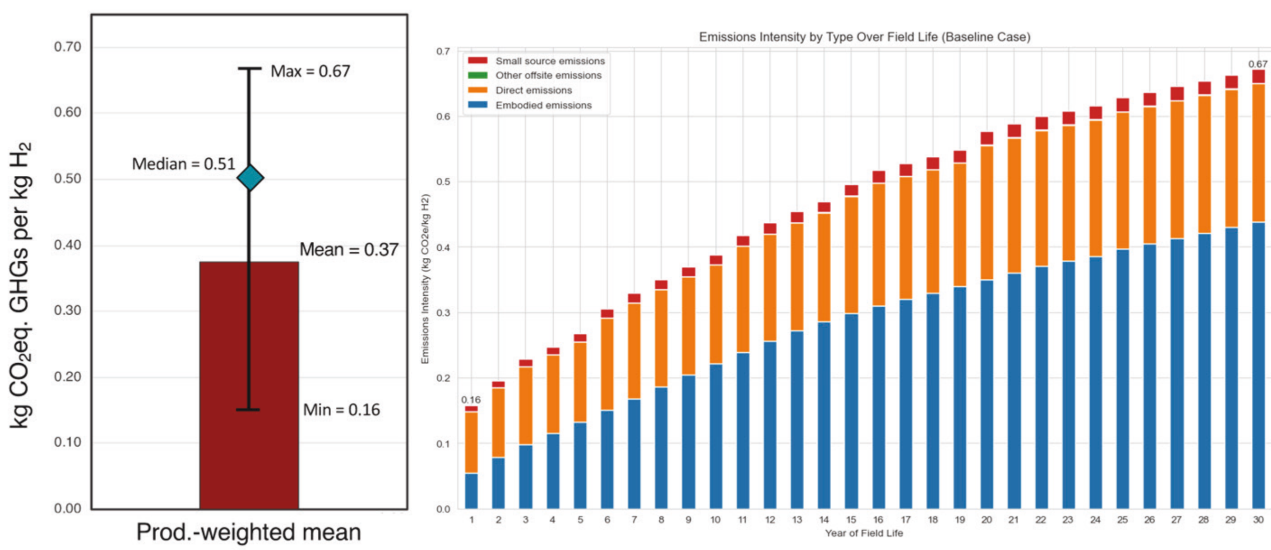


Figure 3.1: Left – Extract of Brandt’s Figure 2 (2023, p. 5), the key figure from this publication. Right – Output from the replicated model produced in this work. This illustrates the clear alignment between the Min, Median, and Max values from Brandt and the Year 1, Year 16, and Year 30 output values from the replicated model.

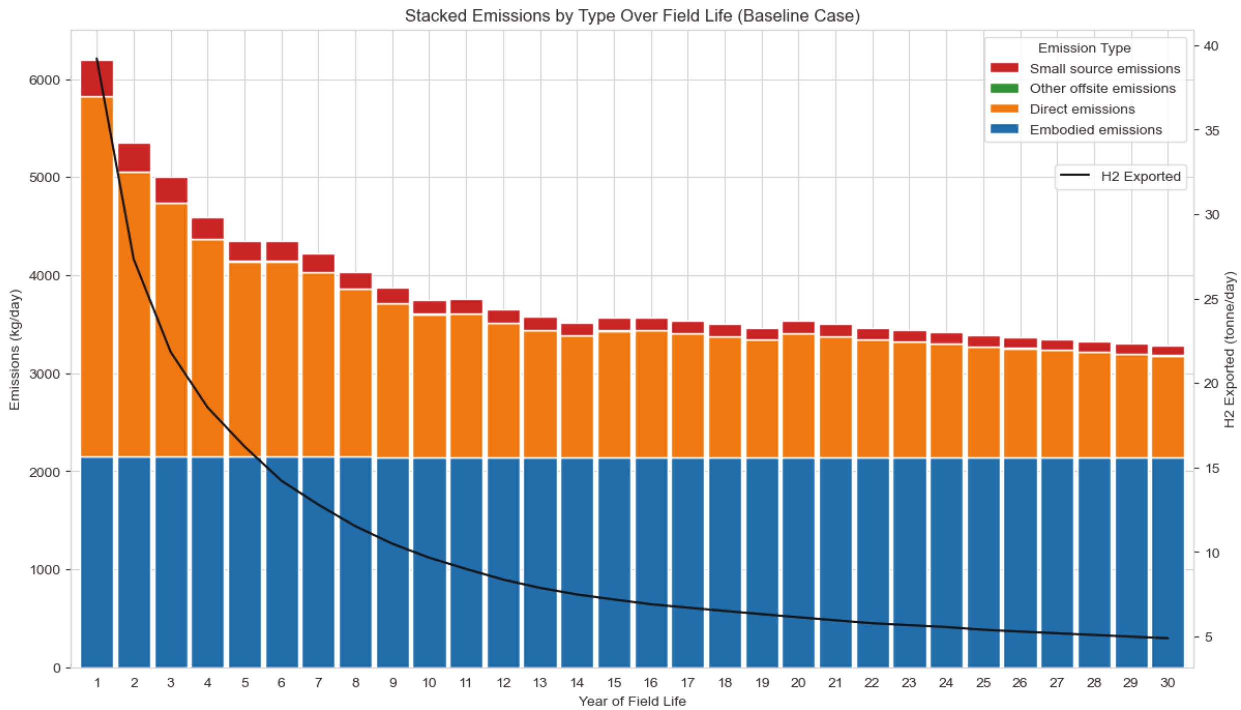


Figure 3.2: Alternative view of the output of the replicated model, showing absolute daily GHG emissions (broken down into four categories of emission types) and hydrogen exports for each year over the 30-year life of the hypothetical resource.
Notice that embodied emissions are assumed to be evenly distributed over the entire life of the asset despite these emissions actually taking place before the start-up of the development (except for the small proportion of these emissions associated with field abandonment).

3.4. Commentary on the Brandt paper

Reverse-engineering Brandt's application of the OPGEE model revealed the strengths and weaknesses of both the broad modelling approach and the OPGEE model itself. These are discussed in detail here.

3.4.1. Strengths and weaknesses of the modelling approach

In this author's view, the main strength of Brandt's modelling approach is the decision to leverage the capabilities and strengths of the OPGEE model, outlined below. Another primary strength of the approach was to generate an array of sensible sensitivity cases to examine the influence of key design decisions and key assumptions. Brandt's thoughtful selection and description of these sensitivity cases are particularly beneficial given the paucity of reliable data for making reasonable assumptions for geologic hydrogen developments.

The selection and implementation of sensitivity cases do, however, raise some concerns. Specifically, several sensitivity cases ostensibly involve changes to a single, key assumption to determine the sensitivity of the emissions intensity results to this assumption. Consider, for example, the “Shallow” and “Low H_2” cases. These cases are, respectively, intended to examine the influence of well depth and gas composition. There is no clear justification to explain why these cases would have assumed productivity different to that of the Baseline case. However close inspection of the supplemental data reveals that these two cases seem both assumed to have ‘raw gas’ EUR rates of 33 BCF, which is half of the Baseline case and equivalent to the ‘Low Productivity’ case. Precluding the ability to distinguish between the impact of depth, hydrogen concentration, and reservoir productivity means that these cases are less useful at best and misleading at worst.

Noting that the sensitivity cases are useful when making claims about an assessment involving high uncertainty, this author argues that Brandt’s approach to modelling uncertainty is one of the major weaknesses of the paper. His argument that “the nascent nature of the industry precludes assigning realistic empirical distributions to the underlying parameters” may be logical but does not justify ignoring uncertainty altogether. Brandt’s argument may be construed as ‘there is very high uncertainty in this assessment, so we ignore uncertainty and report only on deterministic results’. Alternatively, just as reasonable assumptions are made to select deterministic values to include in the model, reasonable assumptions can be made regarding probabilistic distributions for these same values. This approach may yield important insights. Brandt’s decision here is somewhat perplexing, given that the OPGEE model has the native ability to handle uncertainty analysis. See Chapter 5 for a detailed discussion of incorporating uncertainty analysis and the associated insights.

3.4.2. Strengths of the model

The OPGEE model has several strengths relevant to its application to an assessment of geologic hydrogen. These include:

- The model is well-established and reputable, thanks to the nature of its development history. This includes the legitimacy afforded by the peer-review of previous publications based on the model.
- OPGEE’s comprehensive inclusion of potential sources of emissions, including

embodied emissions (prior to operation) and decommissioning activities (well plugging, after operations have ceased).

- The open-source nature of the model and the data/assumptions upon which it is built. This ensures that results generated by the model are maximally transparent and verifiable. Indeed, the premise of this thesis relies on the transparency of Brandt's publication and the OPGEE model itself.
- The model has sophisticated functionality, including the ability to include or exclude modules via simple toggles, the ability to incorporate uncertainty analysis, the inclusion of reasonable default values that may be easily overridden, and internal error-checking. It is also reasonably well-documented via a 402-page operating manual.

3.4.3. Weaknesses of the model

As a counterpoint to its strengths, the OPGEE model also has aspects that are disadvantageous in the context of the lifecycle assessment of geologic hydrogen. These include:

- The 'general purpose' nature of the model. While the flexibility to apply a model to various contexts would ordinarily be considered a strength, the fact that OPGEE was not built with geologic hydrogen resources in mind means that it includes significant capability and structure that is unnecessary for hydrogen assessment(s). This superfluous capability reduces the interpretability of the model and analysis of its results.
- The use of a Microsoft Excel spreadsheet as the primary modelling tool. The OPGEE documentation suggests that this choice of modelling tool ensures that it is highly accessible, given the ubiquity of spreadsheet software and the sophisticated capability that can be created via macros and other automation. The downside is that spreadsheet models are notoriously hard to inspect and validate due to the challenge of interpreting formulas, particularly those that use unnamed cell references and references across different sheets of the model file. In this instance, this difficulty is exacerbated by the previous observation of the inclusion of significant superfluous capability, which makes navigation of the file more complicated than it would otherwise be.

- The model includes citations or allusions to various reference documents, but it does not include a reference list, nor does the reference list in the operating manual capture all of the citations made within the model.

3.5. Significance of minor errors/corrections on conclusions

The reverse engineering of Brandt's OPGEE modelling work revealed the weaknesses mentioned above and served as a detailed check of the logic and mechanics of the various calculations performed by the model. This activity revealed numerous minor errors in both logic and calculation mechanics (e.g. clear typographical errors in cell references). Figure 3.3 shows the individual and cumulative effects of correcting these errors for the Baseline case. The details of each of these errors are explained below.

3.5.1. Corrected the number of injection wells when calculating steel mass

Brandt's OPGEE model clearly states the assumption that there are four gas re-injection wells for each of the assumed fifty production wells (i.e. applying a factor of 25%, rounding up). This results in an assumption of 13 injection wells, for a total of 63 wells. Some of Brandt's calculations are inconsistent with this assumption, where the number of injection wells is assumed to be a factor of "0.25/1.25" (i.e. 20%) of the number of production wells. This inconsistency is not justified or explained and appears to be an error.

3.5.2. Added injection well surface tubing

The "Production and surface processing facilities" section of the "Embodied Emissions" sheet of Brandt's OPGEE model calculates an assumed mass of steel associated with each well. It multiplies this 'per well' amount by the number of production wells and the number of water injection wells. The formula does not include the number of gas injection wells, so the reported total mass (and associated total emissions) only covers the 50 production wells in the Baseline case. The additional 13 gas injection wells will necessarily require piping (between the surface processing facilities and the wellhead), so this calculation appears to be an error.

3.5.3. Corrected equipment sizing calculations

Brandt's approach to sizing surface processing equipment (and thus the determination of the embodied emissions associated with this equipment) is flawed. The reasoning for this flaw is due to a nuance of the design and intended use of the generic OPGEE model, and how Brandt has implemented it for the geologic hydrogen study. Generally, OPGEE is set up to allow parallel analysis and comparison of the estimated emissions of numerous oil and/or gas fields, with the general assumption of constant production flow rates over the life of the field. In Brandt's analysis, he pays close attention to the estimated production decline rates over the assumed 30-year field life by assuming a constant flow rate for each year of operation, with flow rates generally declining over the field life (as indicated by an analysis of historical natural gas well operation data). Brandt models each of the 30 years of operation as a separate field. Each analysis of these 30 years of operation is then aggregated to provide the final results associated with the hydrogen development.

Examination of the OPGEE calculations for embodied emissions reveals that the production flow rate is the main variable considered when sizing the surface processing equipment. This means that Brandt's approach effectively re-sizes the equipment for each year of operation and the aggregation of results 'averages out' this phenomenon. In reality, equipment can only be sized once and, typically, this must consider the most onerous design conditions plus an additional design or safety margin. In general, this means that equipment like pressure vessels will need to be made larger to handle the high flows and pressures of early field life, while equipment like compressors will need to be made larger to deal with the lower pressures at the end of field life.

Specific flaws in equipment sizing are discussed briefly below. As shown in Figure 3.1, each of these changes has an almost negligible impact on the LCA and its final reported value of lifetime emissions intensity for the Baseline case. However, these flaws and corrections become more significant when considering techno-economics, so they are discussed in more detail in Chapter 4.

Separator/PSA sizing

The OPGEE model assumes a three-phase separator is installed directly downstream of the gas-gathering piping from the wellheads. In line with the logic described above, Brandt's modelling re-sizes this separator during each year of operation. In fact, the flow rates and pressures in early field life exceed the ratings of the nominal pressure vessel designs built into OPGEE, so they result in an error, meaning that zero weight is assumed for these years of operation. This significantly underestimates the mass of steel and embodied emissions associated with this equipment. The model generated as part of this work has corrected this error by assuming a conservative design case (i.e. maximum expected flow rate) and a conservative pressure vessel design, based on the nominal designs included in OPGEE. Refer to the relevant sections of the model notebook in Appendix A and Section 4.3.1for detailed explanations.

Further, Brandt's modification of OPGEE to include a PSA unit is implemented simply by assuming the mass of the PSA unit is a multiple of 5 times that of the separation equipment. Accordingly, this magnifies the effect of correcting the flawed separator sizing.

Acid Gas Removal Unit (AGRU or 'gas sweetening unit') included in embodied emissions

The Brandt OPGEE model clearly states, "Turn acid gas removal off, as there is no appreciable concentration of CO_2 or H_2S in this gas." This instruction is followed in the VFF and process flow portion of the model. However, the embodied emissions calculation includes an estimate of the mass of steel associated with "gas sweetening equipment", which is clearly in conflict. Removing this equipment from the embodied emissions calculation reduces the emissions intensity of the development.

Corrected AGRU adsorber sizing

Noting the above observation that gas sweetening equipment, which is primarily centred on adsorber vessels, should be excluded from the embodied emissions calculation, it was also observed that the adsorber sizing logic was flawed. This flaw is similar to the separator sizing flaw, in that Brandt's OPGEE implementation re-sizes the gas-sweetening adsorber pressure vessel at each year of operation. If the inclusion of AGRU/'gas sweetening' is 'turned on' in the model, then correcting this error based on a conservative design case would increase emission intensity due to increased steel mass. More specifically, for the Baseline case, emissions intensity would increase by ~4.7E-5 $kgCO_2e/kgH_2$ or ~0.013%.

Corrected gas dehydration contactor sizing

The sizing of the gas dehydration contactor in Brandt's model suffers from the same sizing flaws as the other pressure vessels. In this case, however, an additional error requires correction. OPGEE generally assumes that pressure vessels are simple cylindrical objects whose mass can be estimated by calculating the volume of steel in the shell of the vessel and multiplying it by a suitable value for the density of steel. In this instance, however, there are significant typographical errors in the spreadsheet formulas intended to calculate the shell volume. The volume calculation did not include pi, nor did it account for any ends on the cylinder. Correcting these errors similarly resulted in increased embodied emissions due to increased estimation of steel mass.

Corrected gas reinjection compressor sizing

The OPGEE model algorithm scales the estimate of the size and mass of the waste gas reinjection compressor to the amount of gas being reinjected. Similar to how vessels are sized, Brandt's OPGEE implementation effectively revises the size and mass of the compressor each year, as production flow rates decline. In reality, the compressor can only be sized once, so it is sensible and conservative to do so for the maximum flow rate. The impact of this change is minimal, calculated at 2.72E-07 $kgCO_2e/kgH_2$. This is the smallest effect of a correction from this chapter and is an order of magnitude smaller than the effect of the second smallest. For this reason, it has been deliberately omitted from Figure 3.3.

3.5.4. Corrected export piping steel allocation

In order to account for embodied emissions of export infrastructure, the default method in OPGEE is to determine the steel intensity of the entire United States crude oil transportation network and apportion (on a volume basis) the embodied emissions associated with this network to the oil development under assessment in the OPGEE instance. In doing so, the calculation estimates the total mass of the U.S. pipeline system steel, as well as an allowance for "ancillary steel (supports, reinforcement, casing and trenching)" equal to 50% of the mass of the pipe. In an apparent typographical error, however, only the mass of the ancillary steel is used to apportion the associated emissions. This means that this estimate is only one-third the amount it should be.

3.5.5. Added gathering piping for gas injection wells

The OPGEE model includes an estimate of embodied emissions associated with the steel used in the "small diameter crude gathering system infrastructure". This calculation is not documented within the operating manual nor clearly explained within the model. However, it appears that this references literature that assigns an assumed length of 'small diameter' piping for each well, possibly as an allowance for transporting produced oil within the surface processing facility. Again, a 'per well' mass of steel is determined and multiplied by the number of wells. In the OPGEE model, the multiple is of the number of production wells as well as the number of water injection wells. This author cannot identify a justification for selecting these two categories of wells so, to be conservative, the revised model applies this factor to all wells (i.e. production as well as gas reinjection, given there are no water re-injection wells as part of the assessment).

3.5.6. Added abandonment plugs for all wells

One of OPGEE's strengths is the consideration of the entire lifecycle of a development, up to and including abandonment. However, it appears the calculations estimating well abandonment emissions have not been carefully constructed. The default OPGEE model assumes that four wellbore plugs are required for abandonment, regardless of the number of wells. The lack of documentation means this logic cannot be checked for correctness. However, it seems likely that this should be a 'per well' factor rather than an absolute factor. Accordingly, the revised model includes an allowance for four plugs for each well involved in the development, including the production wells and the gas reinjection wells.

3.5.7. Corrected typo in "other offsite emissions"

Brandt's modified OPGEE model for geologic hydrogen assessment includes an additional sheet for "Geologic H2 specific results". It is from this sheet that the important annual emissions intensity value is calculated. Within this sheet, however, there are clear typographical errors in the calculation of "Other offsite emissions". First, the formula subtracts a blank cell in the 'GHG Summary' sheet, which means that embodied emissions are double-counted in the final emissions intensity calculation. This error is slightly offset by another error, where the "Other offsite emissions" calculation does not convert the units from 'tonnes CO_2e/day' to align with the 'kg CO_2e/day' units of the other emissions sources referenced in the calculation. Both of these errors have been corrected in the revised model.

3.5.8. Inconsistent assumptions regarding injection reservoir pressure

Brandt's analysis assumes that pressure in the reservoir into which the waste gas is reinjected is identical to the pressure in the production reservoir, i.e. declining over field life. This injection reservoir is not being produced (i.e. the process is not extracting matter from the reservoir), so the assumption of declining pressure is illogical. This assumption would be logical for applications where produced gases are reinjected for enhanced oil production (known as ‘gas lift’), but it contradicts Brandt’s assumptions elsewhere. Expressly, the embodied emissions section of Brandt’s model assumes the mud required for “water injection wells” is zero because no water injection wells are included in the design. The calculation does not consider gas injection wells. If it is inferred that mud for gas injection wells has been deliberately excluded from the model, then this implies there is no reservoir pressure to be contained by the drilling mud.

Two potential corrective measures can be taken:

- Add the requirement/assumption that drilling mud is used during the drilling of the gas reinjection wells. This will increase embodied emissions.
- Assume the pressure in the reinjection reservoir is the chronological reverse of the pressure in the production reservoir. i.e. increasing over time.

For the sake of conservatism, the revised model implements both of these corrections.

3.5.9. Inconsistent handling of fuel gas offtake assumption affects fugitive emissions

The handling and assumptions regarding the ‘fuel gas’ that is assumed to be used to power the reinjection compressors are not consistent throughout the model. Brandt assumes that all fuel gas is taken from downstream of the PSA unit, meaning it is pure hydrogen and has no GHG emissions associated with combustion. However, Brandt’s mass balance approach used to determine fugitive emissions does not properly reflect this assumption. In this case, Brandt’s model shows that the fuel gas driving the reinjection compressor has the composition of a stream taken upstream of the PSA unit, meaning it contains methane (for cases where methane is present in the reservoir), as well as hydrogen. Incorrectly assuming that some of this methane is consumed as fuel gas means that the subsequent assumptions regarding the composition and flow rate of the stream downstream of the compressor turbine are underestimated. Given that fugitive emissions are assumed generally to be in proportion to the mass flow rate, then this incorrect assumption leads to an underestimation of the fugitive emissions downstream of the compressor.

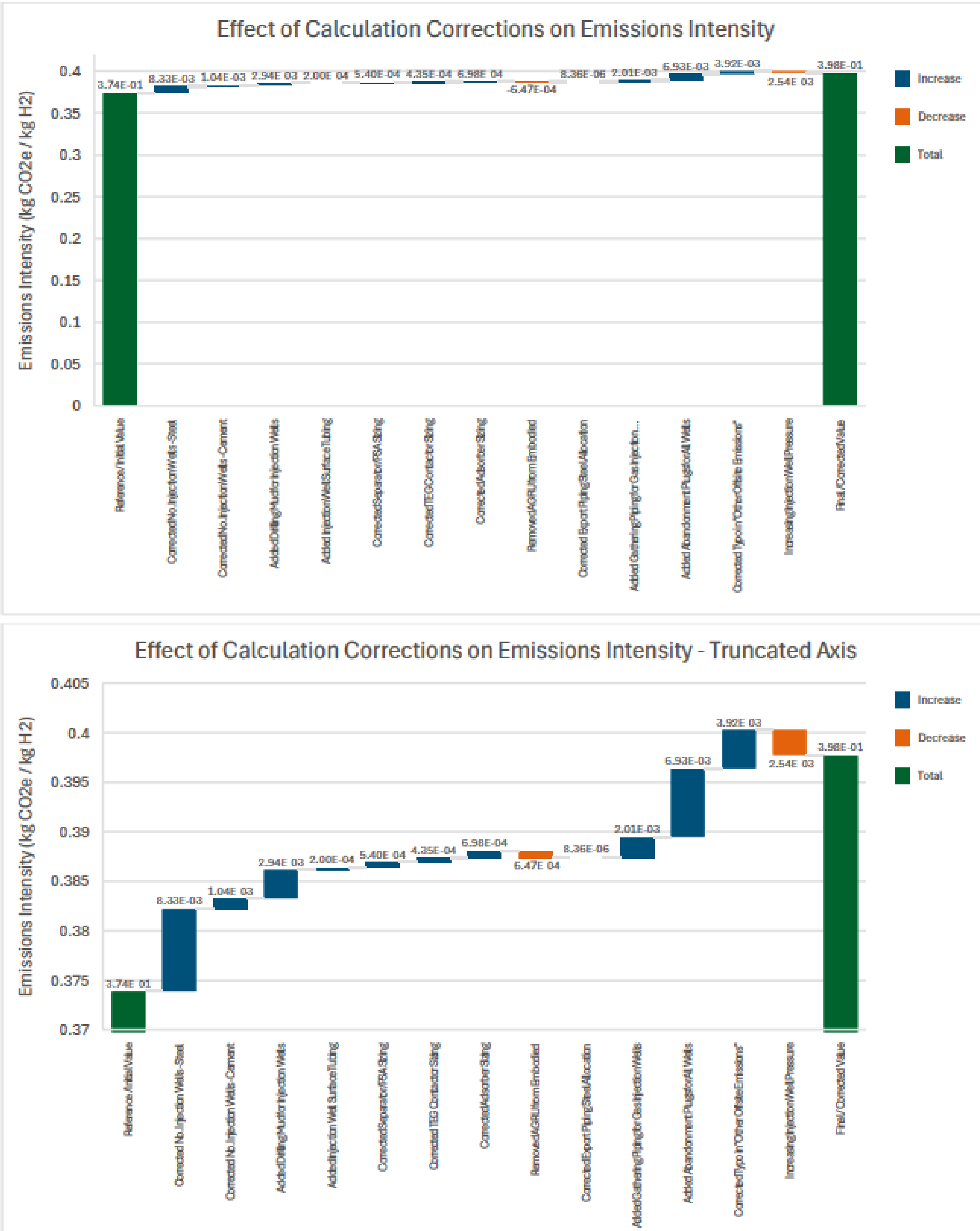


Figure 3.3: Two visualisations of the individual and cumulative effects of a range of calculation corrections on the key metric for this study, production-weighted emissions. The data is identical, but the vertical axis of the lower plot has been truncated to increase the visibility of these small-magnitude changes.

3.6. Summary of impact of minor corrections

As shown in Figure 3.3, implementing the corrections described above has a cumulative effect of increasing the 'headline' emissions intensity result from 0.37 $kgCO_2e/kgH_2$ to 0.40 $kgCO_2e/kgH_2$, or an increase of 6.4%. Given the general uncertainty of many of the necessary parameters, this increase is likely within the confidence interval associated with the calculations. Regardless, correcting basic errors is important to improve confidence in the final results.

3.7. Minor improvements not included in the revised model

In the process of replicating and then revising Brandt's implementation of the OPGEE model, it has become apparent that there are several other opportunities for minor improvements to the model. These have not yet been implemented but are stated here for visibility:

- Add an allowance for the steel and cement used in the foundations and footings of surface equipment. The model uses multiplication factors to 'gross up' the quantity of steel associated with surface processing equipment and account for various ancillary steel; however, it does not include any allowance for the cement in concrete that would very likely be required to establish a permanent operating facility.
- Improve the assumptions used when calculating the geometry of surface processing pressure vessels. Currently, OPGEE assumes pressure vessels are all cylindrical vessels with flat ends. The poor structural performance of this geometry means that it is rarely used, and a more realistic ('better') assumption would be vessels that have hemispherical or elliptical ends.
- The assumptions regarding fugitive emissions associated with well completions and well workovers are inconsistent throughout the model. The calculations for completions emissions take into account hydrogen and assume that there are no emissions from injection wells. Conversely, the calculations for well workovers ignore hydrogen but take into account injection wells. These assumptions are not documented in the OPGEE model, but it is suspected that both of these sources of emissions should include hydrogen and both should consider all types of wells.
- The default sizing algorithm for the dehydration contactor is flow-rate limited. For

high-productivity sensitivity cases (i.e., a combination of high well productivity rate and high well count), the maximum nominal flow rate is exceeded. In these cases, the revised model selects the largest contactor design nominated in the OPGEE algorithm. Thus, these cases underestimate the embodied emissions, however it was shown previously that even large magnitude changes in equipment sizing have only a minimal effect on the headline, final value of emissions intensity of the development.

3.8. Discussion regarding the 'accounting' of embodied emissions

The OPGEE model uses a 'straight-line depreciation' method of accounting for embodied emissions. That is, the model calculates total embodied emissions associated with the development and, together with the assumed lifespan of the development, determines an equivalent daily or annual rate of embodied emissions. While this method is simple and logical, it is unclear if it is the most appropriate. This is because, in reality, embodied emissions (except for those associated with abandonment) are released to the environment in advance of a resource development starting operation. Given the urgent emissions reductions required to achieve Paris Agreement targets, it is questionable that an 'emissions accounting' approach that allows emissions to be apparently 'deferred' by multiple decades would be the best practice. A better approach may be to align this study with the approach and methods used to calculate the so-called 'social cost of carbon' (US EPA, n.d.).

3.9. Conclusions

This review of Brandt's modelling approach and the details of the model itself found that both are sensible and generally of high quality. The correction of minor and typographical errors did not significantly change the major conclusions from the paper. That said, there are more significant changes that can be made to improve the model. Such changes are discussed in detail in Chapter 4.

