Integration of Hydrogen Technology into Large Scale Industrial Manufacturing in Ontario

by

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Author's Declaration

This thesis consists of material all of which I authored or co-authored: See Statement of Contributions included in this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

I understand that my thesis may be made electronically available to the public.

Statement of Contributions

Nicholas Preston was the sole author of chapters 1, 2, 5 and 6 which were written under the supervision of Dr. Michael Fowler and Dr. Ali Elkamel and were not written for publication.

This thesis consists in part of two manuscripts written for publication. Exceptions to sole authorship of material are as follows:

Research Presented in Chapter 3

This work was an expansion on a manuscript originally prepared for the 2018 Power-to-Gas Hydrogen Student Design Contest. Development of the optimization model for this work was supported by Dr. Maroufmashat, and Dr. Mukherjee. Data collection, analysis and background literature review were supported by Hassan Riaz, Sami Barbouti, Peter Tang, and Javan Wang, with Ehsan Haghi formalizing the discussion of relevant policy. It was my role to analyze the results of the optimization, perform sensitivity analysis, calculate financials, and format the final manuscript. Dr. Fowler and Dr. Elkamel consulted on the design of the system and reviewed the manuscript.

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Research Presented in Chapter 4:

This work analyzed the application of Hydrogen Enriched Natural Gas at an automotive manufacturer. Dr. Maroufmashat and Dr. Mukherjee consulted on the optimization approach and costing models. Hassan Riaz, Sami Barbouti, Peter Tang and Javan Wang supported the process design of the power-to-gas system and completed the safety and failure mode and effects analysis. I was responsible for performing the background analysis, developing and refining the optimization, performing technology screening, creating pricing models for individual components, and preparing the final manuscript. Dr. Fowler and Dr. Elkamel consulted on the design of the system and reviewed the final manuscript.

Preston, N.; Maroufmashat, A.; Riaz, H.; Barbouti, S.; Mukherjee, U.; Tang, P.; Wang, J.; Elkamel, A.; Fowler, M. An Economic, Environmental and Safety Analysis of Using Hydrogen Enriched Natural Gas (HENG) in Industrial Facilities. Energies 2021, 14, 2445. https:// doi.org/10.3390/en14092445

Abstract

Power-to-Gas is particularly applicable in Ontario's energy market, due to the abundance of curtailed renewable energy. During off peak hours this results in not only low carbon, but low-cost electricity making hydrogen generation a highly profitable and environmentally friendly venture. Despite the benefits listed above, there has yet to be a full-scale adoption of Power-to-Gas technology both globally and in the local market. This eliminate this hesitation there is a requirement for diverse, profitable proof of concept installations and a public uncertainty regarding the inherent safety of the technology. It is the objective of this thesis to address these concerns by demonstrating the versatility of hydrogen in different energy system configurations, to show how layered revenue streams can produce profits in the face of policy uncertainty and by outlining the risks and control methods available to mitigate the safety concerns associated with Hydrogen.

The first paper presented in this thesis will address the question of whether a business case with strong financial returns is possible for a finished goods manufacture. Here we demonstrate the potential to capitalize on multiple revenue streams under a single investment and highlight some of the ancillary assets including reduction in air pollution and balance of the electrical grid. This design was developed for an automotive manufacturer requiring a total capital investment of $2,620,448 and resulting in a payback period of 2.8 years. Based on a sensitivity analysis, the annual revenue for selling hydrogen at $1.5 to $12 per kgH2 can sum to $54,741 to $437,928. In the modelled carbon tax program, CO2 allowances can be sold at $18 to $30 per tonne CO_2 and the model predicts a CO2 offset of 2359.7 tonnes.

The second paper develops a case study that further expands on the use of a single pathway, the is the use of hydrogen enriched natural gas. This paper analyzes the integration of an electrolyzer unit into a manufacturer's CHP microgrid and both explores the impact a carbon tax has on its feasibility and carries out a failure mode and effects analysis to highlight the safe nature of the technology. Currently realizable capital incentives can see IRRs as high as 13.76% with net present values of approximately $750,000. To realize financial feasibility, the carbon price in Ontario must achieve or exceed a minimum of 60$/ton CO_{2e}. In all economically feasible, cases the system operating under an optimal storage coefficient and operational limit produced an emission offset greater than 3000-ton CO_2 per year.