Chapter 4: Improvements and Extensions to State-of-the-Art LCA

The previous chapter summarised the detailed review of Brandt's (2023) paper and LCA model. It found typographical and other errors that were not individually significant in the context of a 'prospective LCA'. This chapter considers some more significant critiques. It addresses several of these by proposing and implementing means by which they can be addressed in the model. These modifications are then analysed to consider their impact on the conclusions that may be drawn from the model.

4.1. Proposed improvements to the OPGEE LCA of geologic hydrogen

The critiques addressed in the chapter are:

- Expanding on the importance (particularly for techno-economic considerations) of ensuring the model only selects a single design for surface processing equipment rather than effectively 're-designing' the equipment for each year of the field's life, and;
- Examining sensitivity to unjustified assumptions in the original model, especially regarding assumed field lifespan.

The following sections describe these critiques and the remedies included in this author's model.

4.2. Impact of field lifespan on emissions intensity

4.2.1. Introduction

Astute readers of the previous section will have identified that the uncertainty analysis did not include an assessment of another key assumption of Brandt's analysis: the lifespan of the field. In all of Brandt's cases, it is assumed that the field under analysis has an operating life of 30 years. It is further assumed that the flow rate of fluids from the reservoir declines over the 30-year life in amounts represented by the average reported production declines of U.S. natural gas wells (i.e. there is an empirical rather than mathematical sense to the flow rate decline). While using natural gas analogue data is consistent with the assumptions made elsewhere in Brandt's paper, the foundational assumption of 30 years of operation is not explained nor justified.

Brandt may have omitted such an explanation due to concluding that it was not relevant to the lifecycle emissions intensity results. Indeed, if emissions intensity is calculated by dividing lifetime emissions by lifetime hydrogen production, and if everything else is held equal, then the length of the field life will have no effect at all on the emissions intensity result. Pragmatically, however, field productivity and lifespan are likely to be highly correlated under the assumption that a field will continue to operate as long as there are marginal returns to be earned via continued operation (i.e. a field will typically be operated until the revenue earned from the produced hydrogen exceeds the cost of continuing to operate it. This is notwithstanding complicating factors such as operating companies deliberately deferring decommissioning and abandonment activities for financial reasons). With this in mind, it can be assumed that the Baseline case ceases to be sufficiently profitable at the hydrogen production rate in Year 30. For a small or 'failed' development, production rates could drop to this level within years or months, whereas a large, successful development could continue for many decades. This observation suggests that a study linking lifespan and productivity may be informative. Such a study is described below.

4.2.2. Understanding Brandt's assumptions of lifespan and productivity

Brandt states that the "baseline case is meant to represent a ''general'' case with average properties" (2023, p. 11) calculated using a comprehensive dataset of North American (USA and Canada) natural gas wells. The supplementary information explains that productivity (EUR) is calculated on a mean of reported values of 685,661 gas wells. Brandt calculates 1.33 BCF per gas well as the mean of the dataset. The dataset has a clear left skew, with the 75th percentile production rate being 1.21 BCF/well. Brandt indirectly acknowledges this skew by mentioning that the data set includes numerous newer wells and the likelihood that these are highly productive hydraulic fractured gas wells. However, Brandt's baseline case includes only conventional, vertical wells, so the selection of the mean rather than median production rate is worthy of questioning. Brandt addresses potential criticisms of this selection by considering both 'low productivity' and 'very low productivity' scenarios. Like EUR, Brandt calculates production decline rates from the well data set by considering average monthly/annual production from fields with reported production >360 months. This filtering resulted in a smaller set of 160,229 gas wells.

Brandt does not explicitly explain the approach to determining flow rate profiles. However, inspection of the model reveals that these appear to be calculated to fit the previous two assumptions. i.e. An initial flow rate is determined such that, when the empirical production decline rate is applied, the sum of annual flow rates also meets the 1.33 BCF/well total productivity requirement. This approach firmly 'bakes in' the 30-year lifespan assumption into the model.

4.2.3. Approach to lifespan and productivity study

In order to assess the relationship between field lifespan, productivity and emissions intensity, it is first necessary to establish additional assumptions that can 'override' the foundational assumptions linking productivity, production rate decline and flow rates. In this case, Brandt's Baseline case continues to be the reference for the study. First, a mathematical relationship between productivity and lifespan is established by approximating the Baseline flow profile. To do so, the following assumptions are made:

- The Baseline Year 30 flowrate is the minimum flow rate for viable ongoing operations (i.e. the point at which the marginal cost of ongoing production exceeds the marginal benefit) and;
- The Baseline Year 1 flowrate is common, regardless of the total productivity of the reservoir.

Now, noting that Brandt's use of empirical production decline rates is inextricably linked to the assumption of 30-year field life, an exponential decay curve is fit to the Baseline flow curve to mathematically approximate this decline. This least squares regression calculation determined values for the initial flow rate and the exponential decay factor that maximised the closeness of the fit. The qualitative closeness of this fit is shown in Figure 4.1. The general formula for the fit of the equation is as follows:

$$Q(t) = Q_0 e^{(-kt)}$$

Where: $Q(t)$ *is the flow rate in year* t

t *is the number of years since the start of flow from the field*

Q_0 *is the flow rate in Year* 1

k *is the exponential decay factor*

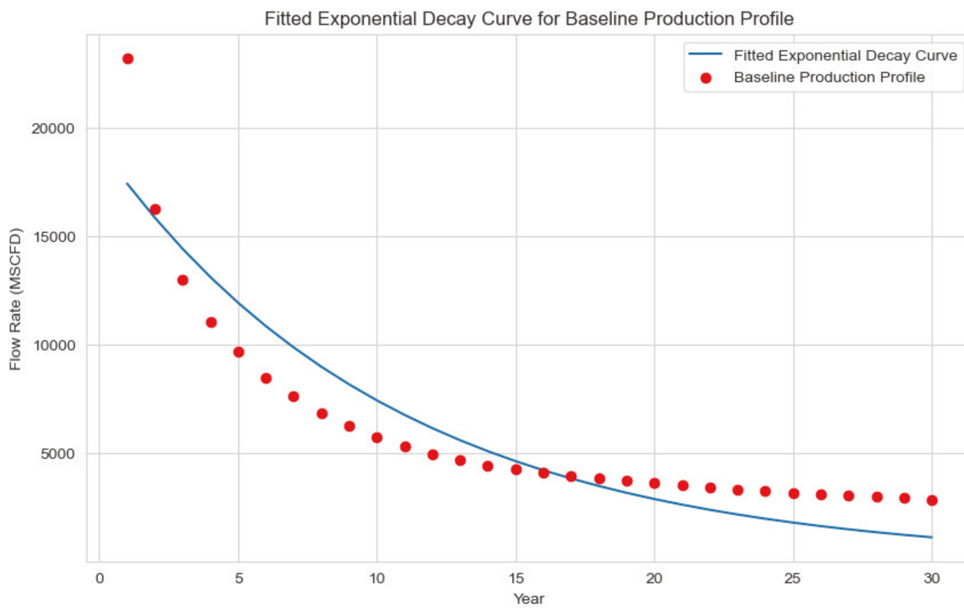


Figure 4.1: A plot showing the empirically determined flow rate profile for the Baseline case (red dots) and the exponential approximation of this profile (blue line), determined via the least sum of squared error method.

While the exponential fit is mathematically convenient to implement, it is obviously an approximation of the Baseline case data. Rather than testing the quality of the fit via statistical means, the fit is tested by assessing the approximated exponential decay curve case's impact on the outputs of the LCA model. Assessing the approximated case with the model shows that the exponential flow approximation is a reasonable representation of key LCA metrics. A specific comparison of the Baseline case's emissions metrics with the approximated case's emissions metrics is shown in Table 4 1.

Table 4-1: Comparison of the approximation of the Baseline case using an exponentially declining flow profile against the unmodified Baseline case. This shows generally good alignment between the Baseline case and the approximation.

Emission Metric	Baseline Value	Exponential Approx Value	Percentage Difference (%)
Min (Year 1) Emissions ($kgCO_2e/kgH_2$)	1.68e-01	2.01e-01	19.5
Max (Year 30) Emissions ($kgCO_2e/kgH_2$)	7.38e-01	1.69e+00	129.2
Percent Embodied to Total Emissions (%)	6.07e+01	6.45e+01	6.3
Total Emissions ($kgCO_2e$/day)	6.64e+03	5.90e+03	-11.1
Total lifetime emissions ($kgCO_2e$)	4.60e+07	4.58e+07	-0.4
Total direct emissions ($kgCO_2e$/day)	3.81e+03	3.14e+03	-17.6
Total small source emissions ($kgCO_2e$/day)	3.81e+02	3.14e+02	-17.6
Total other offsite emissions ($kgCO_2e$/day)	4.52e+01	4.43e+01	-2.1
Total embodied emissions ($kgCO_2e$/day)	2.40e+03	2.40e+03	-0.1
Total emissions excluding embodied emissions ($kgCO_2e$/day)	4.40e+03	3.50e+03	-17.4
Total lifetime emissions excluding embodied emissions ($kgCO_2e$)	1.97e+07	1.95e+07	-0.8
Lifetime Emissions Intensity ($kgCO_2e/kgH_2$)	4.06e-01	4.07e-01	0.2

Noting that the approximation can be considered reasonably representative of the Baseline (30-year lifespan) case, the 30-year approximation case can then itself act as a reference or baseline result for a study that examines the significance of field lifespan on emissions intensity. To do so, the initial and final flow rates of all cases are set to match the exponential approximation of the Baseline case. Then, flow rate decline is calculated according to an exponential decay curve that fits these two points and varies only by the space between the two points, dictated by the lifespan. To illustrate this further, Figure 4.2 provides a visual comparison of the Baseline case flow rate, its exponential approximation, a sample of a case with a shorter-than-baseline lifespan and a sample of a case with a longer-than-baseline lifespan.

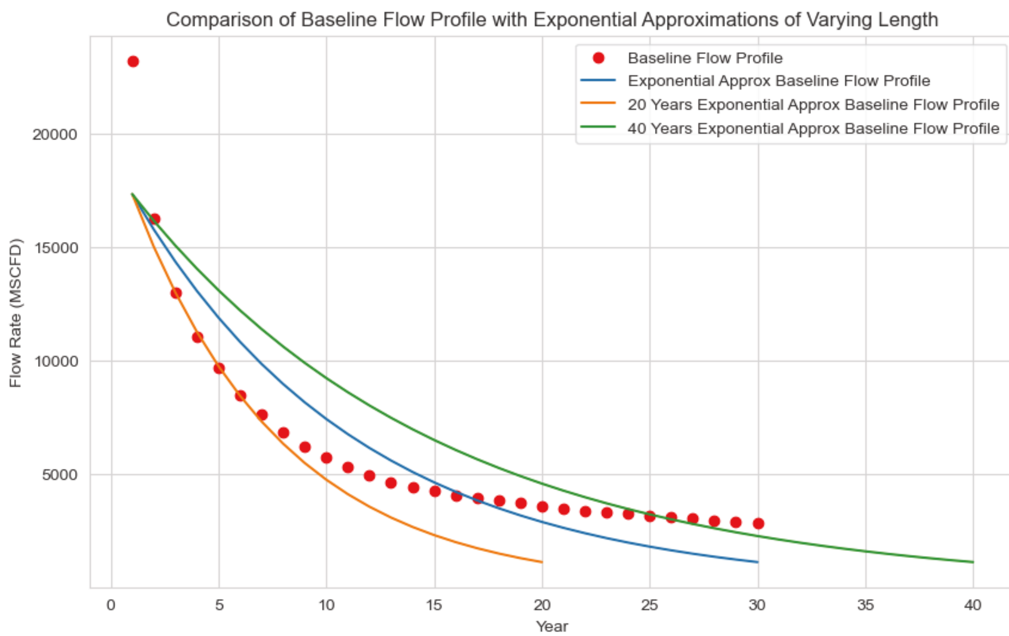


Figure 4.2: Plot comparing the 30-year Baseline case flow profile (red dots) with its exponential approximation (blue line), as well shorter (20-year) and longer (40-year) approximations (orange and green lines, respectively). Notice the exponential approximations all share the same values for initial and final flow rate.

By implementing the approximations in this way, there is an implicit assumption that the total productivity of a development is linked to its lifespan. That is, total productivity is effectively the integral of the flow rate curve (or the area beneath the flow curve). This assumption is consistent with production from either a finite geologic hydrogen resource or production at a rate that exceeds the regeneration rate of a regenerating resource.

4.2.4. Results

With these assumptions defined, assessing field lifespans of any length is possible. For this study, a range of 1 to 50 years was selected. The aggregated results of this study of 50 hypothetical fields, in terms of emissions intensity and total hydrogen exports, are shown in Figure 4.3 and Figure 4.4.

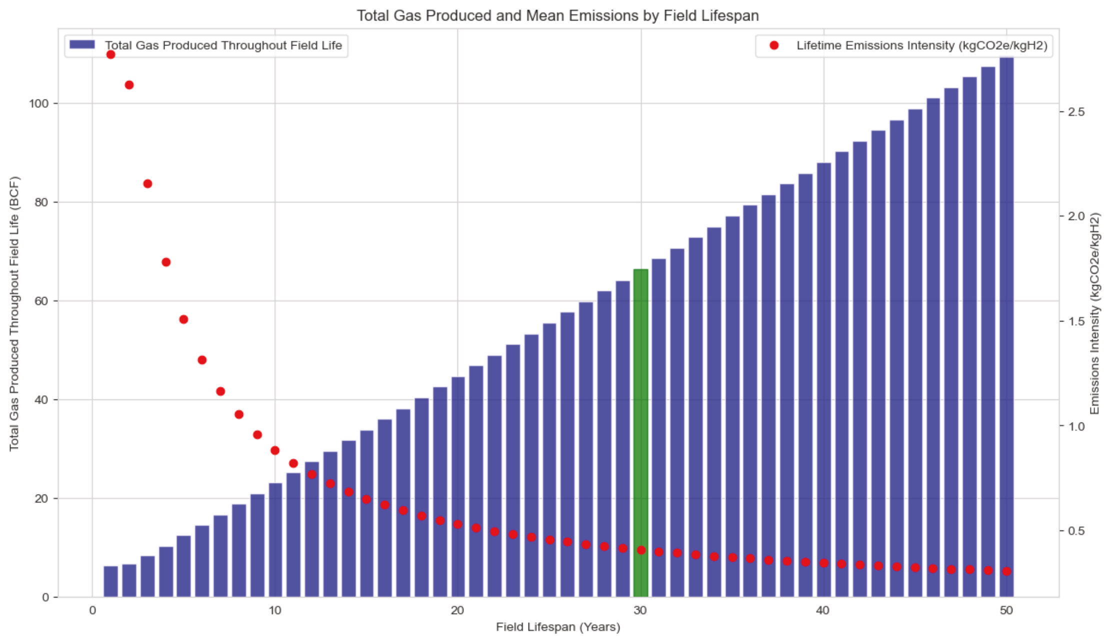


Figure 4.3: Summary of lifespan study based on exponentially decaying flow rate assumption. Note this chart is effectively showing the analysis of 50 different hypothetical field developments. It is **not** showing cumulative production of a field with a 50-year lifespan. The value for total production from the reference, exponential approximation of the 30-year Baseline case is highlighted in green.

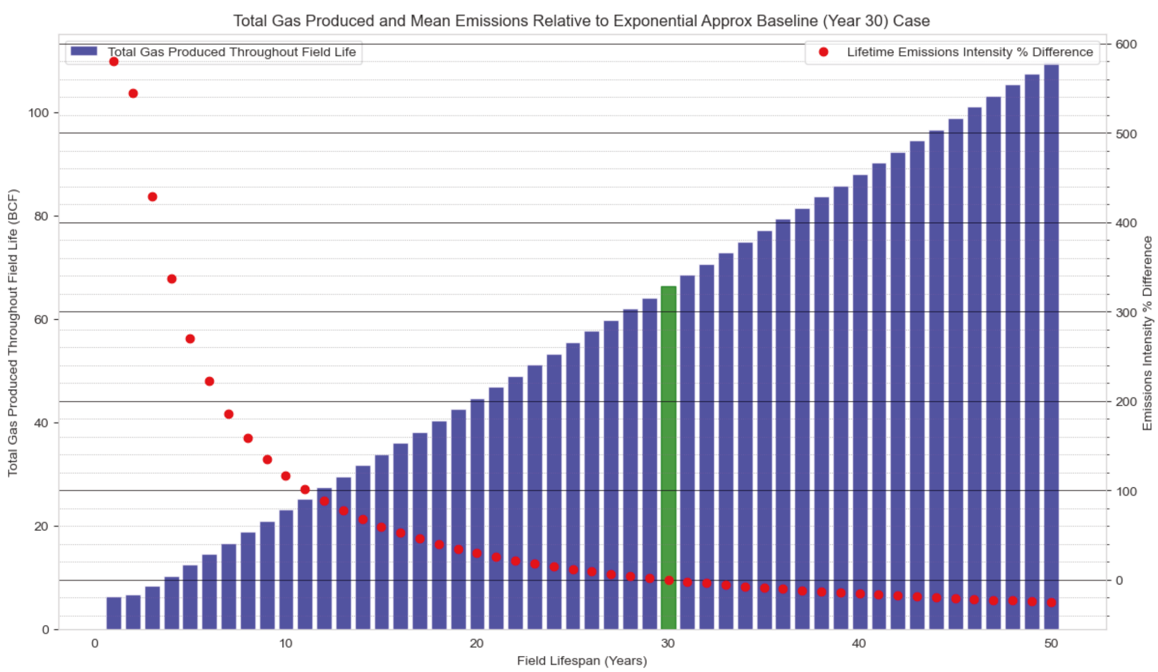


Figure 4.4: An alternative presentation of the previous plot, where emissions intensity values are reported as relative to the Baseline (30-year) case, rather than presented in absolute terms.

4.2.5. Discussion

The results of this analysis confirm a largely intuitive hypothesis. That is, from the perspective of emissions intensity, it is better to operate a large, highly productive resource than to develop what ultimately turns out to be an asset with low productivity and a short lifespan. Much of this finding is due to the 'sunk emissions' associated with embodied emissions, which are assumed to be constant across each of the 50 scenarios.

This analysis reflects the inherent risk and uncertainty associated with developing a geologic resource. The difficulty in characterising the resource means that actual performance (in this case, final emissions intensity) can only ever be truly determined in retrospect. The plot of relative differences reveals, for example, that a field with a 10-year lifespan has 100% higher emissions intensity than the baseline case. Depending on the operating environment of a prospective development, including regulatory and incentive regimes (e.g. production tax credits and/or carbon pricing), the net emissions intensity of an asset may or may not be an important factor when appraising an asset.

The desire to reduce this uncertainty should motivate proponents of geologic hydrogen developments to maximise their ability to appraise and characterise geologic hydrogen reservoirs before committing to a development. Anecdotally, the prevalence of publications focussing on subsurface aspects of geologic hydrogen (including hypothesis on formation mechanisms, exploration techniques and reservoir characterisation methods) suggests that this importance is already well understood. The study above suggests that an ability to estimate lifespan in the decadal timescale may be sufficient to make initial screening decisions.

4.3. Improvements regarding processing equipment sizing

Section 3.5.3discussed the flaws in Brandt's implementation of the OPGEE model and the effects this had on the sizing of the various units of surface gas processing equipment. This was included in Chapter 3 as a 'minor' error due to the minimal resulting impact on the lifetime emissions intensity of the hypothetical development, which was the primary finding of Brandt's study. If emissions intensity was the only metric relevant to the development of such a resource, then it may be sufficient to end the discussion at this point. It is argued here, however, that emissions intensity is only one of numerous important metrics and that the flawed approach to equipment sizing may have a more significant impact on those metrics. Specifically, equipment sizing is often highly correlated to the associated capital cost, as is discussed in detail in Section 6.3.1This perspective means that the error may be considered major rather than minor. It is revisited here in more detail to shed more light on the magnitude of the specific calculation errors, as opposed to limiting the consideration to the magnitude of the effect of the errors on emissions intensity.

4.3.1. Separator and PSA unit sizing

As described in Section 3.5.3, the OPGEE module for embodied emissions includes nominal designs for inlet separator vessels that are distinguished by design pressure and throughput flow capacity. The governing, early-field conditions of Brandt's Baseline case exceed these design conditions. Specifically, the lookup table of separator designs is limited to working pressures of no more than 1440 gauge pounds per square inch (psig), whereas the wellhead pressure in the first year is ~2470 psig.

To accommodate such a wellhead pressure, the separator would need to be custom-designed with a higher working pressure. Basic structural mechanics implies that, while assuming steel of similar strength, the higher-pressure design will require increased wall thickness, resulting in increased mass. Therefore, the following two alternative assumptions are made:

1. The gas-processing capacity of the separators is primarily associated with the vessel geometry (i.e. diameter and length). This means that where the required pressure exceeds the maximum rated pressure, based on the look-up table of designs, the most appropriate geometry from the highest-pressure-rated option will be selected based on gas processing capacity.
2. Increasing the pressure rating for a given geometry will require significantly increasing the wall thickness of the shell. In reality, there is a hyperbolic relationship between pressure and wall thickness of the form ($t = P*R/(S*E - 0.6*P)$, where t is thickness, P is pressure, R is inside radius, S is the allowable material stress, and E is a joint efficiency factor). For simplicity, it is assumed here that the weight of a vessel rated at 2500 psig is 3x that of the vessels rated at 1440 psig.

For the Baseline case, the Year 1 gas production rate is ~23 MMSCF/day. Therefore, of the standard designs referenced in the OPGEE model, the 1440 psig-rated, 36" Outside Diameter x 10' length geometry/design seems the most appropriate. It will further be assumed that this design is appropriate for all cases under examination here.

Because Brandt estimates the mass of the PSA unit as a simple five-fold multiple of the separation unit mass, this correction significantly affects the total mass of steel associated with these two units. More precisely, the separator unit mass, PSA unit mass and total mass of the combination of the two units increases by 1,264%. As described in Section 6.3.1the cost of pressure vessels is correlated with their mass, so it can be inferred that this change in sizing approach will cause a change in the assumed cost of the equipment by multiple orders of magnitude.

Table 4-2: Summary of the impact of increasing conservatism in separator design on total steel mass.

	Separator Unit Mass (lb)	PSA Unit Mass (lb)	Total Mass (lb)
Brandt values	2,538	12,690	15,228
Revised values	34,627.5	173,137.5	173,137.5
Difference	32,089.5	160,447.5	192,537

4.3.2.Gas sweetening absorber sizing

As also described previously, there were two issues with Brandt's approach to accounting for the mass of acid-gas removal or 'gas sweetening' equipment. First, the use of the maximum expected gas flow rate resulted in an approximately 300% increase (from ~27,000 lb to ~80,000 lb) when using the maximum flow rate from the Baseline case, rather than the minimum gas flow rate (as was assumed for the Year 30 'sizing' of the equipment).

Ultimately, however, the model does not 'see' any increase in calculated total steel mass due to this sizing calculation because the model implementation deliberately excludes a gas-sweetening unit from the process design. Accordingly, correcting this error removes 100% of the steel mass associated with gas-sweetening equipment, so the manner and magnitude of the sizing errors are ultimately irrelevant.

4.3.3.Dehydration contactor and equipment sizing

As described in Section 3.5.3, the mass calculations for the sizing of the gas dehydration contactor vessel involved issues two primary issues. The flow rate sizing basis was flawed, and the volume equations included typographical errors. Replication of the Brandt model's Baseline case reveals that the calculations assumed the following values for mass of the dehydration contactor unit:

- Year 1 (i.e. maximum flow) mass: 5,976 lb

- Year 30 (i.e. minimum flow) mass: 851 lb

Correcting to use only the conservative (maximum) flow rate and correcting the volume equations yields a total mass of ~27,500 lb in the revised model. This is an increase of 460% over Brandt's Year 1 result and 3,233 % over the Year 30 result.

4.3.4. Reinjection compressor sizing

The correction of reinjection compressor sizing discussed previously had an almost negligible impact on emissions intensity. The magnitude of the relative effect on steel mass is larger than the effect on emissions intensity, but is also very small. In this case, rather than 'averaging out' Brandt's Year 1 value of 12,740 lb and the Year 30 value of 12,720 lb, the corrected algorithm simply selects the Year 1 value. Therefore, the difference is less than 20 pounds of steel, or less than 0.2%.

4.3.5. Discussion

In aggregate, these calculations show that correcting the equipment sizing logic makes a large difference to the total mass of steel associated with the surface processing equipment. It may not be intuitive that such large differences in steel mass calculations for this equipment can manifest in such small differences in emissions intensity. This apparent incongruence can be explained via reference to Figure 4.5. Here, we note that the mass of steel in the construction of the wells is at least one order of magnitude larger than any other equipment category in the Baseline case.

However, it is important to note that the Baseline case assumes the development involves 63 total wells (50x production wells and 13x injection wells). The proportion of steel associated with equipment versus that associated with wells is clearly linked with this assumption. If the number of wells reduces significantly, the proportion of steel from equipment becomes relatively more significant.

The importance of correcting the equipment sizing logic will become particularly important during the discussion of cost, in Chapter 6. For example, Figure 4.5 shows that the cost estimate for the Baseline case is dominated by the cost of wells, however, the surface equipment cost (based on the corrected sizing logic) is a sizable 15% of total cost. This would have been significantly lower without the corrections to the sizing logic.

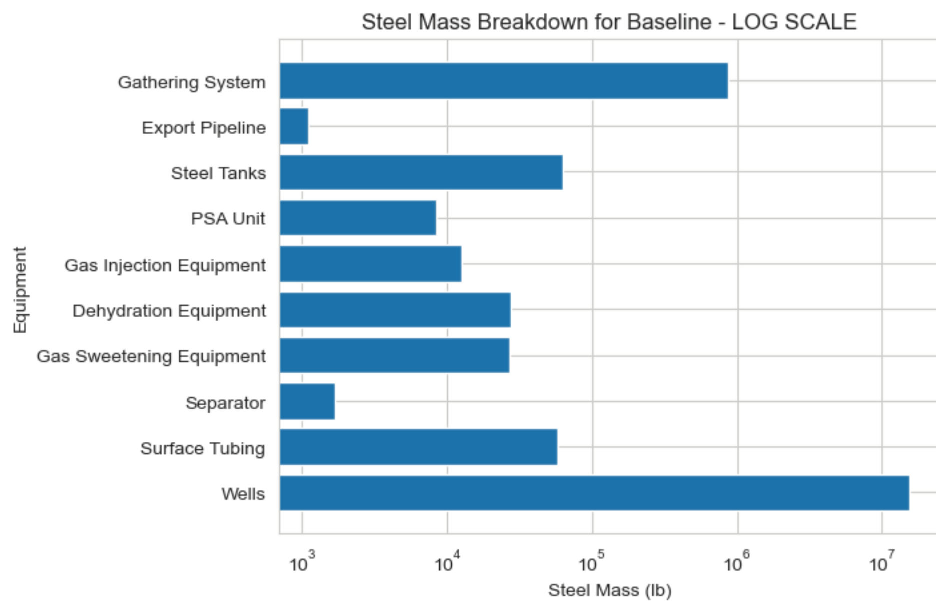


Figure 4.5: Visualisation of the mass of steel calculated with each equipment type. Note the log scale, indicating that the steel associated with wells is the most significant contributor, by at least an order of magnitude over the second largest contributor.

4.4. Summary

This chapter extended Brandt's work by considering the interplay between field lifespan and productivity. It also considered the impacts beyond lifetime emissions intensity of improving the logic used to size surface processing equipment. The embodied emissions of this equipment was dwarfed by that of the wells, and hence these adjustments had only a small impact on the LCA. However, the analysis makes it clear that both of these considerations are critical when assessing the economic viability of a potential geologic hydrogen development. Building on this foundation, economic viability will be examined in more detail in Chapter 6.

Chapter 5: Extension of state-of-the-art LCA to include analysis of uncertainty

The critiques, improvements, and extensions to Brandt's prospective LCA of geologic hydrogen discussed in Chapter 4 are informative but do not address a major omission: assessment of the impact of uncertainty. This chapter addresses this omission by incorporating Monte Carlo simulations to study the sensitivity of final lifetime emissions intensity results to uncertain inputs.

5.1. Introduction and method

As mentioned in Section 3.4.1Brandt simultaneously acknowledges high levels of uncertainty regarding geologic hydrogen developments and argues that the level of uncertainty is too high to include in the analysis. This section challenges that argument by implementing the Monte Carlo method of uncertainty analysis to investigate the sensitivity of key results to uncertain inputs.

In the Jupyter notebook used to implement this model, each calculation that is required to determine emissions intensity has been implemented within Python functions. Each of these Python functions can (optionally) take as input a dictionary of 'sensitivity variables'. The sensitivity variables are those to be included in a given Monte Carlo simulation run. Each entry within the sensitivity variable dictionary is an array of values, with the count of values in each array reflecting the number of simulations to be included in the run.

5.2. Variables included in Monte Carlo simulation

When establishing a framework for a Monte Carlo simulation, it is critical to select suitable variables to include in the analysis. The variables selected as part of this study are described and justified below.

5.2.1. Correction factor for empirically determined venting and fugitive emissions rates

A fundamental assumption of the OPGEE model is that fugitive emissions rates from oil and gas facilities are most accurately modelled using statistics derived from observation of leakage rates from operating facilities. Brandt then further assumes that these empirically derived leakage rates also describe the leakage rates from the hypothetical geologic hydrogen development. Without equivalent empirical observations, it is difficult to evaluate the reliability of this assumption. Accordingly, the revised model has incorporated a 'correction factor' to be used in the algorithm that determines component and site-level leakage rates as a function of the flow rate of fluids through the process. The default assumption is that this factor is equal to 1. That is, the factors are calculated exactly as they would be in the OPGEE model. This correction factor is used exclusively to test the sensitivity of the results to the assume fugitive emissions rates.

5.2.2. Global warming potential of molecular hydrogen (GWP H_2, dimensionless)

Figure 3.1 and Figure 3.2 show that "Direct" emissions are approximately as significant as embodied emissions when determining a geologic hydrogen development's emissions intensity. Direct emissions can otherwise be described as 'venting, fugitive and flaring' (VFF) emissions, where venting is the deliberate release of fluids to the environment, fugitive emissions are those fluids that inadvertently escape the process into the equipment, and flaring is the deliberate destruction via combustion of part of the process stream. For each of these sub-categories of emissions, their GHG effect implications can be normalised to 'equivalent tonnes of carbon dioxide emissions' via their Global Warming Potential (GWP). As described in Chapter 1, existing studies on the GWP of molecular hydrogen have not converged on an agreed value.

5.2.3. Reservoir oil production rate (barrels of oil per day, bbl/day)

The assumed rate of oil production from the geologic hydrogen reservoir was included in the sensitivity study for two reasons:

- First, this is one of the key assumptions made via Brandt's aggregation of natural gas well data. As discussed previously, there is little scientific reasoning to suggest that geologic hydrogen resources will mimic natural gas resources, so it is informative to assess the sensitivity of the analysis to these assumptions.
- Second, the calculation structure of the OPGEE model appeared on initial inspection to make the oil production rate central to assumptions regarding gas flow rate. It seemed possible that the analysis would be highly sensitive to this assumption. However, closer inspection revealed this not to be the case, with the impact of the assumed oil production rate being 'cancelled out' in successive

calculations.

Including this variable in the sensitivity study helped to highlight that the OPGEE model structure means that the rate of oil production is only relevant to the calculation of emissions intensity when it assigns a proportional attribution of embodied emissions of the United States crude oil pipeline network to this incremental production. The effect of this attribution is tiny, even if the oil production rate is assumed to be multiple orders of magnitude larger.

Pragmatically, the more significant impact of high oil production rates on emissions is likely to be on the requirement for more and/or more sophisticated equipment in the processing plant near the wellhead. This would increase the embodied emissions and potentially the fugitive emissions of this plant. In its current state, the model is built assuming the geologic hydrogen resource is a gas resource that requires only minimal liquids handling. It is not sophisticated enough to automatically determine the liquid production rate that would drive a significant change in process design (i.e. mist or liquid-dominated multiphase flow regimes).

5.2.4. Reservoir water production rate (barrels of water per million standard cubic feet of gas, bbl/MMSCF)

Similarly to the oil production rate, the water production rate is another variable that relies on the assumption that natural gas reservoir characteristics are appropriate analogues for geologic hydrogen reservoirs. Accordingly, this variable was included in the uncertainty analysis to evaluate the significance of the assumption.

5.2.5. “Small Source” emissions rate (percent, %)

Brandt’s implementation of the OPGEE model accounts for miscellaneous, "small sources" of emissions (e.g. light vehicles driven around the field location, land clearing and site preparation, embodied energy in labour) as 10% of "direct sources" (Brandt, 2023; Brandt et al., n.d.). That is, emissions from combustion, land use, venting, flaring and fugitives throughout all stages of development (exploration, drilling and development, production & extraction, and surface processing), all of which are calculated elsewhere in the model. The assumption of 10% is not justified, so it is logical to include this in a sensitivity analysis, with the goal of determining if or how significant this assumption is on the conclusions drawn from the model.

5.2.6. Reservoir pressure decline/retention rate (percent, %)

Brandt's supplemental information and model file indicate an assumption that the reservoir pressure declines at a rate of 5% per year of operation. Unlike the other reservoir characteristics estimated via the use of natural gas well analogues, the assumption regarding the rate of pressure decline is not discussed nor justified in any way. This lack of justification makes it a prime candidate for a study of uncertainty and sensitivity.

5.2.7. PSA unit 'slippage' rate (percent, %)

Brandt assumes that the pressure swing adsorption (PSA) unit achieves perfect separation of hydrogen from other gas species, but it does so at the expense of a proportion of hydrogen content entering the waste stream rather than the export stream. This proportion is known as the 'slippage' rate. Brandt acknowledges in the supplemental information that there is little published data regarding PSA hydrogen slippage rates for gas compositions similar to those assumed in the geologic hydrogen model, so 10% is selected as it falls within the 5% to 20% range reported in the literature (Brandt, 2023). This observation makes the assumption of PSA slippage rate an obvious candidate for inclusion in uncertainty and sensitivity analyses.

5.2.8. Number of production wells drilled during development

Brandt's model assumes (for all cases) that the development involves the drilling and completion of 50 identical production wells, plus an allowance for gas reinjection/disposal wells of 25% of the number of production wells (i.e. 13 injection wells, for 63 total wells). Injection wells are assumed, for simplicity, to be identical to production wells. The well-count assumption is not discussed nor justified in any way. In speculating why this assumption was not justified, it is noted that the key well-productivity assumption (1.33 BCF per well) scales with well count. Given that the study is primarily interested in emissions intensity (i.e. quantity of emissions per quantity of product), perhaps Brandt assumed that emissions would scale directly with well-count, meaning that emissions intensity is insensitive to the well-count assumption. While it is reasonable, this work has tested this assumption by including well-count within the uncertainty analysis.

5.3. Assignment of probability density functions to selected variables

Brandt's observation that the nascency of the geologic hydrogen industry renders it difficult to assign probability functions to key uncertain variables is fair. Accordingly, a straightforward approach has generally been adopted for this first-pass attempt at addressing this challenge. This approach assumes that uncertain variables can be described with a uniform probability density function centred on the default assumption from the Baseline case and extends out to ± 50% of the default assumption value. The exceptions to this general approach are:

- **GWP of hydrogen:** Rather than assessing the scientific validity of each of the two estimates for GWP H_2 mentioned by Brandt (i.e. 5.0 and 10.9), the approach taken is to consider them equally valid end bounds to a uniform probability distribution. To allow for further uncertainty of these reported figures, the end bounds are then extended by a further 50% of the lower estimate (i.e. 50% of 5 = 2.5).
- **PSA slippage rate:** As summarised in Brandt's supplemental data, the available literature indicates slippage rates ranging from 5 to 20%, so these have been taken as the bounds of a uniform distribution.

The specific ranges and probability density function (PDF) types used in the uncertainty analysis are detailed in Table 5-1.

Table 5-1: Details of the probability density functions applied to uncertain variables in the Monte Carlo simulations

Variable	PDF Type	Units	PDF Characteristics	Basis
Fugitive emission rate correction factor	Uniform	Dimensionless	Lower Bound: 0.5 Upper Bound: 1.5	+/- 50% of default value
GWP of hydrogen	Uniform	Dimensionless	Lower Bound: 2.5 Upper Bound: 13.4	Range from literature, plus margin
Oil production rate	Uniform	Barrels of oil per day (bbl/day)	Lower Bound: 0.05 Upper Bound: 0.15	+/- 50% of default value
Water production rate	Uniform	Barrels per thousand of standard cubic feet of gas (bbl/mscf)	Lower Bound: 0.5 Upper Bound: 1.5	+/- 50% of default value
"Small source" emissions factor	Uniform	Dimensionless	Lower Bound: 5% Upper Bound: 15%	+/- 50% of default value
Reservoir pressure decline rate	Uniform	Dimensionless	Lower Bound: 2.5% Upper Bound: 7.5%	+/- 50% of default value
PSA unit slippage rate	Uniform	Dimensionless	Lower Bound: 5% Upper Bound: 20%	Range from literature
Number of production wells	Uniform	Integer	Lower Bound: 25 Upper Bound: 75	+/- 50% of default value

5.4. Number of iterations in the simulation

Monte Carlo analyses are, by their nature, computationally expensive. This study did not include a detailed examination of convergence. Rather, it selected a maximum number of iterations that could be run in a reasonable timeframe using available computation power. The results presented below are from a simulation of 1,500 iterations.

5.5. Results

The results of the Monte Carlo analysis are discussed here:

5.5.1. Aggregated response results

The data generated by the simulation is first examined via archetypal visualisations for Monte Carlo analyses. The histogram in Figure 5.1 shows that the results appear approximately normally distributed (i.e. follow a typical 'bell curve' shape). The central limit theorem suggests this should be the case, providing confidence that the model and analysis approach produce valid results.

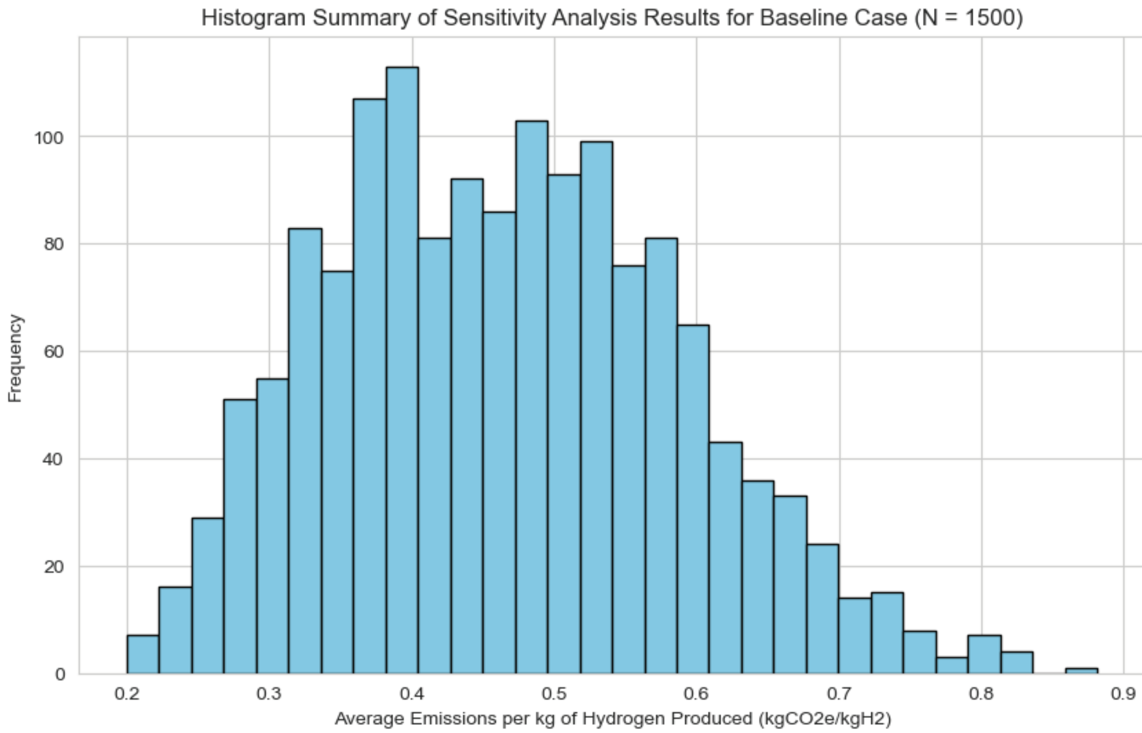


Figure 5.1: Histogram summarising the results of a 1,500 iteration Monte Carlo analysis of the Baseline case, targeting lifetime emissions intensity as the target variable.

This same data is presented in Figure 5.2 to show the classic 'S-curve' shape in the cumulative distribution function (CDF). This figure shows that the median value for lifetime emissions intensity in the Baseline case calculated by the simulation is 0.46 $kgCO_2e/kgH_2$. Further, this plot can be interpreted to indicate that there is a 90% probability that the lifetime emissions intensity of the Baseline case falls within the range of 0.28 to 0.68 $kgCO_2e/kgH_2$. Recalling that these values include embodied emissions and that embodied emissions form the clear majority of emissions in the Baseline case (Figure 3.1 provides an indication of the relative proportion of embodied vs non-embodied emissions), this analysis indicates that geologic hydrogen is highly promising from the perspective of emissions intensity.

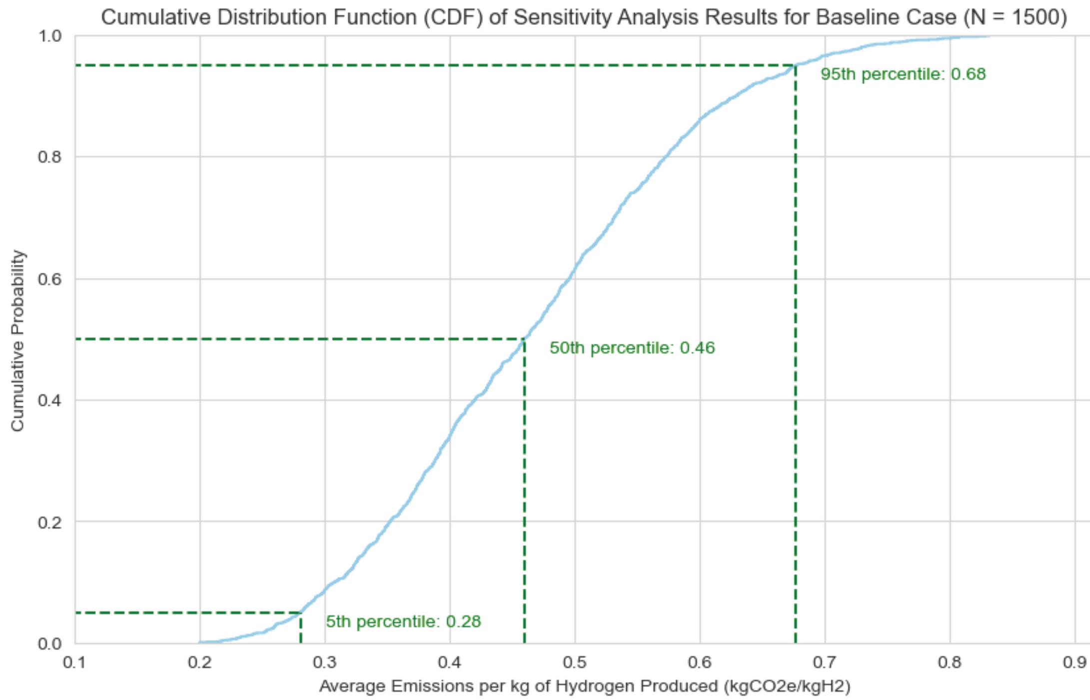


Figure 5.2: CDF plot of the 1,500 iteration Monte Carlo sensitivity analysis results for the Baseline case. This shows that the 90% confidence interval for lifetime emissions intensity is 0.28 to 0.68 $kgCO_2e/kgH_2$ (where the confidence interval is defined according to the 'percentile bootstrap' method).

5.5.2. Individual variable response results, assuming independence

In addition to providing cumulative, aggregated results, Monte Carlo analysis also allows examination of the relative influence of each of the uncertain variables included in the analysis. A simplistic, first-pass method of such an examination can be achieved by first assuming that each of the uncertain variables is completely independent of one another and has independent effects on the target variable (emissions intensity, in this case). Then, the sensitivity analysis can be run while varying only a single uncertain variable at a time, and the magnitude and direction of the results from these separate analyses can be compared to infer the variables to which the result is most sensitive. The results of such an analysis are presented in the so-called 'tornado chart' of Figure 5.3. This analysis technique suggests that the productivity of each well is the most significant variable, followed by the GWP of hydrogen, the emissions factor correction coefficient (i.e. the extent to which fugitive emissions rates from natural gas facilities are applicable to hydrogen facilities), and the separation efficiency of the PSA unit.

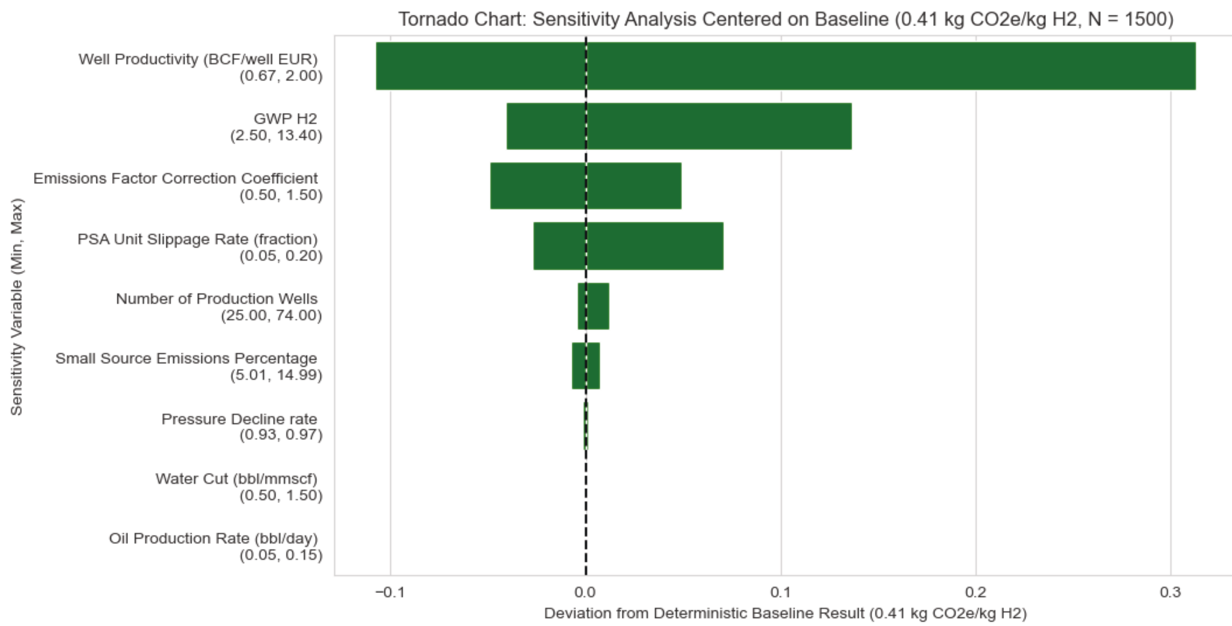


Figure 5.3: Tornado chart showing the range of effect of each sensitivity variable on lifetime emissions intensity. Note that this analysis assumes complete independence between variables.

An alternative presentation of this same data is in the so-called 'spider diagram' shown in Figure 5.4. This diagram shows the emissions intensity response to variation of each variable included in the analysis. Note that the sensitivity variables have differing units of measure, so the horizontal axis of this diagram normalises these units to a measure of 'percentage change'. Recall also that this analysis depends on the assumption of complete independence of the sensitivity variables.

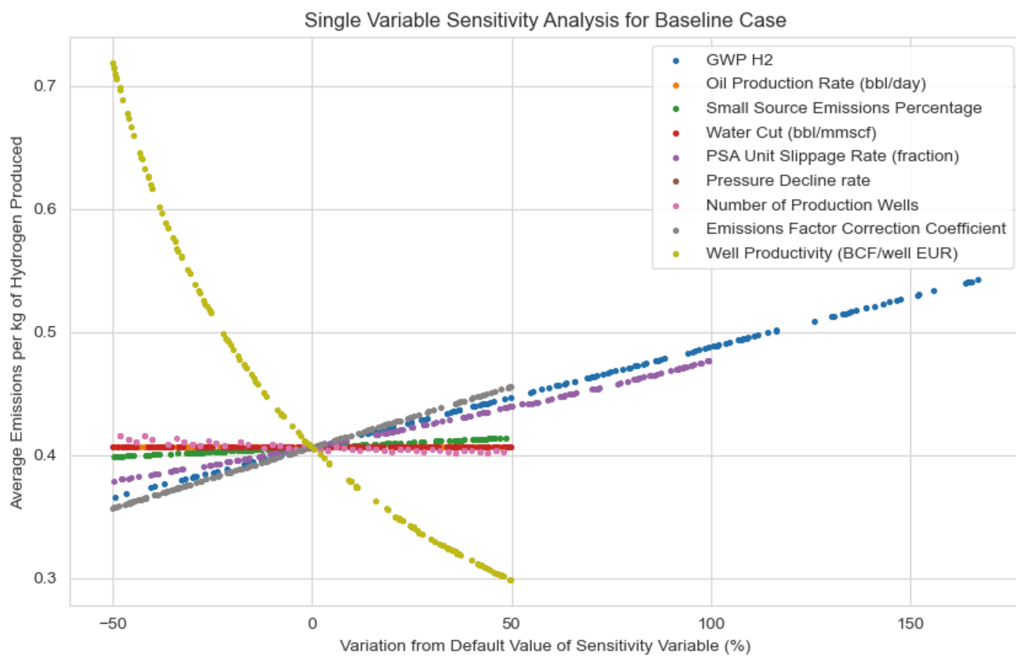


Figure 5.4: 'Spider Diagram' showing the independent effect of each sensitivity variable on lifetime emissions intensity

The assumption of the independence of the sensitivity variables is significant and warrants examination. One approach to assist with this examination is to present so-called 'sensitivity analysis graphs', which present the single-variable response data of a single variable (represented by one bar of the tornado chart or one series of points in the spider diagram) on a separate chart, without normalising the values of the sensitivity variable shown on the horizontal axis. On this same chart can then be plotted the series of points that represent the emissions intensity response of all variables, including the subject variable of a given chart. An example chart is shown in Figure 5.5 and the complete set of charts, one for each of the sensitivity variables, is included in Appendix B. Figure 5.5 indicates that the single-variable response to GWP of H_2 aligns with the trend of the all-variable response. This qualitatively suggests that the GWP of H_2 explains some but not all of the stochastic variation.

The charts in Appendix B show that this result holds generally true for many of the sensitivity variables. Two important exceptions to this observation are the charts that examine the influence of the number of production wells assumed in the development and the total gas productivity per well. These charts are shown in Figure 5.5 and Figure 5.6.

In Figure 5.5, the single-variable study suggests that the number of production wells has only a small impact on emissions intensity. This is intuitive because, when all else is held equal, adding an additional well will result in an incremental amount of hydrogen product as well as an incremental amount of embodied and fugitive emissions. As the well count grows and the surface processing facilities reach their maximum limits (as artificially restricted by the OPGEE model algorithms), it is logical that the lifetime emissions intensity value is not significantly affected. Despite the logic of this intuition, however, inspection of the multi-variable response suggests that there is a significant correlation between the number of production wells and emissions intensity.

The chart for per-well productivity stands in counterpoint to the chart for the number of production wells. In this chart, the single-variable analysis suggests that the value of per-well productivity is highly influential to emissions intensity. Inspection of the multi-variable response, however, does not indicate any obvious association between these two variables. The incoherence of these charts suggests that the original, fundamental assumption of the independence of the input variables may be flawed. This then dictates that an alternative approach is necessary.

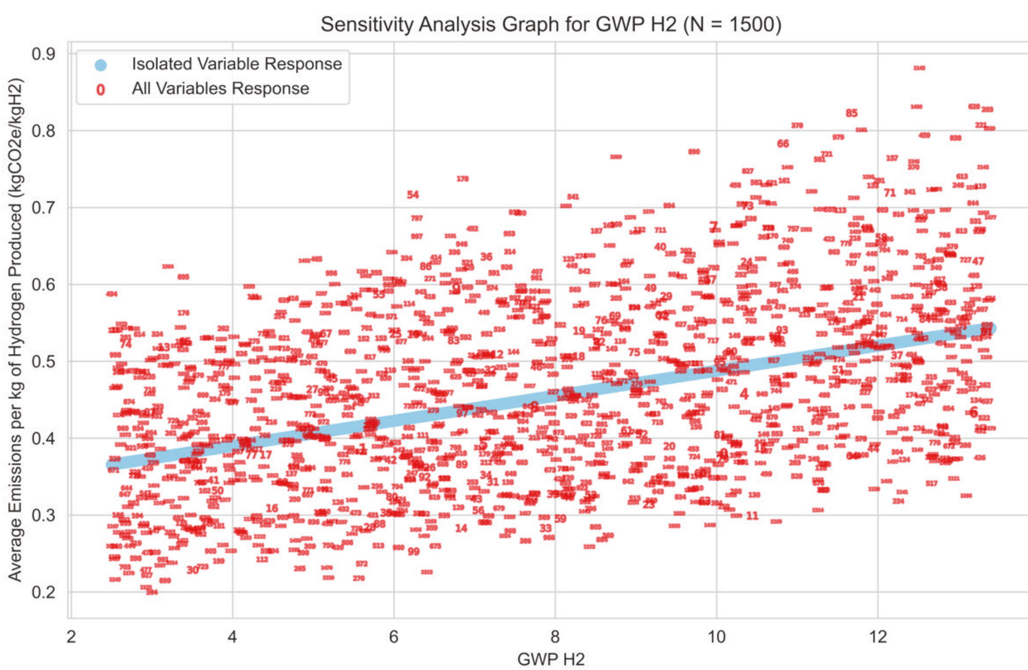


Figure 5.5: Sensitivity Analysis Graph comparing the effect of varying only the GWP of hydrogen against the effects of simultaneously varying all variables.

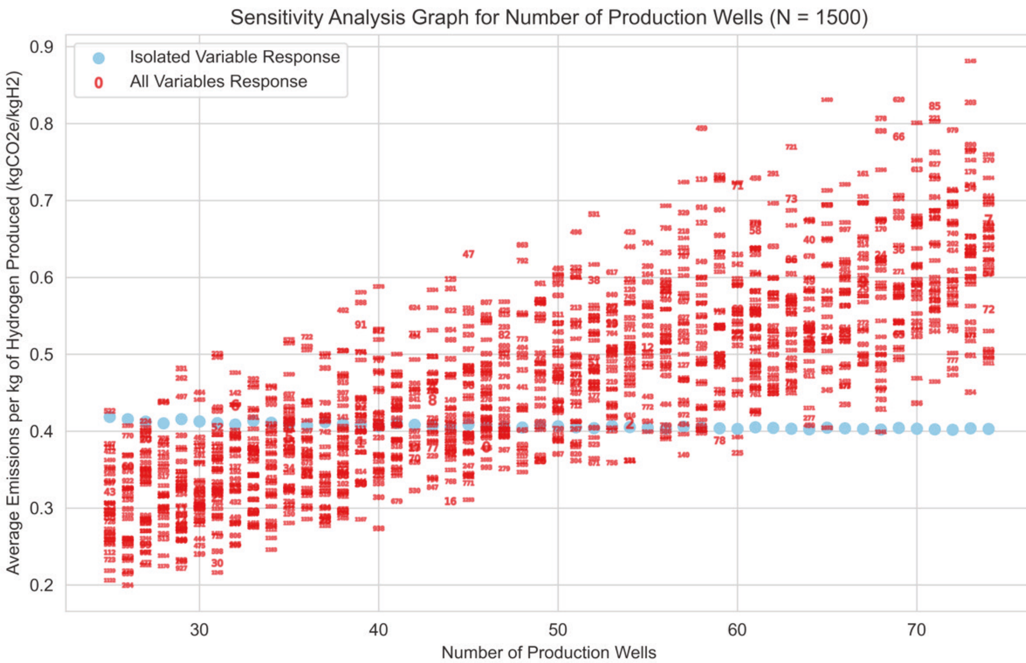


Figure 5.6: Sensitivity Analysis Graph showing the incoherence between the trend of results when varying all variables and the trend when varying only the number of wells.