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1.0 Introduction

There is an increasing international pressure to reduce carbon emissions and in 2019 the Canadian Federal Government responded to this by mandating a $20 per tonne CO_{2eq} carbon tax in all Provinces. That number will increase to $170 per tonne CO_{2eq} by 2030 which means large polluters, such as industrial manufacturers need to decarbonize their processes to maintain competitive in a global market [1]. As part of their built in Ontario action plan that province has mandated a 30% reduction in the industrial manufacturing sector, half of which is assigned to more stringent industry performance standards and the other half to general innovation [2]. Already, major Ontario manufacturers have set aggressive reduction targets that will require either significant modifications to existing processes, or decarbonization of their localized energy hub. As part of this there has been a significant push in recent years towards widespread adoption of clean hydrogen technology, which was most recently exemplified by the development of Ontario's Low-Carbon Hydrogen Strategy discussion paper [3]. This document seeks public consultation on a made-in-Ontario plan to roll out the development of hydrogen infrastructure.

Hydrogen is a diverse energy vector with multiple potential end use applications. While the consumption of hydrogen in end use applications often results in zero emissions, to capitalize on its full potential for decarbonization it must also be produced by green technology. One of the most promising methodologies for this is the application of Power-to-Gas technology. Power-to-Gas is an energy storage concept that involves taking low cost, renewable rich electricity and using it to electrolyze water into its subsequent components, hydrogen, and oxygen. The products of this process in turn generate multiple revenue streams that can be layered to produce highly profitable business cases even with a lower taxation rate on carbon. Such revenue streams include the use of hydrogen in fuel cells for transportation, the blending of hydrogen with natural gas, the direct sale of oxygen and hydrogen for industrial applications and the storage of hydrogen for re-electrification.

Power-to-Gas is particularly applicable in Ontario's energy market, due to the abundance of curtailed renewable energy. During off peak hours this results in not only low carbon, but low-cost electricity making hydrogen generation a highly profitable and environmentally friendly venture. Furthermore, for industrial manufacturers that are labeled as class A consumers under the Province's Global Adjustment program, the percent contribution to the total energy consumption during a year's 5 peak days correlates directly to the percentage of the province's total global adjustment paid [4]. The flexibility to store hydrogen at off peak times and reuse it during these days can lead to significant savings and has key advantages over alternative storage methods, including energy density, footprint, and storage duration.

Despite the benefits listed above, there has yet to be a full-scale adoption of Power-to-Gas technology both globally and in the local market. While installations do exist, for example Enbridge Gas's Markham facility and Canadian Tire's Bolton distribution center, given its attractive environmental and financial returns the uptake has been relatively slow compared to other energy storage alternatives. The two previous examples are targeting the utility and distribution sectors and while these are incredibly promising installations, they account for a niche portion of the province's industry. In this paper we will focus in on the provinces' manufacturing sector which accounts for 11.98% of the GDP (second only to Real estate) and 30% of total carbon emissions [5]. This hesitation is founded primarily in a lack of diverse, profitable proof of concept installations and a public uncertainty regarding the inherent safety of the technology. It is the objective of this thesis to address these concerns by demonstrating the versatility of hydrogen in different energy system configurations, to show how layered revenue streams can produce profits in the face of policy uncertainty and by outlining the risks and control methods available to mitigate the safety concerns associated with Hydrogen.

1.1 Layered Analysis of Multiple Revenue Streams at a Southern Ontario Automotive Manufacturer

The first paper presented in this thesis will address the question of whether a business case with strong financial returns is possible for a finished goods manufacture. Here we demonstrate the potential to capitalize on multiple revenue streams under a single investment and highlight some of the ancillary assets including reduction in air pollution and balance of the electrical grid, as well as begin to identify some of the policy concerns related to efficacy.