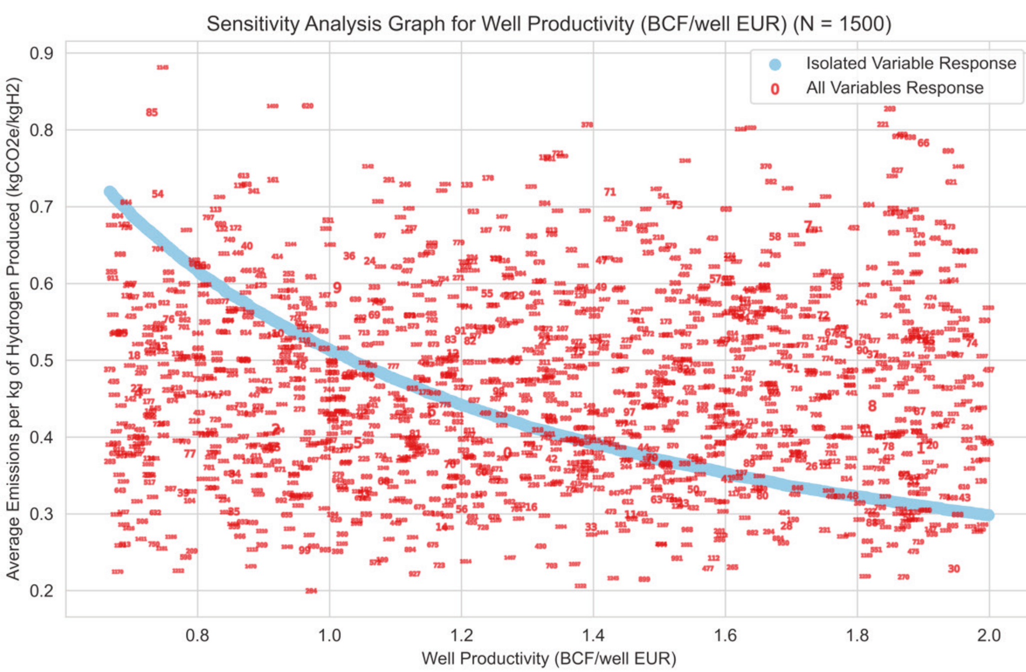


Figure 5.7: Sensitivity Analysis Graph for per-well productivity, showing a similar lack of coherence as the chart for number of production wells.

5.5.3. Multi-variable sensitivity analysis

Rather than assuming the variables are independent, statistical methods can be used to analyse the multi-variable response results and provide an indication of the relative significance of each sensitivity variable. Three different methods are applied in this analysis. First, a Pearson correlation matrix is calculated to determine the strength of the correlation between each of the sensitivity variables and the target variable, emissions intensity. Given that all of the sensitivity variables are generated randomly from uniform probability density functions, there is no multicollinearity present in these variables. There is, however, a notable correlation observed between several of the sensitivity variables and emissions intensity. These results are summarised in Figure 3.1. The results for “Number of Production Wells” and “GWP H2” confirm mathematically what was observed via inspection of Figure 5.6 and Figure 5.5: There is a notable positive correlation associated with each of these two variables. Inspection of the sensitivity analysis graphs for “PSA Unit Slippage Rate” and “Small Source Emissions Percentage” (see Appendix B) also confirms the positive but relatively weaker positive correlation for these two variables. Indication of correlation is important, however it only describes the quality of the ‘fit’ of the observed variables to a monotonically increasing (or decreasing) line. It does not tell us anything about the slope of this line. Put another way, confirmation of correlation does not indicate how much a unit change in the sensitivity variable will cause in terms of emissions intensity.

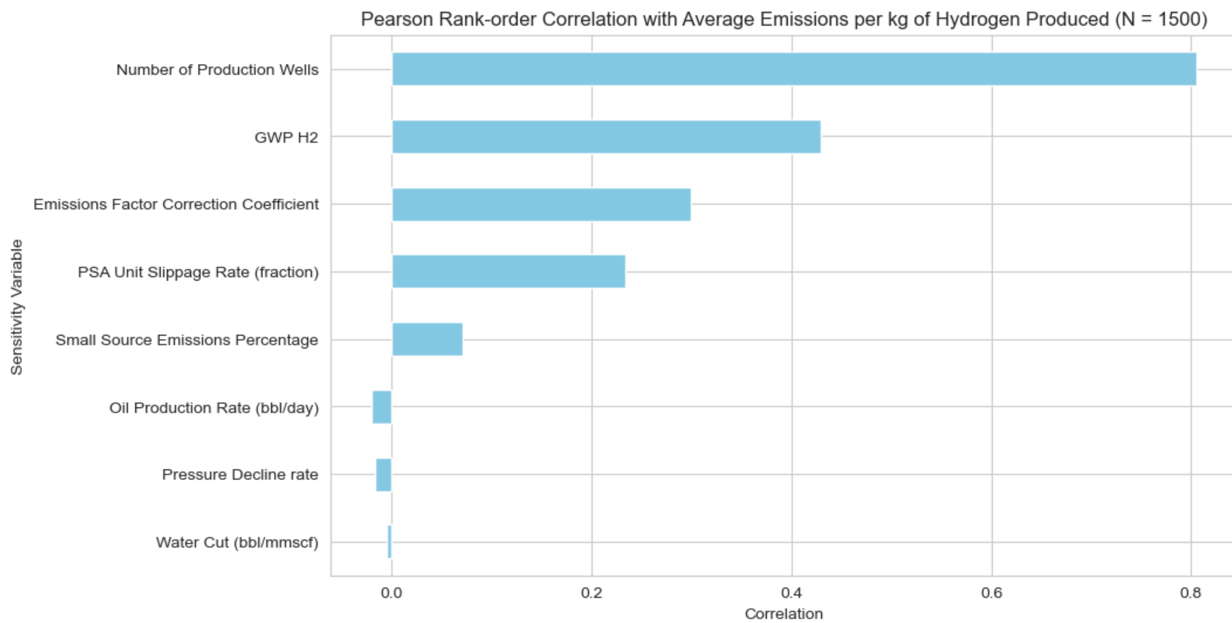


Figure 5.8: Rank-order correlation results from the 1,500 iteration simulation

Fortunately, regression techniques can be used to provide this indication of sensitivity. This study implements two different techniques to do so. The first technique is a 'rank-order regression' analysis. This analysis runs a separate linear regression for each of the sensitivity variables, with emissions intensity as the target variable. The 'R-squared' values of these linear regressions are then used to gain a sense of the proportion of variation within the multi-variable response that can be explained by each of the sensitivity variables. As shown in Figure 5.9, "Number of Production Wells" has the highest R-squared value, equal to 0.65. Simplistically, this implies that the number of production wells explains 65% of the variation in the multi-variable response data. Similarly, the GWP of hydrogen explains approximately 18%, the emissions factor correction coefficient explains approximately 9%, and the PSA unit slippage rate explains approximately 5% of the variation. This provides an indication of the relative importance of each of these variables when seeking to analyse and improve the results produced by the LCA model.

Finally, a multi-variable linear regression is performed to gain a further improved sense of the relative sensitivity of emissions intensity to each of the sensitivity variables. This analysis first involves standardising each of the input variable datasets such that they all have a mean of zero and a standard deviation of one. After doing so, a multi-variable linear regression is run to calculate coefficients for each of the sensitivity variables. These coefficients can then be used to directly compare the sensitivity of the target variable to a change in each of the sensitivity variables. To help visualise the results, the coefficients for each variable are plotted in the bar chart in Figure 5.10. Here, we can see that "Number of Production Wells" has the largest magnitude coefficient, equal to 0.099. This implies that an increase in one standard deviation in production well count (approximately 15 wells) results in an increase in emissions intensity of 0.099 $kgCO_2e/kgH_2$. Similarly, a single standard deviation increase in the GWP of hydrogen (~3.2) causes emissions intensity to increase by 0.054 $kgCO_2e/kgH_2$. Importantly, there is close alignment of the 'rank order' (i.e. from most significant to least significant) of variable sensitivities suggested by both of these analyses and displayed in Figure 5.9 and Figure 5.10.

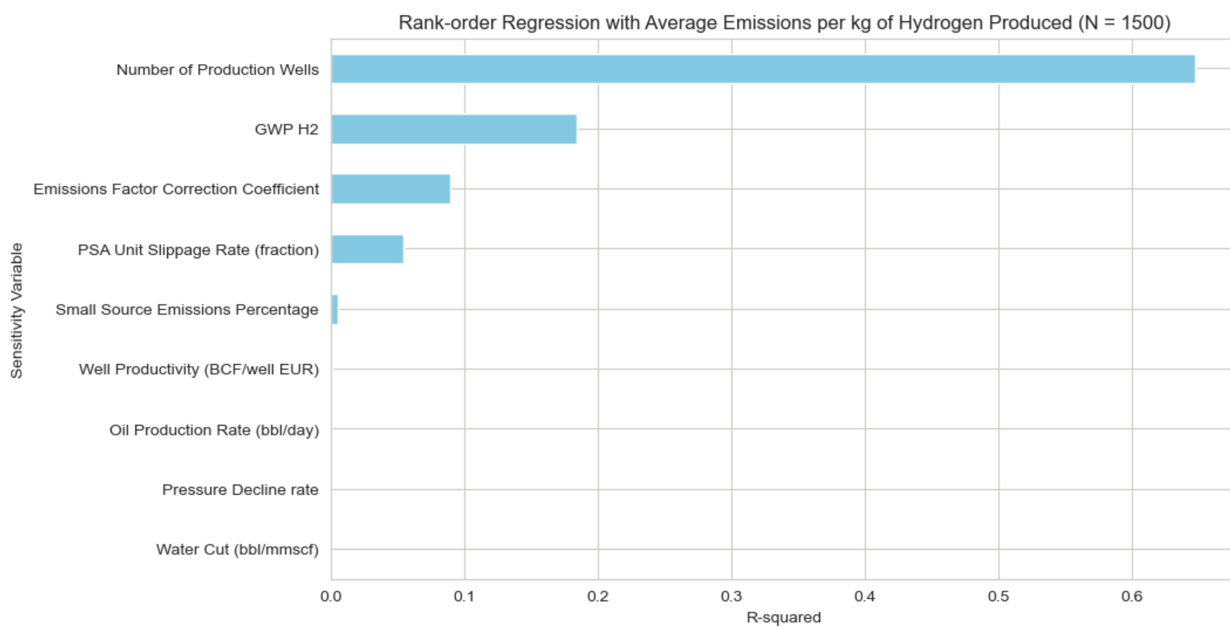


Figure 5.9: Chart showing the relative magnitude of the R-squared value associated with a single variable regression fit with each sensitivity variable with emissions intensity as the target value.

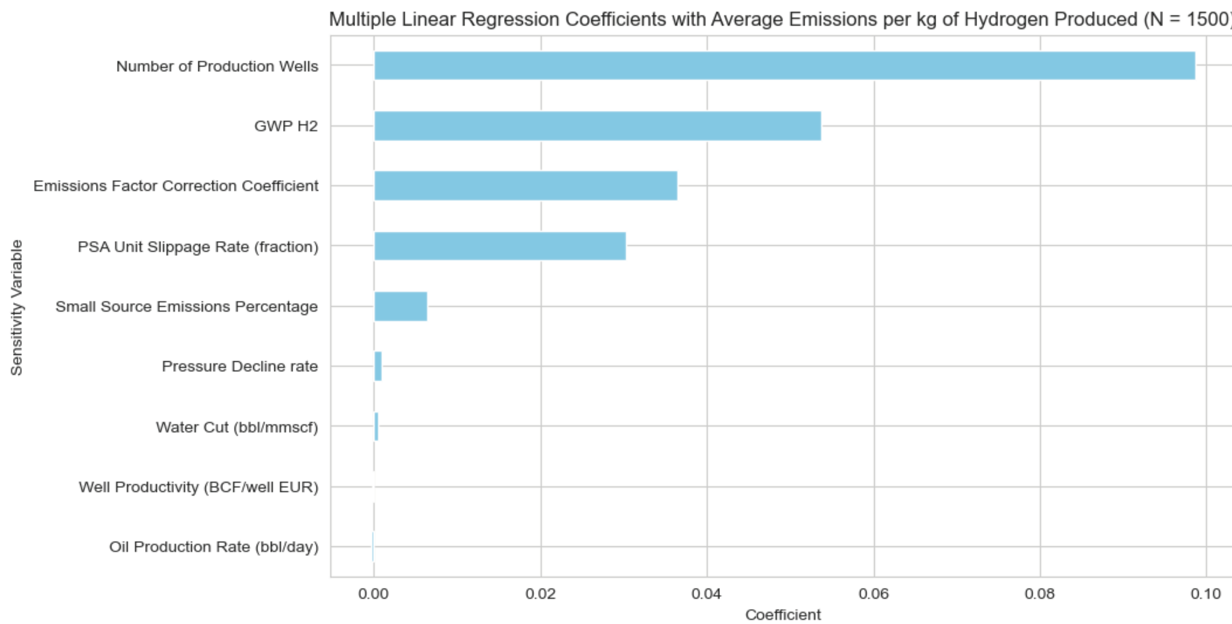


Figure 5.10: Chart showing the relative magnitude of the coefficients from a multi-variable linear regression with the sensitivity variables set as inputs and emissions intensity set as the target variable. Note: To enable direct comparison of the magnitude of each coefficient, input data was standardised to have a mean of zero and a standard deviation of one.

5.5.4. Sensitivity analysis excluding the effect of embodied emissions

The analyses described above all include embodied emissions in the calculation of lifetime emissions intensity to align with LCA best practices. However, as will be discussed in more detail in Section 6.5. some investment incentive regimes such as the United States 45V production tax credit regime, do not require embodied emissions to be included in emissions intensity calculations. In these situations, it may be interesting to consider the relative importance of the sensitivity variables to the value of emissions intensity excluding embodied emissions. This can be achieved via the same means as described previously, but simply amending the target variable accordingly. The results of this revised analysis are shown in Figure 5.11 through Figure 5.14.

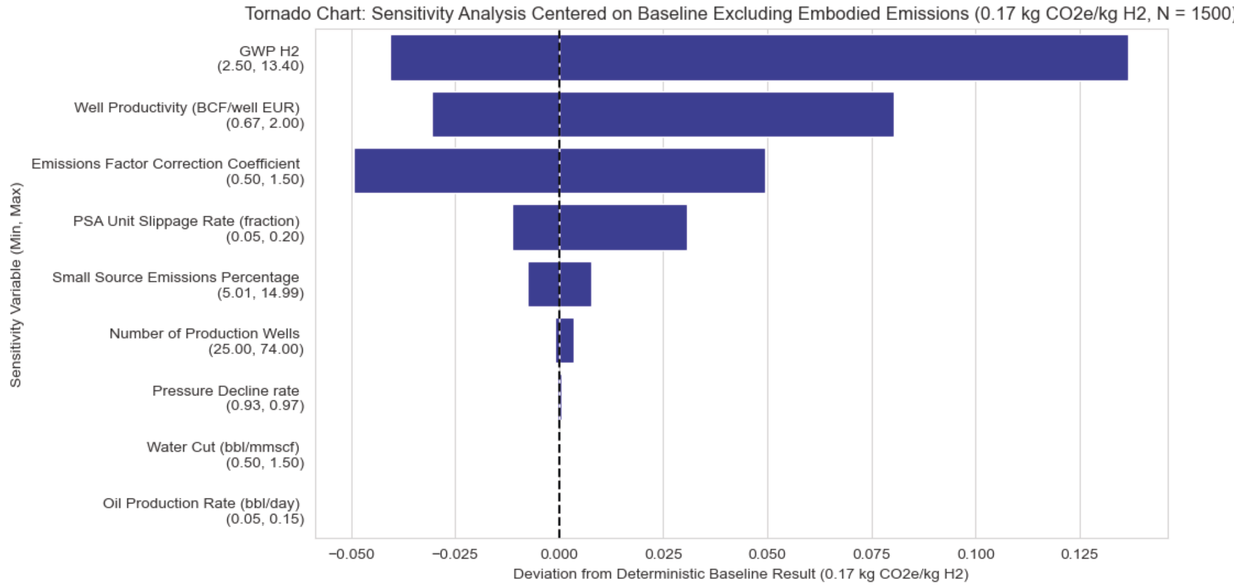


Figure 5.11: Tornado chart indicating the significance of each sensitivity variable in the case that embodied emissions are excluded from calculation of emissions intensity.

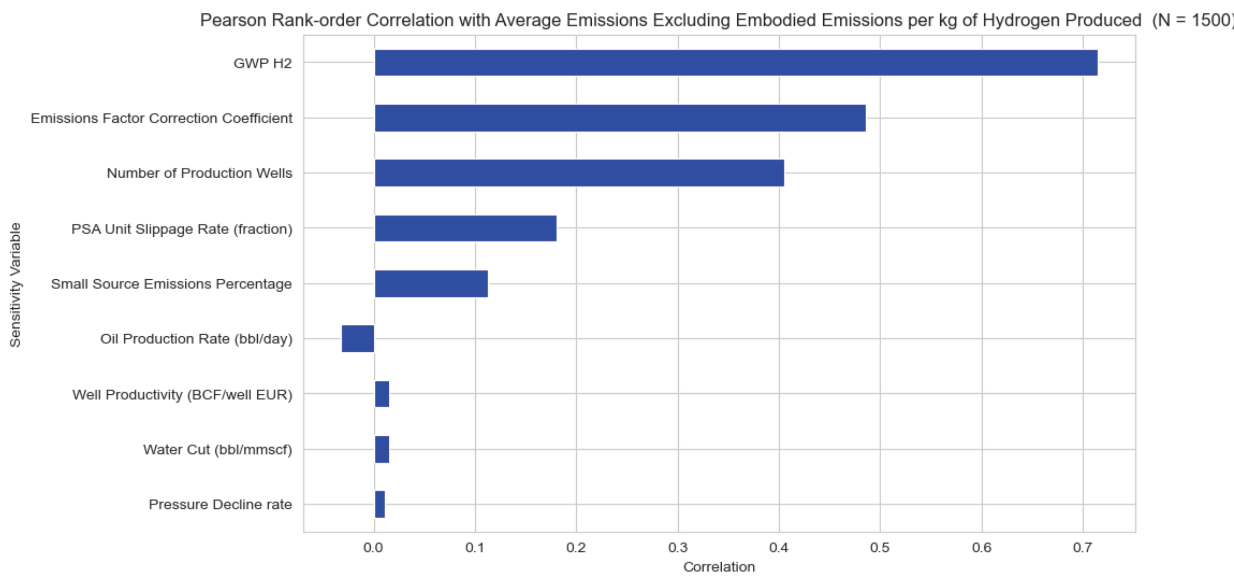


Figure 5.12: Chart of Pearson Rank-order Correlation with target variable of lifetime emissions intensity excluding embodied emissions.

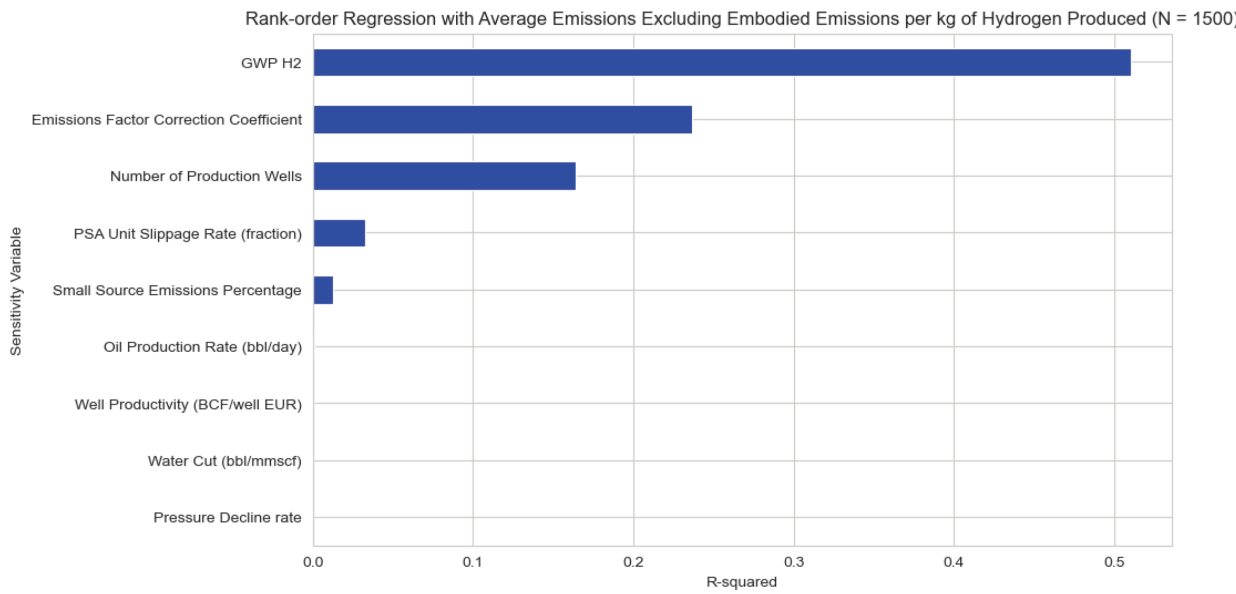


Figure 5.13: Chart of Rank-order Regression with target variable of lifetime emissions intensity excluding embodied emissions.

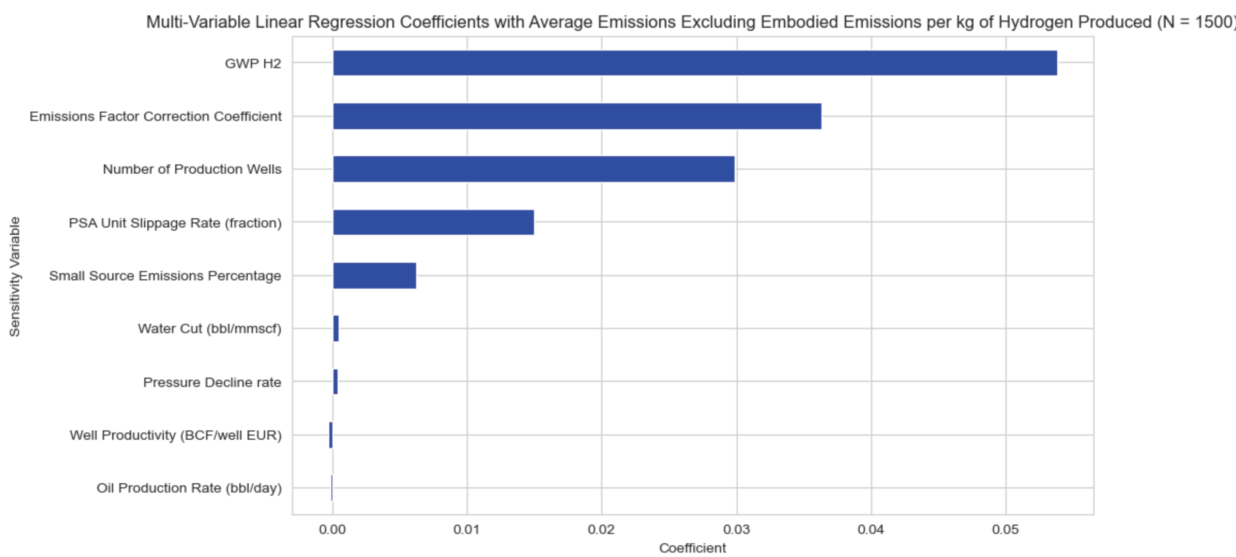


Figure 5.14: Chart showing relative magnitude of coefficients from scaled multi-variable linear regression with target variable of lifetime emissions intensity excluding embodied emissions.

5.6. Conclusions

The analysis in the chapter indicates that, even in a 'worst case' scenario, geologic hydrogen developments are still expected to have lifetime emissions intensity that is among the most compelling of all hydrogen production pathways. The high uncertainty associated with the industry is reflected in this analysis by selecting broad, uniform probability density functions for each of the modelled sensitivity variables.

Understandably, these broad ranges of uncertainty are manifested in a wide confidence interval result for the target value, with a 90% confidence interval having a magnitude of 0.4 $kgCO_2e/kgH_2$, around a median value of 0.46 $kgCO_2e/kgH_2$. Put less formally, the results indicate a 90% chance that the emissions intensity is 0.46 ± 0.2 $kgCO_2e/kgH_2$.

The lack of coherence between the single-variable and multiple-variable trends causes this author significant consternation. In an empirical study using observed data, the existence of multi-collinearities or other explanatory factors is logical to expect. This study, however, generates all data from a single model. Indeed, the single-variable scatter plots are created by calling exactly the same model function as the multi-variable scatter plots. Logic suggests that the root cause of the difference should be readily discernible from the structure and calculations of the model. Despite having made this realisation and expending significant exploration effort, this author has not successfully identified a satisfactory explanation for the phenomenon. This remains a subject of future work.

The confusion regarding the significance of the number of production wells when determining emissions intensity may be less pertinent when considering the economics of a potential geologic hydrogen development. As shown in Chapter 6, drilling and completion costs of wells are expected to comprise the majority of capital expenses associated with a development. This means that proponents of a development will generally be incentivised to minimise the well count. This is particularly true when the assumption of constant productivity per well is examined more closely. Assuming constant productivity implies that more production can always be achieved by simply drilling more wells. In reality, experience from oil and gas reservoirs suggests that there is a limited volume of recoverable product within a reservoir, which naturally results in 'diminishing returns' for the number of wells drilled. Perhaps a more appropriate set of assumptions for future analysis will be to explicitly set the total productivity of the reservoir rather than each well. The analysis in this chapter achieved a similar effect by simultaneously varying per-well productivity with the number of production wells. However, it may be useful in future to make this distinction more explicit.

The sensitivity study of lifetime emissions intensity excluding embodied emissions reveals several insights. For example, this analysis shows that excluding embodied emissions causes factors associated with direct, VFF emissions to dominate the sensitivity study. Here, the value of the GWP of hydrogen is the most influential variable. While this value is currently uncertain, it can effectively be considered a physical constant that simply has not yet been precisely determined. With further research, it is likely that a consensus will form on the 'correct' value for this GWP. This consensus will contribute significantly to the precision of this analysis.

Similarly, the emissions factor correction coefficient becomes more significant. Importantly, it is possible that this factor can be influenced by the design of surface processing facilities. With careful effort to ensure that designs minimise VFF emissions, this factor and overall emissions intensity can be similarly minimised. It is logical to assume, though, that designs that minimise VFF emissions will cost more than designs that do not. Presumably, developers will not incur the extra expense unless there is adequate incentive (or absence of disincentive) to do so.

Chapter 6: Extension of LCA via preliminary TEA

Consistent with the principles of lifecycle analyses, Brandt's paper limits the scope of the study to emissions intensity only. Emissions intensity is undoubtedly an important consideration for prospective energy resource developments. However, it may be argued that economic viability (or attractiveness) is a more critical consideration, particularly for developments being considered by enterprises operating in a free market. Analyses that consider these questions of economic viability are known broadly as techno-economic analyses (TEA) (P. H. Kobos et al., 2020). This chapter extends Brandt's use of the OPGEE emissions model as part of a "prospective LCA" by developing a coarse cost model for the same set of cases assessed by Brandt (and discussed in previous chapters) to form the basis of a 'prospective TEA'. The details of this analysis are described below.

6.1. Introduction and background

This chapter intends to use available, public-domain information to build preliminary cost models for the development and operation of the hypothetical geologic hydrogen resources described by Brandt's Baseline case and a subset of sensitivity cases. The goal of this study is not a comprehensive techno-economic analysis. Such an analysis would require developing detailed revenue and cost models. In this case, developing a revenue model would require forecasting the realised sale price of hydrogen throughout the asset's lifespan. Commodity price forecasting is a challenging and often imprecise activity, even for well-established commodities such as oil and natural gas. Forecasting the hydrogen price across the entire lifespan of a prospective hydrogen development is particularly difficult, given the high uncertainty regarding the growth of both demand and supply. Accordingly, the development of a revenue model is excluded from this study. Instead, it will estimate LCOH and compare it against relevant benchmark technologies to provide an indication of the attractiveness of this means of hydrogen supply to the market versus the more established means of production and supply.

While complete techno-economic analysis is out of scope, this study does extend the LCA and cost analysis to provide indications of economic attractiveness. As an alternative to forecasting revenue to determine the viability of a potential development, this study takes the reverse approach. Specifically, given estimates of cost, estimates of hydrogen production/export rates (developed as part of the LCA), and an organisation's threshold for a minimum acceptable return on investment, one can determine the minimum average price of hydrogen exports that is required to render the investment attractive. A proponent can then consider this price requirement alongside estimates of other costs/prices in the hydrogen 'value chain' (such as transport, storage, and marketing) to develop an estimate of end-customer pricing that is required to make the industry viable.

6.2. Techno-economic analysis approach

The basic approach of this study involves extracting relevant outputs from the LCA and using them as the foundation for a cost model. Specifically, information regarding the size and type of processing equipment and the number and design of wells are used to estimate the necessary upfront capital expenditure (CAPEX). Standard allowances for ongoing operating expenses such as labour and maintenance are used to estimate the ongoing operating expenditure (OPEX).

The source data and assumptions used to build these models are knowingly imprecise, so the models are only intended to be coarse, low-precision estimates. The intent is that they broadly comply with the Association for the Advancement of Cost Engineering International (AACEI) definition of a "Class 5" or "Class 4" estimate (Towler & Sinnott, 2022). The development of more precise and reliable estimates is considered impracticable for a study of this scope for several reasons.

First, precision in cost estimation is associated with the maturity of engineering design. For such a prospective analysis, engineering design is necessarily immature, so cost estimates cannot be precise.

Second, reliable cost estimation depends on access to reliable historical cost data for analogous developments. Such data is generally considered proprietary and unavailable in the public domain. Indeed, research organisations that specialise in techno-economic analyses, such as the Argonne National Laboratory and Sandia National Laboratory, openly acknowledge this challenge and often resolve it by building their own cost databases or commercially engaging third-party engineering consultants to access their cost databases as well as their engineering expertise (P. H. Kobos et al., 2020; Lewis et al., 2022).

Finally, a review of best-practice documentation for techno-economic analysis reveals that the generation of a cost estimate suitable for a meaningful TEA is an activity that requires considerable resources and expertise (P. H. Kobos et al., 2020). The resources available to execute this study are very constrained, so the scope and reliability of the cost modelling are likewise constrained.

6.3. Cost estimation approach

Noting the limitations discussed above, the approach to building the cost model is described here. As mentioned, the first distinction is between CAPEX and operating OPEX. The CAPEX model is composed of two major components:

- A cost estimate for surface processing equipment, per the guidance in Chapter 7 of Towler & Sinnott (2022).
- An estimate of the cost of developing wells (both production and injection wells), which leverages historical data from the United States Energy Information Authority (EIA) (Trends in U.S. Oil and Natural Gas Upstream Costs, 2016).

The OPEX model follows the guidance of Chapter 8 of Towler & Sinnott and is also composed of two major components:

- Variable costs
- Fixed costs

Each of these components of CAPEX and OPEX are described in more detail below.

6.3.1. Approach for estimating the cost of surface facilities

Without access to specialised cost-estimating resources and expertise, this study leverages approaches to cost estimation outlined in Towler & Sinnott's book on chemical engineering design (2022). They describe the workflow as follows (paraphrasing pg. 260):

1. Complete preliminary process design: Prepare material and energy balances; draw up preliminary flowsheets; size major equipment items and select materials of construction.
2. Estimate the purchased cost of the major equipment items.
3. Calculate the ISBL [inside battery limits] installed capital cost… and correcting for materials of construction.
4. Calculate the OSBL [outside battery limits], engineering, and contingency costs

5. Determine the fixed capital investment as the sum of ISBL, OSBL, engineering, and contingency costs.
6. Estimate the working capital as a percentage of the fixed capital investment.
7. Add the fixed and working capital to get the total investment required.

The relevant details of each step in this workflow are described below:

Complete preliminary process design

For this study, Brandt completed the preliminary process design as the foundation of the original study, and this approach has been replicated here. The only element of process design discussed by Towler & Sinnott but not by Brandt is material selection. Primarily due to the small size of hydrogen molecules, the mechanical design of hydrogen processing equipment needs to be particularly conscious of the risk of hydrogen-specific damage mechanisms, such as hydrogen embrittlement. While a detailed material selection process is beyond the scope of this study, it will be assumed that piping and equipment are fabricated from a grade of austenitic stainless steel (such as 304 or 316) that has improved resistance to hydrogen embrittlement compared to plain carbon steel grades.

Cost of major equipment items

Chapter 7 of Towler & Sinnott presents the "cost curve" correlation method for estimating the purchased cost of processing equipment. This processing equipment is also referred to as 'inside battery limit' (ISBL) equipment. The method details a range of equipment types and, using a combination of historical cost data, empirically derived cost constants, a size parameter and an empirically derived, equipment-specific exponent factor, allows estimates of the cost of equipment within defined size parameter ranges. Towler & Sinnott's Equation 7.9 governs the estimate model and is replicated here for clarity:

$$C_e = a + bS^n$$

where: C_e = purchased equipment cost on a U.S. Gulf Coast basis

a, b = cost constants, published in Towler & Sinnot Chapter 7

S = size parameter, published in Towler & Sinnot Chapter 7

n = exponent for that type of equipment, published in Towler & Sinnot Chapter 7

For example, pressure vessels are scaled based on shell mass (in kg) as the size parameter and reciprocal or centrifugal compressors are scaled based on driver power (in kW) as the size parameter. The range of equipment types included in Brandt's process model for geologic hydrogen are all represented in the Towler & Sinnot data, so it is straightforward to apply the listed factors to the scaling variables, which were calculated as part of the LCA.

Once Equation 7.9 has been used to calculate the purchase cost for the equipment, then Towler & Sinnot's Equation 7.12 can use the purchase cost and a range of installation factors to estimate the 'installed cost' of the equipment. This equation effectively assumes that the installed cost of any piece of gas-processing equipment is approximately three times the purchase cost.

It is important to note that the model is based on cost data from the U.S. Gulf Coast, in January 2010. Towler & Sinnot quote the relevant Chemical Engineering Plant Cost Index (CEPCI) for this period as 532.9. This is helpful, as the intent of the CEPCI is to allow meaningful scaling of cost data across time horizons. The most recent CEPCI publication (for 2023) states a value of 797.9 (Anonymous, 2024). Thus, the cost estimates generated using the equation above are scaled into 2023 terms by multiplying by a factor of 797.9/532.9 (i.e. approximately 1.5).

Material selection cost scaling

Importantly, Equation 7.12 incorporates a "materials cost factor", which represents the ratio of purchased costs of equipment in exotic materials to those of that same equipment in carbon steel. For austenitic stainless steel grades 304 and 316, the materials cost factor is listed as 1.3 (i.e. 30% more costly than carbon steel). This factor is included in the cost model built in this study.

Offsites, design and engineering, contingency, and working capital

Towler & Sinnott's method provides guidance regarding allowances for the cost of 'offsite' facilities, including all non-processing equipment that is required to run a facility. These are otherwise referred to as 'outside battery limit' (OSBL) facilities. This term covers a wide range of items such as utility systems like those that provide compressed air and water, buildings containing control rooms, offices and amenities, maintenance workshops, emergency response facilities, boundary fences and security systems and the like. Towler & Sinnott indicate that OSBL costs typically vary from 10% to 100% of ISBL costs. The default value for OSBL costs in Towler & Sinnott's Table 7.5 is 30% of ISBL costs, which is the value that has been adopted here.

Towler & Sinnot make a similar allowance for the cost of design and engineering. Here it is assumed to be 30% of the total of ISBL and OSBL costs. They also include an allowance for contingency costs, which is 10% of the total of ISBL and OSBL costs. This has also been adopted here.

Total fixed capital cost

Total fixed capital cost is simply the sum of the previously calculated costs: ISBL equipment cost, OSBL equipment cost, design and engineering cost, and contingency cost.

Working capital

Towler & Sinnott make allowance for the amount of capital required to be held in order to commence and sustain operation of a plant. This is referred to as working capital. They indicate that this is typically 10% to 20% of total fixed capital cost, so this study has adopted a value of 15%.

Total cost of development

The total capital cost of a development is thus the sum of total fixed capital working capital. This represents the total capital investment required to build and sustain the facility.

6.3.2. Approach for estimating the cost of wells

Ideally, a method analogous to that described for estimating the cost of surface processing equipment would also be used to estimate the cost of drilling and completing the wells associated with the development. Unfortunately, no public-domain method was identified during this research, so an alternative method was adopted. This method relies heavily on the data published in a 2016 report from the United States Energy Information Authority (EIA), titled "Trends in U.S. Oil and Natural Gas Upstream Costs" (Trends in U.S. Oil and Natural Gas Upstream Costs, 2016). This report aggregates cost data for upstream drilling and production costs between 2006 and 2015 across five key onshore regions and the offshore Gulf of Mexico region. Given the significant difference in drilling between onshore and offshore wells, the report treats these two categories completely separately. Brandt's scenarios all assume that the geologic hydrogen development involves only onshore wells, so this study refers only to the onshore sections of the EIA report. The report, authored primarily by the information services provider IHS, discusses the growth of the ‘unconventional’ drilling activities in the U.S., characterised by consistently increasing amounts of horizontal drilling and hydraulic fracturing. These differ from the ‘conventional’, vertically-drilled and unfractured wells assumed in Brandt’s scenarios. The clear focus on unconventional wells means that much of the data in the report cannot be readily adapted to inform meaningful cost estimates for conventional wells. Fortunately, however, there is a small but sufficient amount of data that can be used to develop a coarse cost model for conventional wells. This model is described below.

Determine drilling cost per foot of vertical depth

First, the report details historic (up to 2014) and forecast (from 2014 to 2018) drilling cost per “Total Depth”, which is distinguished from horizontal drilling. The relevant chart has been duplicated here in Figure 6.1. For this study, it is assumed that Total Depth cost rates are a suitable representation of drilling costs for vertical wells. 2014 is selected as the benchmark year, as this is the data year from the chart, with data in subsequent years representing forecast rather than actual costs. In the spirit of replicating Brandt’s LCA approach of geologic hydrogen wells being an analogue of the ‘average’ natural gas well, a drilling cost rate for hydrogen wells of $150/ft is selected as an approximate average of the reported 2014 regional cost rates.

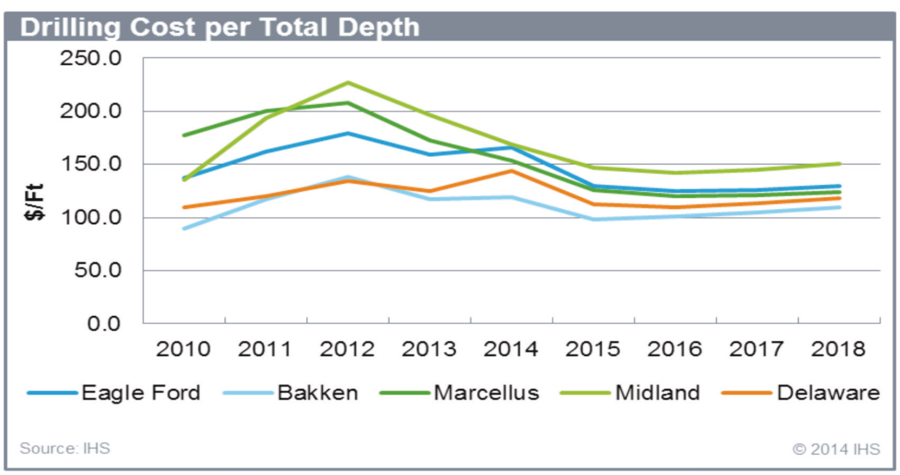


Figure 6.1: Extract of Figure 2-17 from EIA's Trends in U.S. Oil and Natural Gas Upstream Costs report (2016, p. 31)

Scaling drilling cost to total well cost

The EIA/IHS report also states that “Before the expansion of horizontal drilling within unconventional plays, drilling costs ranged from 60% to as much as 80% of a well’s cost” (2016, p. 17). Accordingly, this study conservatively assumes that drilling costs represent only 60% of the total well cost. This logic can be extended to estimate total well cost, as per the following equation:

$$Total\ well\ cost = \frac{Drilling\ cost}{Drilling\ cost\ as\ proportion\ of\ total\ cost} = \frac{\$150/ft}{0.6} = \$250/ft$$

The report describes the IHS cost model for wells consisting of four components; drilling, completions, facilities, and operations. The report does not make it clear which of these four components are captured by the $250/ft value calculated above. In the absence of this clarity, it is assumed in this study that this cost value covers all and only costs associated with drilling and completions. Costs for facilities are assumed to be captured by the costs calculated in Section 6.3.1 Costs for operations are assumed to be captured by the calculations in Sections 6.3.3and 6.3.4

Scaling 2014 cost data to 2023 basis

Given that the costs for surface equipment have been scaled to represent 2023 values, it is important that costs for wells are also scaled this way. The EIA/IHS report discusses the use of cost indexes for this specific purpose and makes use of the CERA Capital Cost Index to do so as part of the analysis. S&P Global now maintains this index, referred to as the Upstream Capital Cost Index (UCCI). Thus, the UCCI is considered appropriate for scaling the total well cost from 2014 to 2023 dollars. The relevant data points are as follows:

- Mean UCCI value for 2014: 232
- Mean UCCI value for 2023: 220

These values imply that upstream costs in 2023 are approximately 5% lower than those in 2014. To be conservative, this study assumes that 2014 and 2023 cost data are equivalent. i.e.:

$$Total\ well\ cost\ in\ 2023 = Total\ well\ cost\ in\ 2014 = \$250/ft$$

Validation of estimation approach

There is precious little data available to enable validation of this estimation approach, with the exception of one case within the EIA/IHS report. The report refers to “small vertical wells accessing the stacked pay zones in the Sprayberry costing only $2.5 MM per well” (2016, p. 20). This sentence provides a reference point for vertical wells against which the estimation method can be validated.

The report also explains that the Sprayberry 'sub-play' is in the Permian 'play' (region). We can see in Figure 6.1: Extract of Figure 2-17 from EIA's Trends in U.S. Oil and Natural Gas Upstream Costs report (2016, p. 31)Figure 6.1 that the 2014 drilling rate for the Permian play was $170/ft. Further, Table 8-1 from the report reveals that the model for the Sprayberry sub-play involved well depth of 8,996 ft (2016, p. 96). Applying the logic from above gives:

$$Total\ well\ cost = \frac{\$170}{ft} * 8{,}996ft * \frac{1}{0.6} = \$2.55\ million/well$$

The close alignment with the stated cost for these wells of "only $2.5 MM per well" gives some level of confidence that the modelling approach, while simple, may be considered suitably representative for the purposes of this research.

Summary cost calculations

This analysis in this study only considers three discrete scenarios for well depths. 'Shallow' wells of 1,500 ft, the Baseline case of 6,000 ft wells and the 'Deep' case of 12,000 ft wells. This means the calculation of estimated drilling cost and total cost per well is trivial. This is summarised as follows:

Drilling cost per well:

Shallow = 1,500 ft * $150/ft ~= $225k/well

Baseline = 6,000 ft * $150/ft ~= $900k/well

Deep = 12,000 ft * $150/ft ~= $1.80 million/well

Total cost per well:

Shallow ~= 0.225/0.6 ~= $0.4 million/well

Baseline ~= 0.9/0.6 ~= $1.5 million/well

Deep ~= 1.8/0.6 ~= $3 million/well

6.3.3. Approach to modelling variable operating costs

Towler & Sinnot (2022) describe their approach to modelling variable operating costs in Chapter 8.4. The components they describe as contributing to variable operating expenses are listed below, along with a brief explanation as to how the components are treated in this analysis:

- Raw materials (e.g. feedstock)
  - Brandt's process model does not include the consumption of any raw materials, so this cost is assumed to be zero.

- Utilities (e.g. fuel for turbines and generators, electricity)
    - The LCA calculates electricity demand, so the cost model applies the a cost in US Dollars per kWh, taken from the EIA's reported average electricity price for industrial customers in April 2024 ($0.08/kWh) (*Electric Power Monthly - U.S. Energy Information Administration (EIA)*, 2024).
- Consumables (e.g. chemicals, catalysts, corrosion inhibitors etc.)
    - The cost model assumes that the process doesn't require any consumables, so this is assumed to be zero.
- Effluent disposal
    - The primary 'effluent' involved in this assessment are the waste (non-hydrogen) gases produced from the reservoir. These are assumed to be reinjected into a disposal reservoir, which is powered by self-consumption of produced hydrogen. Accordingly, the additive cost of this process (as opposed to the opportunity cost of lost/reduced quantity of exported hydrogen) is assumed to be zero.
- Packaging and shipping
    - This 'well to gate' analysis, specifically excludes transportation infrastructure from both emissions and cost analysis, so this cost is set to zero.

6.3.4. Approach to modelling fixed operating costs

Towler & Sinnot outline a similar approach for fixed operating costs in their Chapter 8.5. The components of fixed costs are listed as:

- Operating labour and supervision;
- Overhead for direct employees;
- Maintenance (including material and labour);
- Property taxes and insurance;
- Rent of land and/or buildings;
- General plant overhead;
- Environmental charges;
- Running license fees and royalty payments;

- Capital charges, and;
- Sales and marketing costs.

The approach taken for each of these components is described below:

Operating labour and supervision

Towler & Sinnot provide specific guidance for estimating labour and supervision cost, based on the nature of the facility. Here, the following assumptions are made:

- 3x shift positions are required.
    - This is a conservative selection, based on the assumption of one control room operator, one field operator, and one product shipping area operator. With sufficient automation, this could potentially be reduced to a single control room operator position.
- 4.8 operators employed per shift position
    - This provides "a four-shift rotation with allowance for weekends, vacations and holidays, and some use of overtime" (Towler & Sinnott, 2022, p. 295).
- Operator annual salary of USD $50,000
- Cost of supervision salaries is estimated at 25% of total operator salaries

Overhead for direct employees

These costs represent non-salary costs associated with employees, including non-salary benefits and training. Towler & Sinnot suggest this typically varies between 40% and 60% of labour plus supervision costs, so this study assumes a value of 50%.

Maintenance (including material and labour)

Here, Towler & Sinnots' guidance for gas plants is that annual maintenance expense can be estimated as 3% of capital costs. This includes the cost of materials, equipment and labour required to complete the maintenance program.

Annual property costs

Annual property costs consist of property taxes, rent, and insurance. Towler & Sinnot indicate that, as a first approximation, the cost of each of these categories can be estimated at 1% of capital costs.

General plant overhead

These are charges to a facility to cover corporate overhead functions such as human resources, research and development (R&D), information technology and the like. Here we account for most of these costs in an annual "General and Administrative (G&A)" category, which is approximated as 65% of the total labour costs of the facility (i.e. labour plus supervision plus overhead, described above). While Towler & Sinnot propose estimating R&D costs as 1% of revenue, for simplicity we assume here that it is instead 1% of processing equipment costs (applied annually).

Environmental charges

Towler & Sinnot acknowledge the "Superfund Act", which taxes chemical and petroleum industries to fund the remediation of uncontrolled or abandoned hazardous waste sites. Here this cost is estimated as 1% of surface processing equipment CAPEX, applied annually.

Running license fees and royalty payments

An allowance is suggested for running of proprietary processes and payment of royalties. Given the simplicity of the proposed process design, it is assumed that these fees to not apply to this study.

Capital charges

If the development of an asset is funded by debt, then repayment of this debt will form part of the fixed cost of the asset. For simplicity, we assume here that there are zero capital charges (i.e. the development is funded by cash not debt).

Sales and marketing costs

Given this hydrogen is expected to be a commodity product, special sales and marketing expenses are not expected (unlike the production of specialist cosmetic or pharmaceutical products). Any necessary expense is assumed included in the G&A overhead, so this line item is set to zero.

6.3.5. Key assumptions

Noting the range of assumptions made above, there are several assumptions that are considered particularly critical to the magnitude of the estimates. These include:

- Wells are vertical only – It is expected that horizontal wells will add significantly to the cost. However, if horizontal drilling increases the productivity per well, then it may be required to estimate and consider a trade-off curve to optimise the profitability of the development.

- No hydraulic fracturing – Fracking adds the cost of fracturing pumps and proppant (Trends in U.S. Oil and Natural Gas Upstream Costs, 2016).
- Surface processing equipment is assumed to be fabricated from austenitic stainless steel (grade 304 or 316). These grades are assumed to have 30% higher purchase cost than basic carbon steel.
- All operating costs are assumed to be subject to annual inflation of 3%.

6.4. Cost estimate results

Figure 6.2 summarises total and component-level costs estimated for the Baseline case. Clearly, the cost associated with developing the 50 production wells and 13 injection wells dominates this estimate. The balance of the cost is approximately divided between capital costs associated with processing equipment and fixed costs. The results indicate that variable costs (associated with electricity consumption from the grid) are essentially negligible. Dividing the total present value of all costs by the total hydrogen exports from the asset gives cost value of \$1.45/kgH_2.

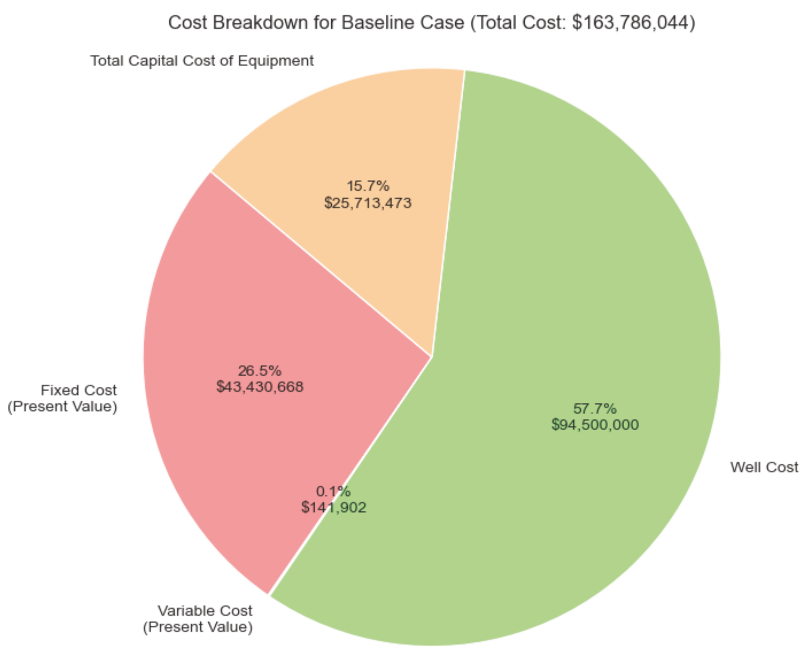


Figure 6.2: Visualisation of the components contributing to the total cost estimate for the Baseline case.

6.5. Consideration of United States hydrogen PTC regime

As discussed in Chapter 1, the United States government has incentivised the production of low-carbon intensity hydrogen via the 45V PTC regime. Given the size of the United States economy, its related importance to the global economy and the significant geologic hydrogen startup activity within that country, this study attempts to value the PTCs associated with the hypothetical geologic hydrogen development that forms the basis of Brandt's paper.

Also as discussed previously, the LCA portion of this study calculated estimates of the annual emissions intensity of the hydrogen produced in each year of the asset's life. If it is assumed that the 45V PTC regime requires or allows an annual calculation basis for determining eligibility for the tiers within the PTC regime, then these estimates can be readily repurposed to estimate the potential value of the associated tax credits. It is not clear to this author if the United States legislation and regulations allow or require such annual accounting, or if PTCs will be granted based on a calculation of forecast lifetime emissions intensity.

The repurposing of annual emissions intensity values and consideration of lifetime emissions intensity values have both been implemented in the revised model. For the sake of academic interest (as opposed to the sake of investment analysis or policy setting), the calculations have been run considering both the situation where embodied emissions are excluded from the PTC eligibility calculation (as is currently the situation) as well as the situation where embodied emissions are included in the eligibility calculation. While the latter of these situations is clearly not in line with the relevant legislation, it may be argued that considering embodied emissions is a valid and necessary progression for this type of incentive or stimulus, because, from the perspective of atmospheric physics and chemistry, embodied emissions are as relevant as any other form of emissions. Lastly, the fivefold increase in the value of PTCs associated with meeting the relevant employment conditions is also modelled.

In general, it is found that the emissions intensity of geologic hydrogen developments are sufficiently low such that the inclusion or exclusion of embodied emissions in the calculus is irrelevant. That is, even with the inclusion of embodied emissions, average annual emissions intensity over the first ten years of operation is below the most onerous (lowest) tier of emissions intensities, for which the highest tax credits are earned. This means that the PTC values are identical and maximised in either situation. Figure 6.3 shows the undiscounted value of PTCs for the Baseline case and makes it clear that the reported values are unaffected by the inclusion or exclusion of embodied emissions. It also shows that the use of annual or lifetime emissions intensity does not affect the value of PTCs earned, in this case. Here, the fivefold value increase when the stipulated employment conditions are satisfied manifests as a simple fivefold increase, regardless of whether embodied emissions are included or whether emissions intensity is determined on an annual or lifetime basis.

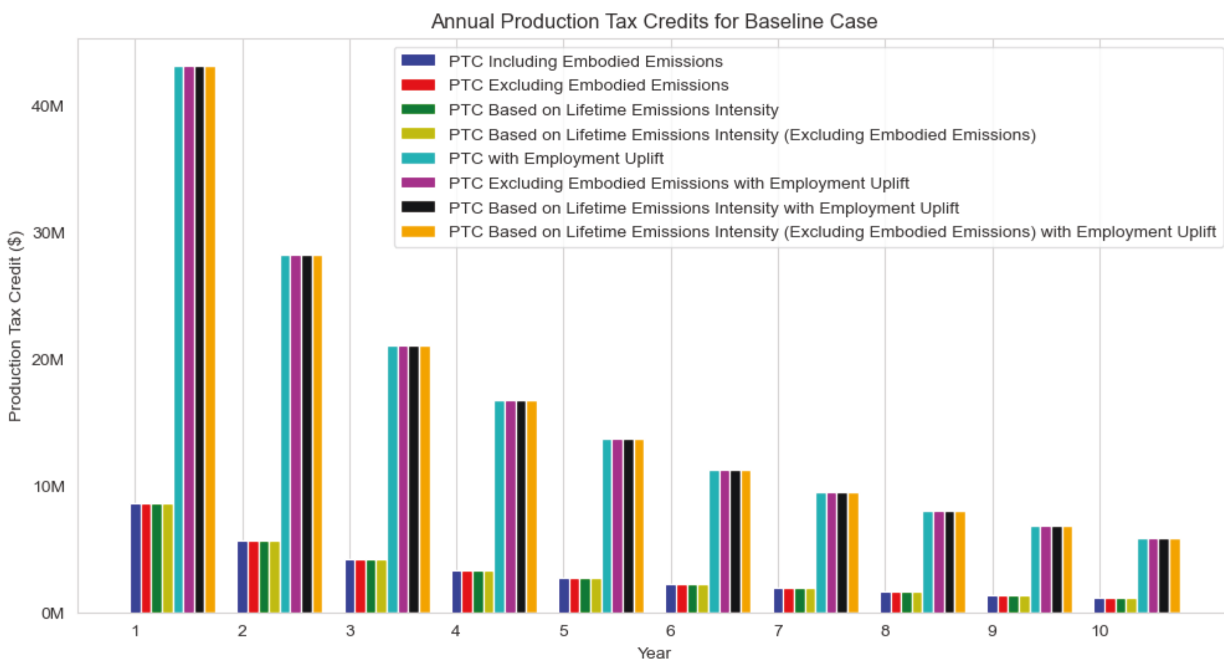


Figure 6.3: Plot of the undiscounted value of Production Tax Credits for the Baseline case. Notice the value is not affected by the inclusion or exclusion of embodied emissions.

It is not to say, however, that the inclusion or exclusion of embodied emissions is irrelevant in all cases. Figure 6.4, for example, demonstrates the significant difference in PTC values when including versus when excluding embodied emissions from the emissions intensity calculations in the 'Low Productivity' case. The figure also shows that the basis of annual versus lifetime emissions intensity can significantly affect the value of PTCs granted.

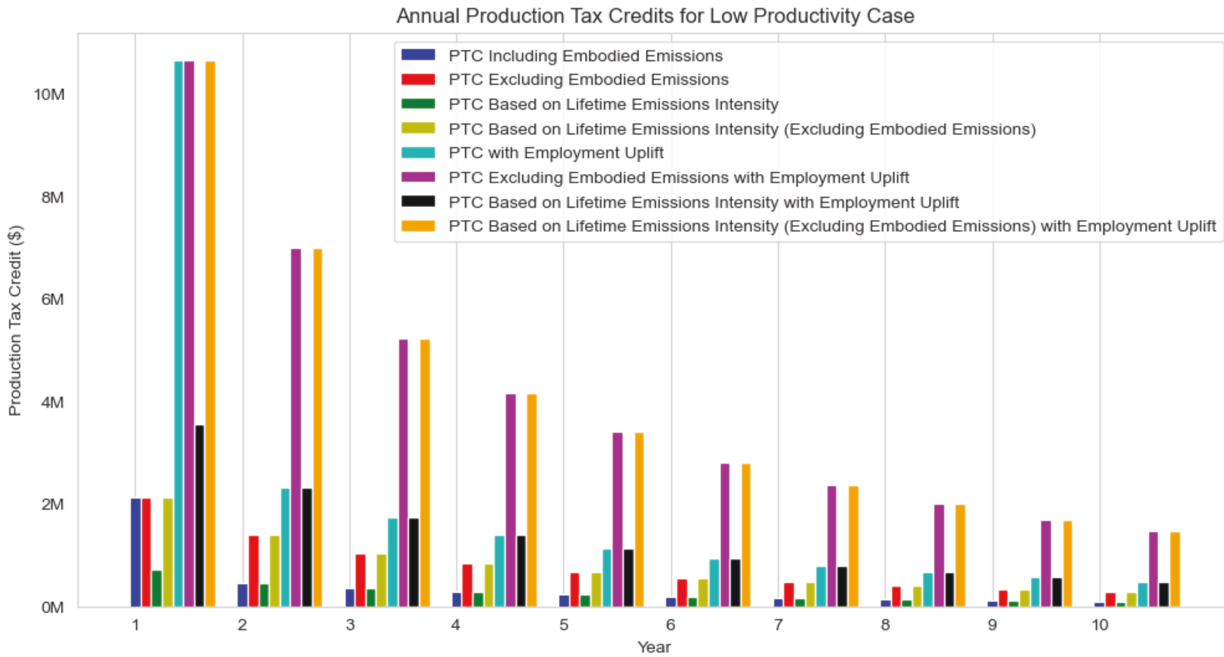


Figure 6.4: Plot of the undiscounted value of Production Tax Credits for the "Low Productivity" case.

Notice that the reduced quantity of export hydrogen increases the emissions intensity relative to the Baseline case, and the value of PTCs is significantly eroded by the inclusion of embodied emissions. Similarly, basing the PTC calculation on a single value of lifetime emissions intensity (rather than annual emissions intensity) is highly impactful when embodied emissions are included. When these are excluded, the emissions intensity drops such that the maximum PTC benefit is realised for all 10 years.

It is also interesting to consider the value of the PTCs relative to the costs of developing a geologic hydrogen asset. If, for example, the value of the PTCs completely offsets the development cost, then the decision to develop the asset would be inherently low risk. In this example, the development would be profitable regardless of the realised hydrogen price and there would be enormous 'upside risk', where the asset's value increases proportionally with the price of hydrogen. Figure 6.5 shows that this scenario is realistic under the current United States PTC regime if the requirements regarding employment conditions are satisfied and the fivefold benefit 'uplift' is applied. With or without the uplift, the value of PTCs is an important factor in the 'business case' and investment attractiveness of potential geologic hydrogen developments. Section 6.7. examines this significance in more detail.

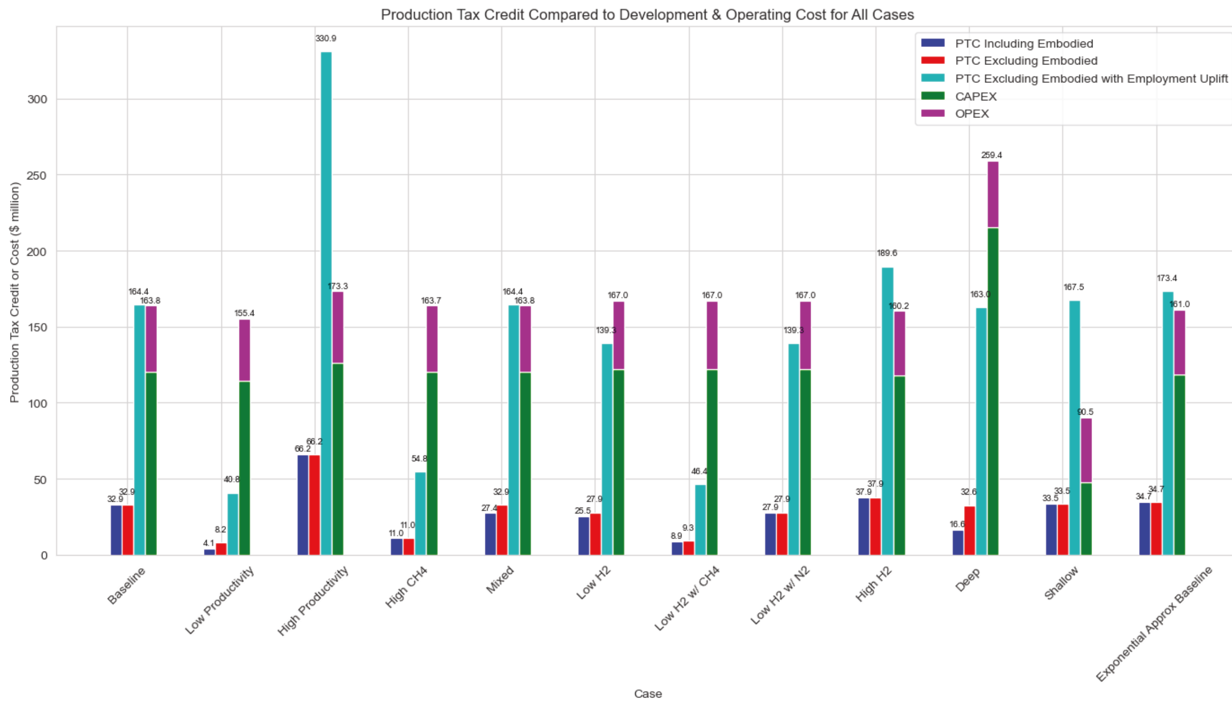


Figure 6.5: Plot of estimated present-value costs against present-value PTC benefit for a subset of sensitivity cases.

6.6. Effect of lifespan and total productivity on levelized cost of hydrogen

Just as the effect of lifespan and its link to total productivity (EUR) was interesting to study as part of the LCA, it is also interesting to consider as part of TEA. This analysis maintains the simplifying assumptions regarding flow rate at the start and end of field life, as well as the assumption of exponential flow rate decline between these two flow rates. Figure 6.6: Plot summarising the effect of increasing lifespan (and associated estimated total productivity) on the levelised cost of hydrogen for the Baseline case. Figure 6.6 summarises these results, where the levelized cost decreases with increasing productivity (and lifespan) in the same hyperbolic manner as did emissions intensity. This reinforces the conclusion that proponents should seek to develop maximally productive and long-lived geologic hydrogen developments.

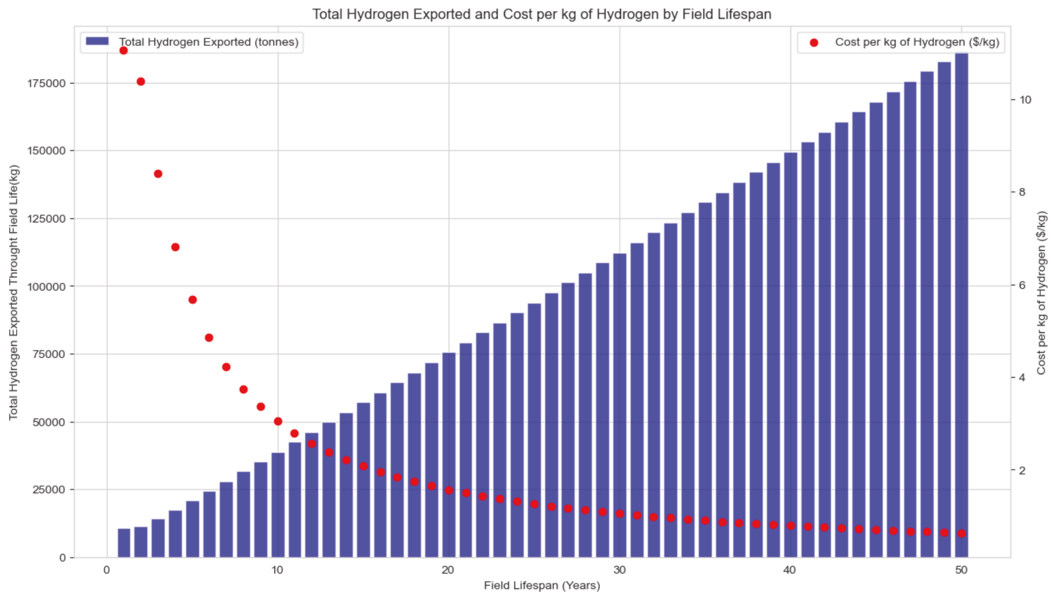


Figure 6.6: Plot summarising the effect of increasing lifespan (and associated estimated total productivity) on the levelised cost of hydrogen for the Baseline case.

6.7. Preliminary assessment of investment metrics vs average realised price of hydrogen

In a market economy, firms are incentivised to seek maximal returns on investments. There are a range of methods to evaluate and estimate the potential return delivered by a potential investment. Each of these methods requires three basic elements: an estimate CAPEX, an estimate of OPEX, and an estimate of ongoing revenue generation. With these basic elements and a discount rate that appropriately represents the ‘time value of money’, an estimated net present value (NPV) of the investment can be calculated. NPV is simply the present value of revenues less the present value of costs, and rational investors typically seek to maximise NPV (or at least ensure that it is not negative). A thorough determination of NPV will use a discount rate set equal to a firm’s real weighted average cost of capital (WACC), which is a calculation that weighs the relative costs and benefits of debt and equity financing, including tax advantages (P. Kobos et al., 2020). This calculation involves details that are more specific than are worth considering in this study, so a common default discount rate of 10% has been adopted instead.

In this study, estimates of CAPEX and OPEX have been generated as per the discussion in Section 6.3. Annual rates of hydrogen exports have also been calculated, so annual gross revenue can be estimated as the production rate multiplied by an assumed realised price (i.e. the price received by the producer, typically equivalent to the cost to their customer). As indicated in Section 1.4.2, forecasting of hydrogen pricing is beyond the scope of this study (and the opinion of this author is that any third-party forecasts are unlikely to be at all reliable, given the expected growth of the hydrogen market). Instead, the approach taken here is to consider the effect of investment attractiveness 'hurdle rates', and calculate the price of hydrogen exports over the asset's life that would see these hurdle rates met or exceeded. The hurdle rates are explained in more detail below.

6.7.1.Hurdle rates

Internal Rate of Return (IRR)

The Internal Rate of Return is the discount rate such that, when calculating NPV, the resultant NPV equals zero. Simplistically, the IRR needs to be at least as much as a WACC to be considered attractive. As discussed above, while WACC can be calculated for an individual firm and an individual investment, 10% is often selected as a reasonable benchmark hurdle rate.

Discounted Profitability Index (DPI)

The Discounted Profitability Index (DPI) is an alternative way to assess the attractiveness of a potential investment. DPI is calculated as the NPV of an investment, divided by the upfront capital expenditure (CAPEX). In this case, the discount rate used in the NPV calculation is fixed, typically at the proponent's WACC (with 10% often assumed as a reasonable default). DPI enables the comparison and prioritisation of competing investment alternatives with differing capital investment requirements. It can be considered a 'risked' metric because, while the calculation of NPV accounts for CAPEX, it doesn't account for the uncertainty in the cash flow model that is also required to calculate NPV. Put simply, DPI suggests that proponents should and will prefer to minimise the capital investment required to achieve a given value of NPV. A common benchmark value for minimum acceptable DPI (i.e. a DPI hurdle rate) is 1.3.

Handling of Production Tax Credits

For simplicity, this analysis treats PTCs as a source of revenue in the Discounted Cash Flow model that forms the basis of NPV calculations. This implies that the proponent has a sufficiently large tax liability to avail themselves of the full value of the PTCs. For academic interest, the study considers the impact of PTC values excluding embodied emissions (as per the current U.S. legislation) as well as those including embodied emissions (as would be best practice from the perspective of minimising environmental impact).

6.7.2. Limitations/notes

It is acknowledged that the approach adopted here is unsophisticated. It is intended to provide only a preliminary view as to the potential investment attractiveness of geologic hydrogen in comparison to other production pathways.

When considering the fivefold increase to the PTC due to the satisfaction of the employment condition requirements, this analysis considers the ‘upside’ effect of the additional benefit. It is reasonable to assume that satisfying these conditions would only be possible at additional cost to the firm. The ‘downside’ effect of these costs have not been considered or included in the cost modelling approach in this study.

As mentioned, this approach calculates a single price for each hurdle rate included in the study. This is not to suggest that the price of such a commodity product will ever be stable over a 30-year lifespan; rather, it is the ‘production-weighted mean price’ above which the hurdle rate will be satisfied. Due to both the expected rapid decline in production rates in early field life, and the effect of the time value of money, the prices realised early in the field life will dominate the investment attractiveness.

6.7.3. Results

Rather than report values for a single hurdle rate for each of the metrics of investment attractiveness, this study calculated values for a ‘sweep’ of potentially-viable hurdle rates. Resultant prices are reported for scenarios both excluding and including embodied emissions in the calculation of PTC values. These results are shown in Figure 6.7 and Figure 6.8.

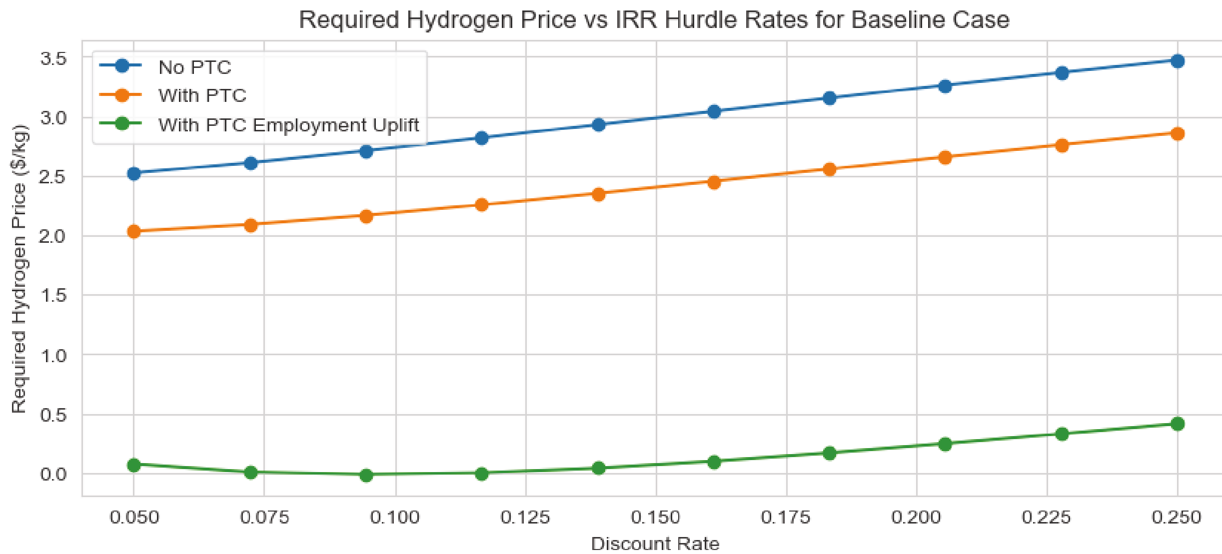


Figure 6.7: Plot of the lifetime mean hydrogen price required to meet a range of IRR hurdle rates.

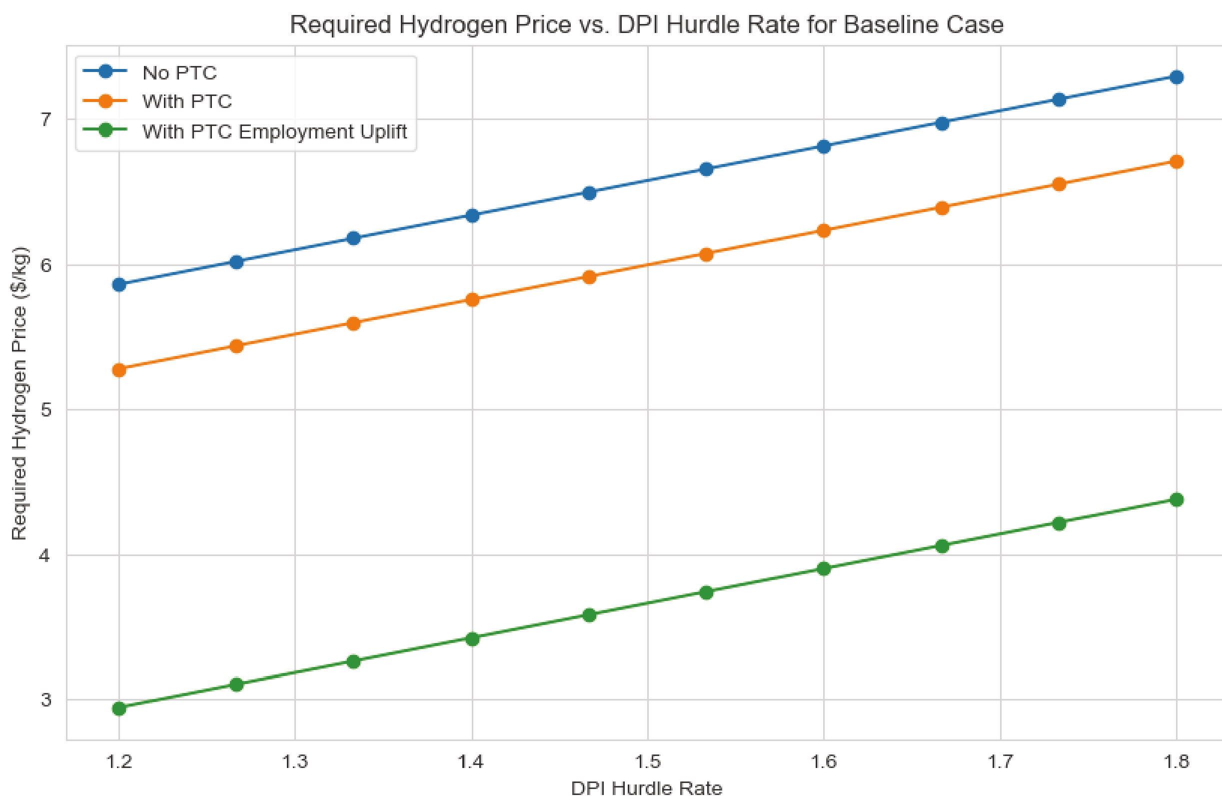


Figure 6.8: Plot of the lifetime mean hydrogen price required to meet a range of DPI hurdle rates.

6.7.4.Discussion

The most obvious observation from these results is that the use of DPI as a metric of investment attractiveness is significantly more onerous (i.e. requires significantly higher realised hydrogen prices) than IRR. Given the large estimated capital investment required to develop the geologic hydrogen field, this is a logical finding.

A second important observation is that the pricing referred to above is at the ‘gate’ of the hydrogen production facility. The price to the end user of the hydrogen will thus need to account for the cost of so-called ‘midstream’ services, such as transportation and storage. Examples of the estimated magnitude of these midstream costs include (Murdoch et al., 2023):

- $0.1/kg to $0.4/kg for ‘best in class compression’
- $0.1/kg for 7 days of salt cavern storage
- $0.8/kg for 7 days of tank storage
- $0.1/kg for transportation via pipeline
- $0.7/kg to $1.5/kg for transportation via trucking

Ultimately, the hydrogen economy will need to find an equilibrium such that the price paid by end consumers is sufficiently high to compensate both hydrogen producers and those firms providing midstream services.

Assuming that midstream costs will be approximately equivalent for any of the hydrogen production pathways, it is the cost of production (or the ‘gate’ price) that will ultimately distinguish the viability, attractiveness and competitiveness of a development that uses a particular production pathway (or set of pathways). The coarse modelling of this study suggests that the cost of geologic hydrogen production (in the Baseline case) is $1.45/kg.

It is interesting to compare the cost profile of geologic hydrogen to other hydrogen production pathways. This study suggests that geologic hydrogen is capital-intensive, but that operating costs are mostly governed by the cost of labour. Comparisons with electrolytic (“green”) hydrogen developments are particularly interesting. Consider first those developments that install dedicated electricity generation capacity (e.g. solar panels and energy storage). It is likely that these could be similarly capital-intensive, and the magnitude of the relative capital expense per unit of production may be an important metric. Electrolytic hydrogen developments that procure electricity from third-party suppliers will require significantly lower capital investment but involve significantly higher operating expenses, and will be subject to pricing/cost risk. For reference, a Lazard study of various electrolyser technologies and plant capacities indicated a range of Levelised Cost of Hydrogen (LCOH) between \$1.40/kg and \$2.90/kg(*Lazard's Levelized Cost of Hydrogen Analysis*, 2021).

While this study's cost estimate for geologic hydrogen is coarse, it indicates that the technology may be as attractive as the lowest cost 'green' hydrogen assets. This promising result suggests that further work on the topic is warranted.

Chapter 7: Conclusions and Future Research

7.1. Findings and discussion

This thesis established that the magnitude of the potential societal benefits of naturally occurring geologic hydrogen is matched by the magnitude of the many uncertainties that surround the feasibility of its economic development. It came to this conclusion by:

- Thoroughly reviewing the first publication to attempt to use LCA to quantify potential lifetime emissions intensity of geologic hydrogen developments;
- Finding that Brandt's LCA approach is logical and that the modelling work did not identify any errors that caused major differences in reported emissions intensity results, nor changes to the overall conclusions of the paper;
- Finding that the correction of minor errors increased the headline value of lifetime emissions intensity by approximately 6%, to 0.40 $kgCO_2e/kgH_2$.
- Extending Brandt's work to consider the correlation between field EUR and field lifespan, and the associated impacts on lifetime emissions intensity. This confirmed quantitatively the intuitive presumption that longer-lived, higher-productivity assets are generally preferred. It indicated that lifespans on the 'decadal' timescale are necessary to achieve competitive, compelling emissions intensity results;
- Correcting significant flaws in the LCA model's equipment sizing algorithms. It was recognised that these flaws had minimal influence on the LCA outcomes and that they would have a much more significant impact on TEA;
- Extending Brandt's LCA modelling approach to include analysis of uncertainty via the Monte Carlo method;
- Building coarse cost models to align with the scenarios set out in Brandt's paper, and using these models as the foundation of a cost-centric 'prospective TEA'. This calculated a levelized cost of hydrogen from geologic hydrogen of $1.45/kg, which may render it competitive with the lowest-cost, lowest-emissions of alternative hydrogen production pathways.
- Completing preliminary investment modelling to suggest 'at gate' prices (realised by the owner of the geologic hydrogen production facility) at which investments in geologic hydrogen developments would likely be considered attractive.

More generally, the modelling work here provides numerical support for insights that may be otherwise considered intuitive. These include that:

- Large resources with long field lives are the most appealing, from both an environmental, emissions intensity perspective and from a techno-economic, investment attractiveness perspective.
- Developers should try to minimise the number of wells in a development:
    - Drilling and completing wells has the most significant impact on both embodied emissions and total development cost. In a regime where embodied emissions have no impact on project economics (such as the USA's 45V PTC regime), the cost impact will almost certainly be the most significant consideration for proponents.
    - Thus, maximising productivity per well is essential to maximise the attractiveness of the development.
    - Given the use of natural gas as an analogue for this study, and considering that the natural gas industry has spent decades developing techniques to maximise well productivity (most notably horizontal drilling and hydraulic fracturing) this is not a surprising finding. When the geological/geophysical nature of geologic hydrogen reservoirs are better understood, it will likely be wise to consider if or how these techniques may be applied to similarly maximise well productivity in this nascent industry.

While this work has sought to make meaningful contributions to the body of knowledge, it is self-evident that any conclusions are limited by the inputs to the model. With this in mind, perhaps the most important contribution of this work is not the results produced by the replicated, improved and updated LCA and TEA model. Rather, the creation of this new, open-source tool may itself be considered a more important contribution.

7.2. Research Limitations

This work was governed by numerous limitations. Many of these are shared by Brandt's work but some are unique to this study. These are as follows:

- Reliance on natural gas historical data for reservoir characteristics to compensate for the absence of suitable data specific to geologic hydrogen

- Reliance on natural gas fugitive emission rates
    - The uncertainty analysis shows that this assumption is influential, and there are valid hypotheses (particularly the small size of hydrogen molecules relative to methane molecules) that fugitive emission rates from hydrogen facilities will be different, and probably more severe, than those from natural gas facilities.
- Equipment sizing calculations that are generic/preliminary
- Reliance on multiplication factors to estimate total mass of steel and cement
- Cost estimation is coarse, relying on information in the public domain.
    - Even public research institutes (such as U.S. National Laboratories) tend to rely on proprietary data

7.3. Future Research

The promising findings of this research, coupled with the high levels of uncertainty that it acknowledges means that there are abundant opportunities for further research in the field of geologic hydrogen generally, as well as the more specific areas of LCA and TEA. These opportunities include:

- Continued refinement of the 'prospective' LCA and TEA model developed as part of these research. There are both minor and major opportunities for refinement:
    - Minor
        - Add iteration to solve for the reduced requirement for gas injection when part of waste gas is consumed as fuel gas
        - Add implementation of the OPGEE calculations that were deliberately excluded from the revised model, as described in Section 3.7.
    - Major
        - Where possible, replace assumptions of natural gas analogues with updated findings from geologic hydrogen literature and/or industry
        - Refine cost models based on more detailed engineering and specialist cost-engineering data
        - Incorporate more sophisticated engineering software into the model to improve estimates associated with surface processing equipment.

  Proprietary tools such as *Aspen HYSYS* should improve the reliability of the process and equipment design but will reduce the open-source nature of the model. Future work should consider how best to manage this trade-off.
  - Incorporate into the cost model the implications of achieving the employment conditions that avail a firm of the fivefold increase in PTC benefits. Intuitively, this is expected to raise the cost by a non-trivial amount.
  - Extend cost analysis to include assessment of uncertainty. Much like this study extended Brandt's LCA work, the prospective TEA study completed here will be significantly improved by quantifying the impacts of uncertain assumptions.
  - Consideration of implementing a means of accounting for embodied emissions that is more temporally representative of actual emissions, such as those used to calculate the 'social cost of carbon' (as discussed in Section 3.8.).
- Considerations regarding co-processing of H_2 and He. Answering the question 'how does the presence of He affect the carbon intensity and economic attractiveness of a development that is nominally targeting geologic hydrogen?' Similarly, 'is there a driver to consider the carbon intensity and techno-economics of helium production?'
- Addition of a sensitivity case that uses low carbon intensity steel and cement technology. This has the potential to significantly reduce the quantity of embodied emissions, particularly of the wells.
- Estimates of emissions intensity and LCOH for stimulated geologic hydrogen production (so-called 'orange' hydrogen)

The expectation is that the modified OPGEE model developed by Brandt and extended here could be further modified and/or extended to consider stimulated production. Some key differences are expected to include:

- A default assumption of horizontal drilling and hydraulic fracturing for stimulated production

- Additional surface/processing equipment for water injection and pre-injection water treatment
- Possible elimination of the requirement for a re-injection compressor and associated equipment

A separate branch of research in this area should consider the impact of a geologic hydrogen development on the techno-economics of the broader energy system of a region, using tools such as capacity expansion models. A key characteristic of geologic hydrogen is that, due to the nature of geology, the location of the resource (i.e. the source of hydrogen supply to the market) is fixed. It is unclear if these locations will be conveniently located to end-users of the hydrogen. If they are not, the hydrogen 'value chain' will need to consider 'midstream' aspects (and costs) of transportation and storage. This is distinctly different to electrolytic hydrogen, where proponents can choose to locate hydrogen generation adjacent to end-user facilities (indeed, end-user facilities could well install their own hydrogen generation facilities) and instead 'transport' the electricity they need to generate the hydrogen. A direct, parametric comparison of geologic hydrogen and co-located electrolytic hydrogen would make for an interesting study. Such a study could potentially determine a maximum distance away from an end-user that a geologic hydrogen development could be located to maintain techno-economic and emissions intensity viability. Knowledge of this distance could then feasibly help proponents of geologic hydrogen developments prioritise their exploration efforts accordingly.

In conclusion, this thesis highlights the significant potential of naturally occurring geologic hydrogen as a future energy source, balanced by the numerous uncertainties that must be addressed to fully realise its economic and environmental benefits. Through replicating and extending Brandt's OPGEE model, this research has underscored the importance of accurate lifecycle and techno-economic analyses in evaluating geologic hydrogen. Future research should aim to refine these models further, reducing uncertainties and exploring the long-term viability of geologic hydrogen. By advancing our understanding of this promising energy source, we take a crucial step toward sustainable and low-emission energy alternatives, contributing to global climate goals and energy security.

References

26 USC 45V: Credit for production of clean hydrogen. (n.d.). Retrieved July 5, 2024, from https://uscode.house.gov/view.xhtml?req=granuleid:USC-prelim-title26-section45V&num=0&edition=prelim

Aldersey-Williams, J., & Rubert, T. (2019). Levelised cost of energy – A theoretical justification and critical assessment. *Energy Policy*, *124*, 169–179. https://doi.org/10.1016/j.enpol.2018.10.004

Anonymous. (2024). Economic Indicators. *Chemical Engineering*, *131*(4), 60.

Brandt, A. R. (2023). Greenhouse gas intensity of natural hydrogen produced from subsurface geologic accumulations. *Joule*, *7*(8), 1818–1831. https://doi.org/10.1016/j.joule.2023.07.001

Brandt, A. R., Masnadi, M. S., Rutherford, J. S., El, H. M., Langfitt, Q., Vafi, K., Chen, Y., & Duffy, J. (n.d.). *Oil Production Greenhouse Gas Emissions Estimator OPGEE v3.0b*.

Busch, P., Kendall, A., & Lipman, T. (2023). A systematic review of life cycle greenhouse gas intensity values for hydrogen production pathways. *Renewable and Sustainable Energy Reviews*, *184*, 113588. https://doi.org/10.1016/j.rser.2023.113588

Calvin, K., Dasgupta, D., Krinner, G., Mukherji, A., Thorne, P. W., Trisos, C., Romero, J., Aldunce, P., Barrett, K., Blanco, G., Cheung, W. W. L., Connors, S., Denton, F., Diongue-Niang, A., Dodman, D., Garschagen, M., Geden, O., Hayward, B., Jones, C., … Péan, C. (2023). *IPCC, 2023: Climate Change 2023: Synthesis Report. Contribution of Working Groups I, II and III to the Sixth Assessment Report of the Intergovernmental*

Panel on Climate Change [Core Writing Team, H. Lee and J. Romero (eds.)]. IPCC, Geneva, Switzerland. (First). Intergovernmental Panel on Climate Change (IPCC). https://doi.org/10.59327/IPCC/AR6-9789291691647

Derwent, R. G., Stevenson, D. S., Utembe, S. R., Jenkin, M. E., Khan, A. H., & Shallcross, D. E. (2020). Global modelling studies of hydrogen and its isotopomers using STOCHEM-CRI: Likely radiative forcing consequences of a future hydrogen economy. *International Journal of Hydrogen Energy*, *45*(15), 9211–9221. https://doi.org/10.1016/j.ijhydene.2020.01.125

Derwent, R., Simmonds, P., O'Doherty, S., Manning, A., Collins, W., & Stevenson, D. (2006). Global environmental impacts of the hydrogen economy. *International Journal of Nuclear Hydrogen Production and Applications*, *1*(1), 57–67. https://doi.org/10.1504/IJNHPA.2006.009869

Dugamin, E., Truche, L., & Donze, F. (2019). *Natural Hydrogen Exploration Guide*.

Electric Power Monthly—U.S. Energy Information Administration (EIA). (2024, April). https://www.eia.gov/electricity/monthly/epm_table_grapher.php

Elgowainy, A., Frank, E. D., Vyawahare, P., Ng, C., Bafana, A., Burnham, A., Sun, P., Cai, H., Lee, U., Reddi, K., & Wang, M. (2022, October). *Hydrogen Life-Cycle Analysis in Support of Clean Hydrogen Production*. Argonne National Laboratory.

Ellis, G., & Gelman, S. E. (2022, October 12). *A PRELIMINARY MODEL OF GLOBAL SUBSURFACE NATURAL HYDROGEN RESOURCE POTENTIAL*. GSA Connects 2022 meeting in Denver, Colorado.

https://gsa.confex.com/gsa/2022AM/webprogram/Paper380270.html

Fankhauser, S., Smith, S. M., Allen, M., Axelsson, K., Hale, T., Hepburn, C., Kendall, J. M., Khosla, R., Lezaun, J., Mitchell-Larson, E., Obersteiner, M., Rajamani, L., Rickaby, R., Seddon, N., & Wetzer, T. (2022). The meaning of net zero and how to get it right. *Nature Climate Change*, *12*(1), 15–21. https://doi.org/10.1038/s41558-021-01245-w

Fertilizer Market Size & Share | Growth Forecast Report – 2032. (2024, January). Global Market Insights Inc. https://www.gminsights.com/industry-analysis/fertilizer-market

Gawer, A., & Cusumano, M. A. (2008). How Companies Become Platform Leaders. *MIT Sloan Management Review*. https://sloanreview.mit.edu/article/how-companies-become-platform-leaders/

Gawer, A., & Cusumano, M. A. (2014). Industry Platforms and Ecosystem Innovation. *Journal of Product Innovation Management*, *31*(3), 417–433. https://doi.org/10.1111/jpim.12105

Giovanniello, M. A., Cybulsky, A. N., Schittekatte, T., & Mallapragada, D. S. (2024). The influence of additionality and time-matching requirements on the emissions from grid-connected hydrogen production. *Nature Energy*, *9*(2), 197–207. https://doi.org/10.1038/s41560-023-01435-0

Granger, B. E., & Pérez, F. (2021). Jupyter: Thinking and Storytelling With Code and Data. *Computing in Science & Engineering*, *23*(2), 7–14. Computing in Science & Engineering. https://doi.org/10.1109/MCSE.2021.3059263

Intergovernmental Panel On Climate Change (Ipcc). (2023). *Climate Change 2021 – The Physical Science Basis: Working Group I Contribution to the Sixth Assessment Report* *of the Intergovernmental Panel on Climate Change* (1st ed.). Cambridge University Press. https://doi.org/10.1017/9781009157896

Kobos, P., Drennen, T., Outkin, A., Webb, E., Paap, S., & Wiryadinata, S. (2020). *Techno-Economic Analysis: Best Practices and Assessment Tools* (SAND--2020-13473, 1738878, 692989; p. SAND--2020-13473, 1738878, 692989). https://doi.org/10.2172/1738878

Kobos, P. H., Drennen, T. E., Outkin, A. V., Webb, E. K., Paap, S. M., & Wiryadinata, S. (2020). *Techno-Economic Analysis: Best Practices and Assessment Tools* (SAND-2020-13473). Sandia National Lab. (SNL-CA), Livermore, CA (United States); Sandia National Lab. (SNL-NM), Albuquerque, NM (United States); Hobart and William Smith Colleges, Geneva, NY (United States). https://doi.org/10.2172/1738878

Lazard's Levelized Cost of Hydrogen Analysis. (2021, June). https://www.lazard.com/media/12qcxl1j/lazards-levelized-cost-of-hydrogen-analysis-vf.pdf

Lefeuvre, N., Truche, L., Donzé, F.-V., Ducoux, M., Barré, G., Fakoury, R.-A., Calassou, S., & Gaucher, E. C. (2021). Native H2 Exploration in the Western Pyrenean Foothills. *Geochemistry, Geophysics, Geosystems*, *22*(8), e2021GC009917. https://doi.org/10.1029/2021GC009917

Lévy, D., Roche, V., Pasquet, G., Combaudon, V., Geymond, U., Loiseau, K., & Moretti, I. (2023). Natural H $_2$ exploration: Tools and workflows to characterize a play. *Science and Technology for Energy Transition*, *78*, 27. https://doi.org/10.2516/stet/2023021

Lewis, E., McNaul, S., Jamieson, M., Henriksen, M. S., Matthews, H. S., Walsh, L., Grove, J., Shultz, T., Skone, T. J., & Stevens, R. (2022). *Comparison of Commercial, State-of-the-Art, Fossil-Based Hydrogen Production Technologies* (DOE/NETL-2022/3241). National Energy Technology Laboratory (NETL), Pittsburgh, PA, Morgantown, WV, and Albany, OR (United States). https://doi.org/10.2172/1862910

Liu, W., Zuo, H., Wang, J., Xue, Q., Ren, B., & Yang, F. (2021). The production and application of hydrogen in steel industry. *International Journal of Hydrogen Energy*, *46*(17), 10548–10569. https://doi.org/10.1016/j.ijhydene.2020.12.123

Maiga, O., Deville, E., Laval, J., Prinzhofer, A., & Diallo, A. B. (2023). Characterization of the spontaneously recharging natural hydrogen reservoirs of Bourakebougou in Mali. *Scientific Reports*, *13*(1), 11876. https://doi.org/10.1038/s41598-023-38977-y

McDonald, N. (2024, February). *Gold Hydrogen: Aiming to Develop Naturally Occurring Australian Hydrogen and Helium*. https://announcements.asx.com.au/asxpdf/20240201/pdf/05zzq0p481g6x7.pdf

Murdoch, H., Munster, J., Satyapal, S., Rustagi, N., Elgowainy, A., Penev, M., Crane, D., Cummins, K., Klembara, M., Chan, V., Tian, L., Shah, J., & Wagner, J. (2023). *Pathways to Commercial Liftoff—Clean Hydrogen*. https://liftoff.energy.gov/wp-content/uploads/2023/05/20230523-Pathways-to-Commercial-Liftoff-Clean-Hydrogen.pdf

Net Zero by 2050—A Roadmap for the Global Energy Sector. (2021).

Ocko, I. B., & Hamburg, S. P. (2022). Climate consequences of hydrogen emissions. *Atmospheric Chemistry and Physics*, *22*(14), 9349–9368. https://doi.org/10.5194/acp-22-9349-2022

OPGEE: The Oil Production Greenhouse gas Emissions Estimator | Environmental Assessment and Optimization Group. (n.d.). Retrieved July 7, 2024, from https://eao.stanford.edu/research-project/opgee-oil-production-greenhouse-gas-emissions-estimator

Pironon, J., & Donato, P. de. (2023, September 7). *How we chanced upon what may be the world's largest white hydrogen deposit*. The Conversation. http://theconversation.com/how-we-chanced-upon-what-may-be-the-worlds-largest-white-hydrogen-deposit-212499

Prinzhofer, A., Tahara Cissé, C. S., & Diallo, A. B. (2018). Discovery of a large accumulation of natural hydrogen in Bourakebougou (Mali). *International Journal of Hydrogen Energy*, *43*(42), 19315–19326. https://doi.org/10.1016/j.ijhydene.2018.08.193

Ramsden, T., Ruth, M., Diakov, V., Laffen, M., & Timbario, T. A. (2013). *Hydrogen Pathways: Updated Cost, Well-to-Wheels Energy Use, and Emissions for the Current Technology Status of Ten Hydrogen Production, Delivery, and Distribution Scenarios* (NREL/TP-6A10-60528, 1107463; p. NREL/TP-6A10-60528, 1107463). https://doi.org/10.2172/1107463

Sand, M., Skeie, R. B., Sandstad, M., Krishnan, S., Myhre, G., Bryant, H., Derwent, R., Hauglustaine, D., Paulot, F., Prather, M., & Stevenson, D. (2023). A multi-model assessment of the Global Warming Potential of hydrogen. *Communications Earth & Environment*, *4*(1), Article 1. https://doi.org/10.1038/s43247-023-00857-8

The white gold rush and the pursuit of natural hydrogen. (2024, March 12). [Press Release].

Rystad Energy. https://www.rystadenergy.com/news/white-gold-rush-pursuit-natural-hydrogen

Towler, G., & Sinnott, R. (Eds.). (2022). Chemical Engineering Design (Third Edition). In *Chemical Engineering Design (Third Edition)* (p. i). Butterworth-Heinemann. https://doi.org/10.1016/B978-0-12-821179-3.01001-3

Trends in U.S. Oil and Natural Gas Upstream Costs. (2016). U.S. Energy Information Administration.

Truche, L., & Bazarkina, E. F. (2019). Natural hydrogen the fuel of the 21 st century. *E3S Web of Conferences*, *98*, 03006. https://doi.org/10.1051/e3sconf/20199803006

Truche, L., Donzé, F.-V., Goskolli, E., Muceku, B., Loisy, C., Monnin, C., Dutoit, H., & Cerepi, A. (2024). A deep reservoir for hydrogen drives intense degassing in the Bulqizë ophiolite. *Science*, *383*(6683), 618–621. https://doi.org/10.1126/science.adk9099

United Nations Framework Convention on Climate Change. Paris Agreement. Article 2(a). (2015). https://unfccc.int/process-and-meetings/the-paris-agreement/the-paris-agreement

U.S. Department of Energy Clean Hydrogen Production Standard (CHPS) Guidance. (n.d.).

US EPA, O. (n.d.). *The Social Cost of Carbon* [Reports and Assessments]. Retrieved August 8, 2024, from https://19january2017snapshot.epa.gov/climatechange/social-cost-carbon

U.S. National Clean Hydrogen Strategy and Roadmap. (2023).

Vyawahare, P., Ng, C., & Elgowainy, A. (2023, October). *Hydrogen Production from Methane Pyrolysis*. Argonne National Laboratory. https://greet.anl.gov/publication-methane_pyrolysis

Warwick, N., Griffiths, P., Archibald, A., & Pyle, J. (2022). *Atmospheric implications of increased hydrogen use*.

World Energy Outlook 2023. (2023).

Yedinak, E. M. (2022). The Curious Case of Geologic Hydrogen: Assessing its Potential as a Near-Term Clean Energy Source. *Joule*, *6*(3), 503–508. https://doi.org/10.1016/j.joule.2022.01.005

Zgonnik, V. (2020). The occurrence and geoscience of natural hydrogen: A comprehensive review. *Earth-Science Reviews*, *203*, 103140. https://doi.org/10.1016/j.earscirev.2020.103140

Zhang, M., & Li, Y. (2024). The role of geophysics in geologic hydrogen resources. *Journal of Geophysics and Engineering*, gxae056. https://doi.org/10.1093/jge/gxae056

Appendix A: Replicated and Extended OPGEE Model

The replicated and extended model has been developed using open-source Python coding packages and presented in a Jupyter notebook format. A Jupyter notebook was chosen for the following reasons:

- It is open-source, extending the accessibility of the original OPGEE model
- It allows the inclusion of rich text explanatory notes via markdown language cells. These cells facilitate the interpretation of the code by third parties.
- The markdown list numbering schematic also forms a convenient means of navigating the notebook via hyperlinks in supported Integrated Development Environments (e.g. Visual Studio Code).
- The ability to execute individual cells within the notebook in isolation (rather than running a full script) facilitated rapid iterations during model development.

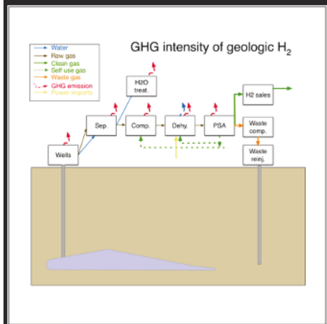
For the sake of limiting the length of this thesis document, a full copy of the notebook has been omitted from this appendix. Rather, the code has been developed via a GitHub repository, preserved via the Zenodo platform. This repository can be accessed via the link below. The screenshots below show several of the early cells of the notebook and provide a sense of its structure.

https://zenodo.org/doi/10.5281/zenodo.13270812

Background / Introduction

This notebook intends to replicate the Lifecycle Assessment (LCA) of geologic hydrogen produced by Brandt (2023) in order to perform a review of its methods and assumptions, as well as the conclusions published in the associated paper.

The Brandt paper considers a comprehensive range of potential emissions sources throughout the whole 'well pad' process, from the wellhead to the 'gate', including emissions embodied in the efforts required to discover the resource and produce/install the associated equipment. The paper displays the process in the following block diagram:



This notebook also builds on top of Brandt's work in three ways. First, it incorporates assessments of sensitivity to uncertainty regarding key assumptions. Second, it estimates costs of development, aligned with the scenarios assessed in the LCA portion. Third, it estimates the value of the Production Tax Credits (PTC) that may be associated with each of the scenarios, under the United States' current PTC regime. Finally, it estimates the prices that a producer of geologic hydrogen would need to realise in order for a geologic hydrogen to be considered an attractive investment.

Import Python Packages

```python
# Capture the start time, for the purpose of measuring the time taken to run the script
import time
start_time = time.time()
```

✓ 0.0s Python

Input Data Specific to Geologic H2

The following section establishes input data specific to the estimation of emissions from production of geologic hydrogen.

Key assumptions are:

- Well pressure calculated as depth (in ft) by a factor 0.42
- Initial Baseline raw gas rate is given (23,100 MSCFD) and declines at a manually-defined rate.
- Low pressure case is assumed to be 75% of baseline
- High pressure case is assumed to be 125% of baseline
- "High productivity" wellhead pressure is assumed to be 200% of baseline
- "Deep" and "Shallow" pressures are calculated based on assumed depths of 12,000 and 1,500 ft, respectively.

Constants/Assumptions for Calculations

```python
well_productivity_default = 1.3333 #BCF/well. Default assumption in Brandt's analysis

GWP_H2_default = 5 #Global Warming Potential of H2, relative to CO2, to enable CO2e calculations. From Brandt OPGEE file: "Low value from Derwent et al. 2020, of 5.0. High
GWP_CH4 = 25 #Global Warming Potential of methane. 100-year basis, IPCC 2007 AR4, per Brandt OPGEE file.

LHV_H2 = 113.958057395143 #mmbtu/tonne. Lower Heating Value of hydrogen. OPGEE source listed as Mechanical engineer's handbook - Energy & Power (3rd edition). John Wiley &
LHV_CH4 = 47.5055187637969 #mmbtu/tonne. Lower Heating Value of methane.

number_well_workovers = 4 # Number of well workovers per well, over the lifetime of the well. Default assumption in OPGEE model.

#LHV Energy Densities for gases:
# OPGEE states as the source: Mechanical engineer's handbook - Energy & Power (3rd edition). John Wiley & Sons. Chapter 17: Gaseous Fuels, Table 2
LHV_data = {
    'Gas': ['N2', 'O2', 'CO2', 'H2O', 'CH4', 'C2H6', 'C3H8', 'C4H10', 'CO', 'H2', 'H2S', 'SO2'],
    'LHV (MJ/kg)': [
        0.0000000000,  # LHV for N2, Ar
        0.0000000000,  # LHV for O2
        0.0000000000,  # LHV for CO2
        0.0000000000,  # LHV for H2O
        50.1206975717,  # LHV for CH4
        47.5867143488,  # LHV for C2H6
        46.4501483444,  # LHV for C3H8
        45.8352847682,  # LHV for C4H10
        10.1242877483,  # LHV for CO
        120.2314484547,  # LHV for H2
        15.2434928256,  # LHV for H2S
        0.0000000000   # LHV for SO2
    ]
}
```

```python
# Create the DataFrame
LHV_density_gases_metric = pd.DataFrame(LHV_data)
# Set 'Gas' as the index instead of a column
LHV_density_gases_metric.set_index('Gas', inplace=True)

# Molecular weights of gases:
# Taken directly from OPGEE
MW_data = {
    'Gas': ['N2', 'O2', 'CO2', 'H2O', 'CH4', 'C2H6', 'C3H8', 'C4H10', 'CO', 'H2', 'H2S', 'SO2'],
    'Molecular Weight (g/mol)': [
        28.0134,  # Molecular weight of N2
        31.9988,  # Molecular weight of O2
        44.0095,  # Molecular weight of CO2
        18.0153,  # Molecular weight of H2O
        16.0425,  # Molecular weight of CH4
        30.0690,  # Molecular weight of C2H6
        44.0956,  # Molecular weight of C3H8
        58.1222,  # Molecular weight of C4H10
        28.0101,  # Molecular weight of CO
        2.01588,  # Molecular weight of H2
        34.0809,  # Molecular weight of H2S
        64.0638   # Molecular weight of SO2
    ]
}
# Create the DataFrame
molecular_weights_gases = pd.DataFrame(MW_data)
# Set 'Gas' as the index instead of a column
molecular_weights_gases.set_index('Gas', inplace=True)

# Constants required to calculate psuedo-critical properties of gas mixtures:
# Taken directly from OPGEE
pseudo_crit_data = {
    'Gas': ['N2', 'O2', 'CO2', 'H2O', 'CH4', 'C2H6', 'C3H8', 'C4H10', 'CO', 'H2', 'H2S', 'SO2'], # N2 is actually "N2 / Ar"
    'Tc_Pc': [0.461366863, 0.380013661, 0.511577965, 0.363255567, 0.515156062, 0.778343949, 1.081331169, 1.390483109, 0.471270936, 0.317056323, 0.517230769, 0.678388792],
    'sqrt_Tc_Pc': [0.679239915, 0.616452481, 0.715246786, 0.602706867, 0.71774373, 0.882238034, 1.039870746, 1.179187478, 0.68649176, 0.563077546, 0.719187576, 0.823643607
    'Tc_Pc_Constant_K': [10.24504569, 10.28145905, 16.74197022, 20.56873505, 13.29861182, 20.68843488, 26.83793382, 32.62750172, 10.61667885, 4.349569036, 18.6490206, 22.9
}
# Create the DataFrame
pseudo_crit_constants = pd.DataFrame(pseudo_crit_data)
# Set 'Gas' as the index instead of a column
pseudo_crit_constants.set_index('Gas', inplace=True)

# Specific heat constants:
# Taken directly from OPGEE, which states: "Source: Heat capacities from EngineeringToolbox.com, accessed Sep 2018"
# Define the data
specific_heat_data = {
    'Gas': ['N2', 'O2', 'CO2', 'H2O', 'CH4', 'C2H6', 'C3H8', 'C4H10', 'CO', 'H2', 'H2S', 'SO2'],
    'Specific heat C_p': [1.04, 0.919, 0.844, 1.97, 2.22, 1.75, 1.67, 1.67, 1.02, 14.32, 1.01, 0.64],
    'Specific heat C_v': [0.793, 0.659, 0.655, 1.5, 1.7, 1.48, 1.48, 1.53, 0.72, 10.16, 0.76, 0.51]
}
# Create the DataFrame
specific_heat_df = pd.DataFrame(specific_heat_data)
# Set 'Gas' as the index instead of a column
specific_heat_df.set_index('Gas', inplace=True)

#Various physical constants:

steel_density = 0.30 #lb/in^3
mmbtu_to_MJ = 1055.05585 #conversion factor
btu_per_MJ = 947.817 #conversion factor
Pounds_per_kg = 2.20462 #conversion factor
mol_per_SCF = 1.1953 # At standard conditions

# Various assumptions regarding gas processing and equipment:

dehy_reflux_ratio = 2.25 #Dehydration reflux ratio. Default assumption in OPGEE model.
dehy_regen_temp = 200 #F. Regeneration temperature for dehydration. Default assumption in OPGEE model.
TEG_water_ratio_dehydrator = 2.00 # gal TEG/lb H2O. Default assumption in OPGEE model.
moisture_outlet_dehydration = 7.00 #lb H2O/mmscf. Default assumption in OPGEE model.
dehy_reboiler_eta = 1.25 # btu consumed per btu delivered

eta_compressor = 0.75 #Compressor efficiency. Default assumption in OPGEE model. For the time being, assume all compressor types have the same efficiency (this is the defa

ng_engine_efficiency_data = { #Data taken from OPGEE model. Based on a linear regression of data from an engine manufacturer. OPGEE states: "Source: Caterpillar technical
    'bhp': [0, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000, 1100, 1200, 1300, 1400, 1500, 1600, 1700, 1800, 1900, 2000, 2100, 2200, 2300, 2400, 2500, 2600, 2700, 28
    'Efficiency btu LHV/bhp-hr': [7922.40, 7862.05, 7801.70, 7741.35, 7681.00, 7620.65, 7560.30, 7499.95, 7439.60, 7379.25, 7318.90, 7258.55, 7198.20, 7137.85, 7077.50, 70
}
ng_engine_efficiency_data_df = pd.DataFrame(ng_engine_efficiency_data)
ng_engine_efficiency_data_df.set_index('bhp', inplace=True)

reciprocating_compressor_ng_emissions_factor = 68193.5860604127 #gCO2eq./mmbtu. OPGEE quoting GREET. This is the emissions factor for reciprocating compressors powered by

#Factors related to drilling calculations:
heavy_duty_truck_diesel_intensity = 969 #btu LHV/ton mi (Paper does not cite source of this figure)
weight_land_survey = 25 #tonnes. Weight of land survey vehicle. Default assumption of OPGEE model.
distance_survey = 10000 #miles. Distance of travel for survey. Default assumption of OPGEE model. "Estimate accounting for long-distance travel of specialized equipment"
emissions_factor_trucks = 78908.518237706 #gCO2eq./mmbtu. OPGEE quoting GREET.
emissions_factor_diesel_exploration = 78823.3589186562 #g GHGs/mmbtu LHV. OPGEE quoting GREET, but using the values for "Barge diesel" rather than "Truck Diesel". It is ur
emissions_factor_diesel_drilling = 78490.5078472298 #g GHGs/mmbtu LHV. OPGEE quoting GREET, but using the values for "Barge diesel" rather than "Truck Diesel". It is uncle

#Pre-production Wells:
number_dry_wells = 1 #Number of dry wells drilled per discovered field.
number_exploration_wells = 3 #Number of exploratory/scientific wells drilled after discovery of the field.
```

```python
diesel_energy_density = 128450 #LHV btu/gal. Source: GREET1_2016, obtained from "Fuel_Specs" worksheet.

#Production Wells:
number_production_wells_default = 50 #Key assumption
#Injection Wells:
number_injection_wells_default = math.ceil(0.25*number_production_wells_default) #Assumption is the number of injection wells is 25% of the number of production wells. Rou
#Total Wells:
total_number_wells_default = number_production_wells_default + number_injection_wells_default
# print(total_number_wells)

#Liquid unloading considerations:
wells_LUnp = 0.068996621 #Fraction of wells with non-plunger liquids unloadings. Default assumption in OPGEE model, "from US EPA (2020) Greenhouse Gas Inventory, based on
wells_LUp = 0.1 #Fraction of wells with plunger liquids unloadings

PSA_unit_slippage_rate_default = 0.1 #Brandt assumes that the PSA unit only separates 90% of the H2 from the gas stream.

drilling_fuel_per_foot_vertical = 0.325964356060972 #gal diesel fuel/ft. This figure taken direct from OPGEE model and assumes Moderate complexity wells drilled at Medium

steel_emissions_intensity = 2747.8545357015 / 2.204 #gCO2/lb. This is the emissions intensity of steel production, as calculated in the OPGEE model. Conversion factor of 2

cement_emissions_intensity = 36587.7935725105 #gCO2/ft^3. This is the emissions intensity of cement production, as calculated in the OPGEE model.
```

✓ 0.0s Python

Key Variables / Inputs

```python
### Gas Densities. Define a dataframe:

# Define the data as a dictionary
data = {
    'Gas': ['N2','CO2', 'CH4', 'H2','H2O'],
    'Density tonne/MMSCF': [33.480353, 52.605153, 19.1738073, 2.4097248, 21.527353]
}
# Create the DataFrame
gas_densities = pd.DataFrame(data)
# Set 'Gas' as the index instead of a column
gas_densities.set_index('Gas', inplace=True)

#Brandt's OPGEE model assumes all cases produce 0.1 bbl/day of oil. The significance of this assumption will be checked via sensitivity analysis.
oil_production_default = 0.1 #bbl/day
water_production_default = 1 #bbl/mmscf of gas

field_lifespan_default = 30 #years

small_source_emissions_percentage_default = 10 #%

# Set a toggle for inclusion or exclusion of Acid Gas Removal Unit (AGRU) (aka Gas Sweetening Unit) in embodied emissions calculations
AGRU_included = False # NOTE: If this is set to True, then the VFF section should be updated to include losses from the AGRU. This capability is not implemented in this nc

# Assumptions for economic analysis:

inflation_rate_default = 0.03 # Assumed 3% rate of long term inflation.
discount_rate_default = 0.10 # Assumed 10% rate of discount (Weighted Average Cost of Capital) for economic analysis.
```

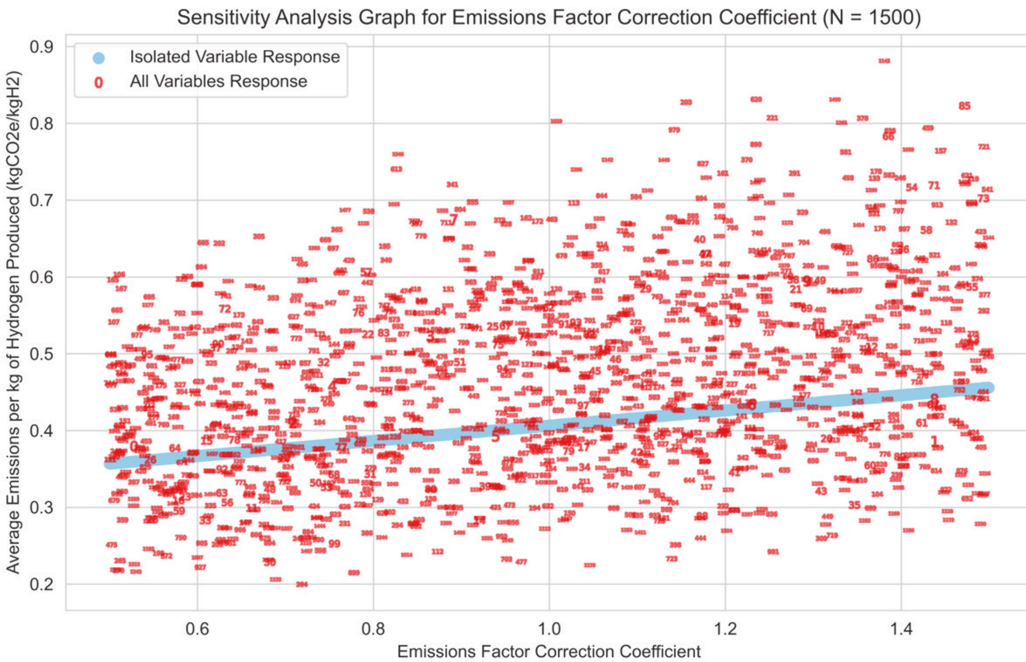
✓ 0.0s Python

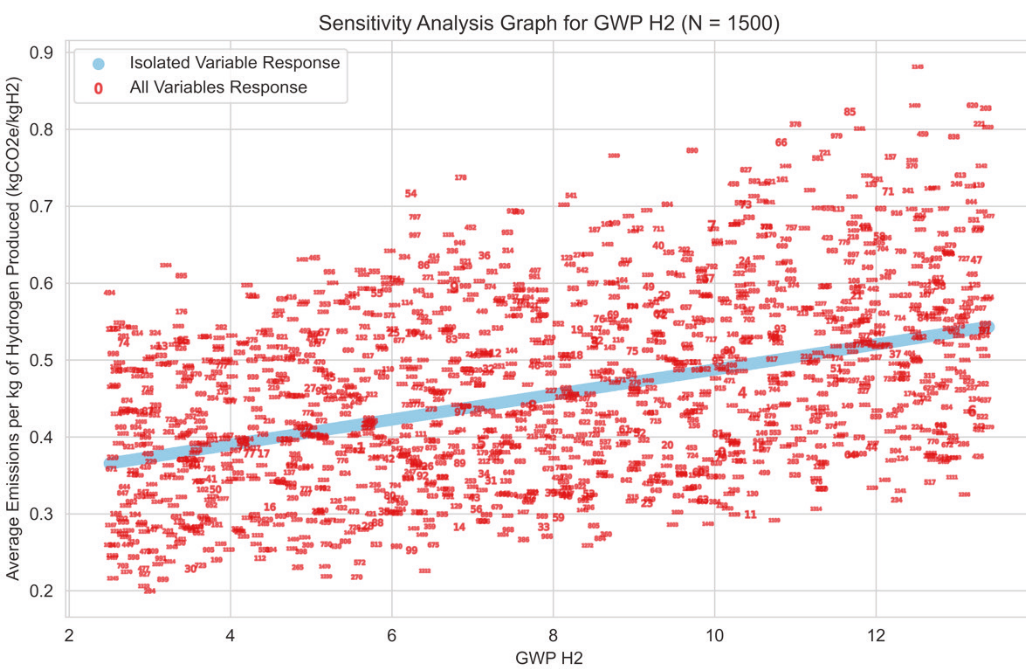
Define/Assume Reservoir Conditions for Analysis

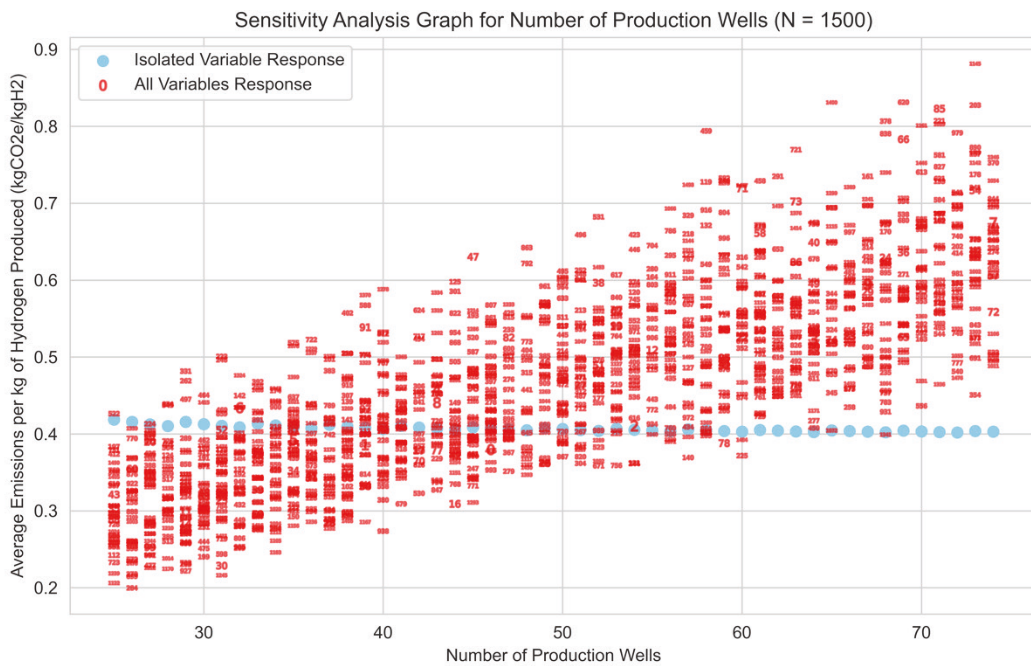
```python
# Data for the Reservoir Conditions DataFrame
# These are all the cases set out in the Brandt paper and the associated supplementary data OPGEE model excel file.



# Data for the Gas Composition DataFrame
gas_composition_data = {
    'Case': ['Baseline', 'Low Productivity', 'High Productivity', 'High CH4', 'Mixed', 'Low H2', 'Low H2 w/ CH4', 'Low H2 w/ N2', 'High H2', 'Deep', 'Shallow', 'Exponentia
    'H2': [85.0, 85.0, 85.0, 85.0, 85.0, 75.0, 75.0, 75.0, 95.0, 85.0, 85.0, 85.0],
    'N2': [12.0, 12.0, 12.0, 1.5, 8.5, 20.0, 0.0, 22.5, 4.0, 12.0, 12.0, 12.0],
    'CH4': [1.5, 1.5, 1.5, 12.0, 5.0, 2.5, 22.5, 0.0, 0.5, 1.5, 1.5, 1.5],
    'C2+': [0.0] * 12,
    'CO2': [0.0] * 12,
    'Ar/oth inert': [1.5, 1.5, 1.5, 1.5, 1.5, 2.5, 2.5, 2.5, 0.5, 1.5, 1.5, 1.5]
}
gas_composition_df = pd.DataFrame(gas_composition_data)
gas_composition_df.set_index('Case', inplace=True)

cases = gas_composition_df.index

def generate_reservoir_data(sensitivity_variables=None):

    if sensitivity_variables:
        well_productivity = sensitivity_variables.get('Well Productivity (BCF/well EUR)', well_productivity_default)
        number_production_wells = sensitivity_variables.get('Number of Production Wells', number_production_wells_default)
    else:
        well_productivity = well_productivity_default
        number_production_wells = number_production_wells_default

    nominal_raw_gas_EUR = well_productivity * number_production_wells
```

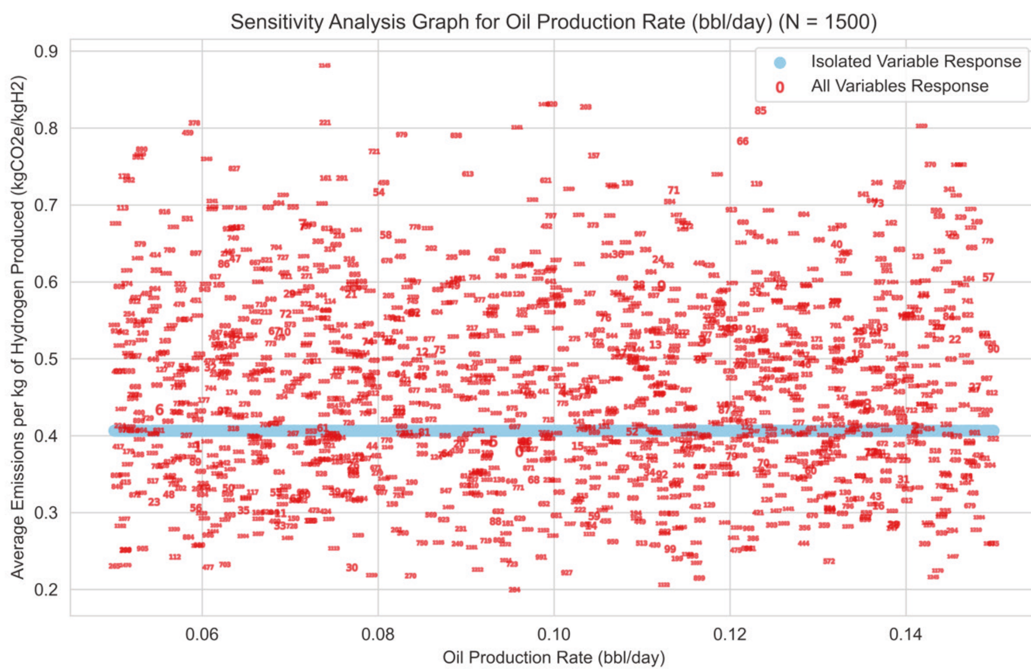
```python
    # #Debugging print statements:
    # print('Well productivity in generate_reservoir_data:', well_productivity)
    # print('number_production_wells in generate_reservoir_data:', number_production_wells)

    reservoir_data = {
        'Case': cases,
        'Depth, ft': [6000, 6000, 6000, 6000, 6000, 6000, 6000, 6000, 6000, 12000, 1500, 6000],
        'Initial Reservoir Pressure, psi': [2520, 2520, 2520, 2520, 2520, 2520, 2520, 2520, 2520, 5040, 630, 2520]
    }

    # Creating the DataFrame & setting 'Case' as the index to make slicing based on Case easier
    reservoir_df = pd.DataFrame(reservoir_data)
    reservoir_df.set_index('Case', inplace=True)

    # Calculate the 'Raw Gas EUR, BCF' for each case
    raw_gas_EUR_values = [
        nominal_raw_gas_EUR, nominal_raw_gas_EUR * 0.5, nominal_raw_gas_EUR * 2, nominal_raw_gas_EUR,
        nominal_raw_gas_EUR, nominal_raw_gas_EUR * 0.5, nominal_raw_gas_EUR, nominal_raw_gas_EUR,
        nominal_raw_gas_EUR, nominal_raw_gas_EUR, nominal_raw_gas_EUR * 0.5, nominal_raw_gas_EUR
    ]

    # Ensure 'raw_gas_EUR_values' is a valid list of floats
    reservoir_df['Raw Gas EUR, BCF'] = raw_gas_EUR_values

    # # Debugging: Print to check values
    # print("Raw Gas EUR, BCF values:")
    # print(reservoir_df['Raw Gas EUR, BCF'])

    # Calculate the 'H2 EUR, BCF' using the gas composition
    h2_EUR_values = reservoir_df['Raw Gas EUR, BCF'] * gas_composition_df['H2'] / 100
    reservoir_df['H2 EUR, BCF'] = h2_EUR_values

    #     # Debugging: Print to check values
    # print("H2 EUR, BCF values:")
    # print(reservoir_df['H2 EUR, BCF'])

    try:
        reservoir_df = reservoir_df.astype({
            'Raw Gas EUR, BCF': float,
            'H2 EUR, BCF': float,
            'Depth, ft': int,
            'Initial Reservoir Pressure, psi': int
        })
    except ValueError as e:
        print("Error converting data types:", e)
        print("DataFrame before conversion:")
        print(reservoir_df)
```

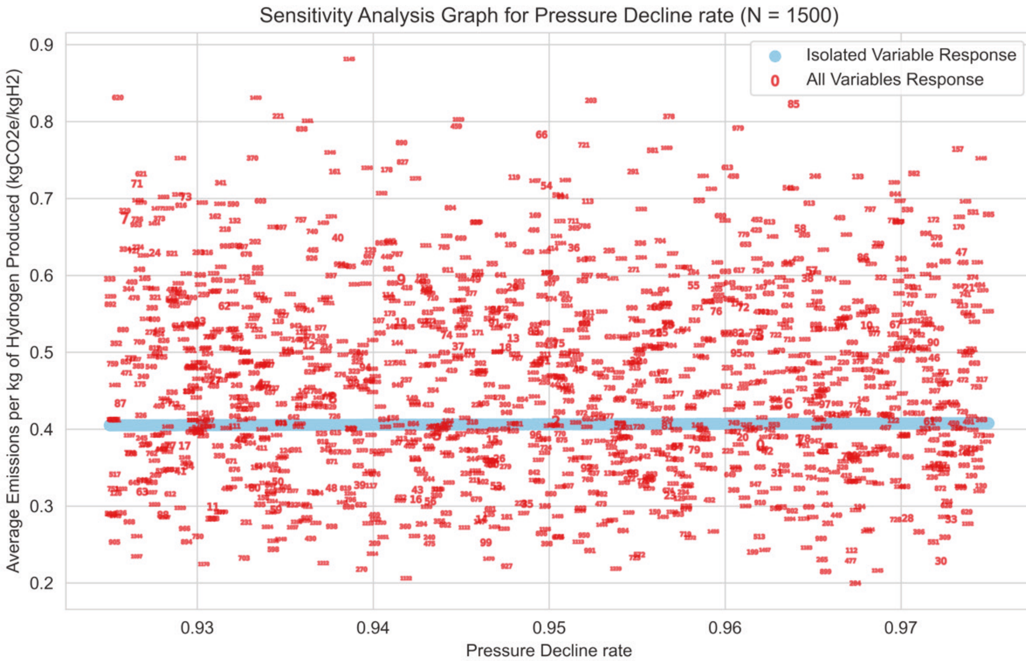
Appendix B: Sensitivity Analysis Graphs

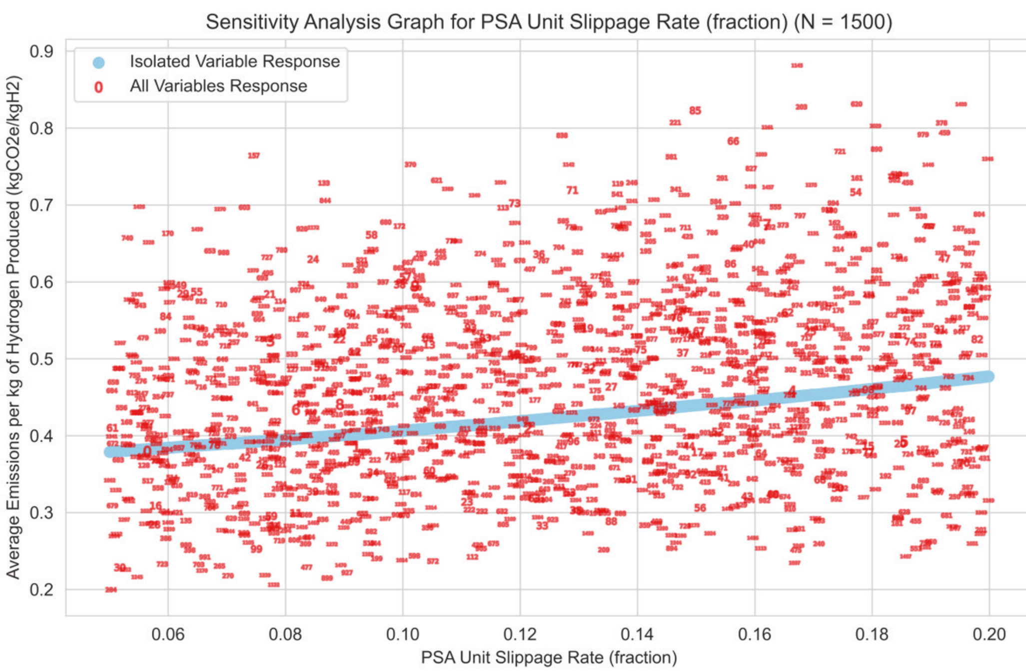


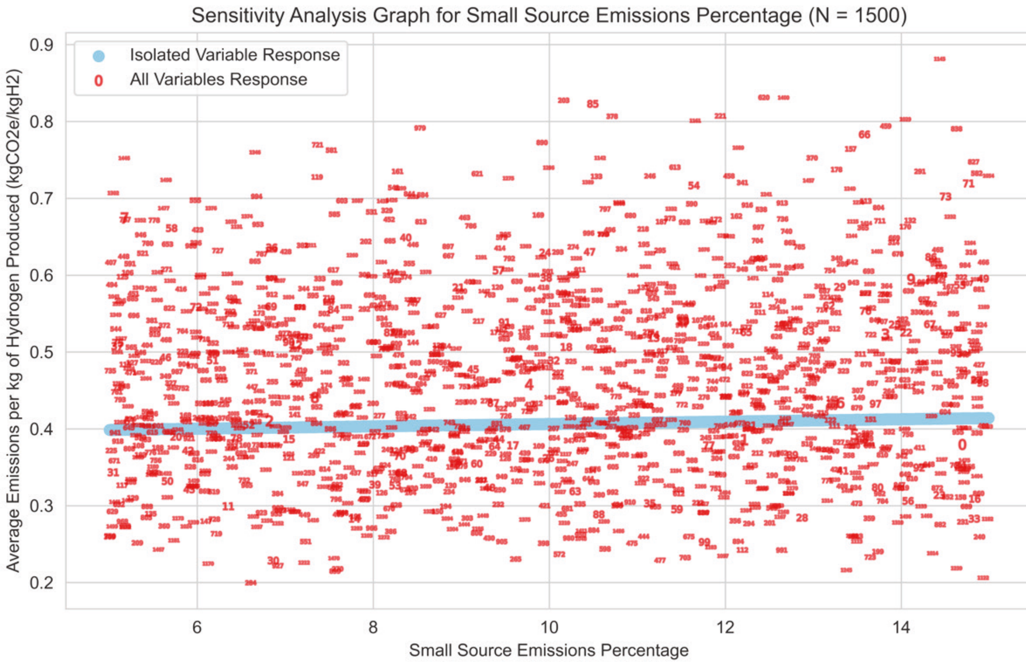


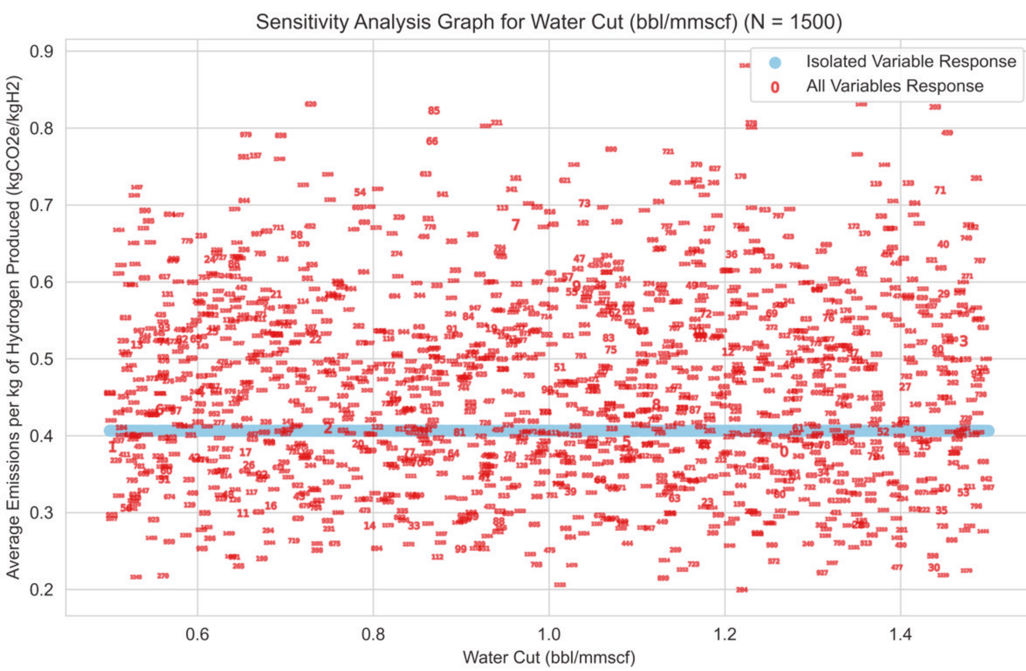

Sensitivity Analysis Graph for Number of Production Wells (N = 1500)
Isolated Variable Response
All Variables Response
Average Emissions per kg of Hydrogen Produced (kgCO2e/kgH2)
Number of Production Wells

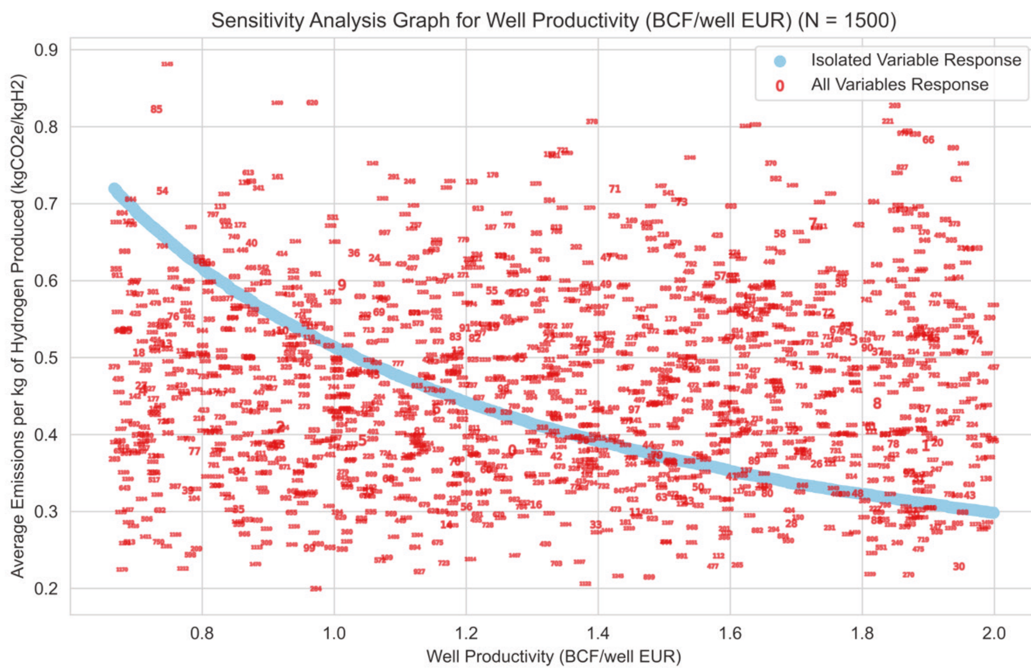

Sensitivity Analysis Graph for Oil Production Rate (bbl/day) (N = 1500)
Isolated Variable Response
All Variables Response
Average Emissions per kg of Hydrogen Produced (kgCO2e/kgH2)
Oil Production Rate (bbl/day)


Sensitivity Analysis Graph for Pressure Decline rate (N = 1500)
Isolated Variable Response
All Variables Response
Average Emissions per kg of Hydrogen Produced (kgCO2e/kgH2)
Pressure Decline rate
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
0.93
0.94
0.95
0.96
0.97


Sensitivity Analysis Graph for PSA Unit Slippage Rate (fraction) (N = 1500)
Isolated Variable Response
All Variables Response
Average Emissions per kg of Hydrogen Produced (kgCO2e/kgH2)
PSA Unit Slippage Rate (fraction)
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
0.06
0.08
0.10
0.12
0.14
0.16
0.18
0.20


Sensitivity Analysis Graph for Small Source Emissions Percentage (N = 1500)
Isolated Variable Response
All Variables Response
Average Emissions per kg of Hydrogen Produced (kgCO2e/kgH2)
Small Source Emissions Percentage


Sensitivity Analysis Graph for Water Cut (bbl/mmscf) (N = 1500)
Isolated Variable Response
All Variables Response
Average Emissions per kg of Hydrogen Produced (kgCO2e/kgH2)
Water Cut (bbl/mmscf)


Sensitivity Analysis Graph for Well Productivity (BCF/well EUR) (N = 1500)
Isolated Variable Response
All Variables Response
Average Emissions per kg of Hydrogen Produced (kgCO2e/kgH2)
Well Productivity (BCF/well EUR)
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
0.8
1.0
1.2
1.4
1.6
1.8
2.0