This work applies a mixed integer linear programming model developed in GAMS to simulate the integration of Power-to-Gas infrastructure into an industrial manufacturer's energy system subject to the existing thermal and electrical energy demands, as well as a third hydrogen energy profile. This work is novel in that it assesses the challenges and economic incentives available to make feasible the installation of a hydrogen-based energy storage systems within the Province of Ontario from a techno-economic, policy and environmental perspective.

The energy hub analyzed in this work uses electricity from the power grid and solar panels to meet the manufacturer's demands, while converting the excess to hydrogen gas, which is used across an array of pathways to generate revenue. This includes a blend of hydrogen for fuel cell vehicles (FCVs), hydrogen for forklifts, and the direct injection of hydrogen into the facility's natural gas, adding renewable content to the heating, and manufacturing processes. Our primary objective was to implement a safe design that minimizes capital and operating costs, resulting in a favorable business case for producing hydrogen, and providing ancillary grid services. However, Power-to-Gas creates a net-emission reduction that can be used not only to sell emission allowances in the provincial carbon tax program for up to \$30/t-CO_{2eq} but to assist the Company in achieving their strategic emission reduction targets.

1.2 Profit Sensitivity to Policy Condition and Technological Safety Analysis

The second paper develops a case study that further expands on the use of a single pathway, the is the use of hydrogen enriched natural gas. This paper analyzes the integration of an electrolyzer unit into a manufacturer's CHP microgrid and both explores the impact a carbon tax has on its feasibility and carries out a failure mode and effects analysis to highlight the safe nature of the technology.

The enrichment of natural gas with hydrogen has been identified as a promising pathway for power-to-gas with the potential to reduce emissions while achieving feasible return on investment. The evolving regulatory market in the province of Ontario motivates the analysis of business cases for hydrogen on the industrial microgrid scale. This paper aims to investigate the financial and environmental returns associated with producing and storing electrolytic hydrogen for injection into the natural gas feed of a manufacturer's combined heat and power plants (CHPs). A mathematical methodology was developed for investigating the optimal operation of the integrated system (power-to-gas along with the current system) by considering hydrogen-enriched natural gas. The result of this simulation is an operation plan that delivers optimal economics and an estimate of greenhouse gas emissions. The simulation was implemented across an entire year for each combination of generation price limit and storage coefficient. Because the provincial grid imposes a lesser carbon footprint than that of a pure natural gas turbine, any offset of natural gas by hydrogen reduces the carbon intensity of the system. From an environmental perspective, the amount of carbon abated by the model fell within a range of 3000-ton CO_2/year. From a policy perspective, this suggests that a minimum feasible carbon price of \$60/ton CO_{2e} must be set by applicable regulatory bodies. Lastly, a Failure Modes and Effects Analysis was performed for the proposed system to validate the safety of the design.

2.0 Background & Literature Review

It is becoming very clear that hydrogen technology will play a major role in our integrated energy systems in the years to come. In May 2021 the International Energy Agency (IEA) released a roadmap for achieving Net Zero Carbon Emissions by 2050 which recommended increasing worldwide hydrogen investment from $1B to $40B by 2030 [6]. They cite that hydrogen fuel combined with some carbon capture can eliminate more than half of all heavy industry, including manufacturing's carbon output. Currently in relation to industries that rely on Hydrogen, such as refineries, and chemical producers, end-use manufacturing is negligible. However, the demand is anticipated to increase to over 5% of market share or nearly 40MT by 2050 [6].

Over that same time period the share of net renewable electricity generation is project to rise to 53% and the amount curtailed by 32%. With a projected requirement for 60% of hydrogen to be generated by electrolysis this suggests that self-generation is likely an attractive venture [6]. In general Power-to-gas is seen as one of the most promising storage options because of its sheer capacity, storage duration, density, portability, and cost. However, a global survey conducted by Thema et. al. showed only 153 existing, ongoing or future Power-to-Gas installations between 1993 and 2050 which is further corroborated by Patel S. that lists only 143 active sites [7,8]. Of these, 7 were Canadian based with 1 within the manufacturing sector. While several case studies of European pilots have been conducted it is important to develop sounds business cases within the local market to act as a demonstration of the fundamental soundness of the technology.

In 2020 Walker, S. et al. attempted to identify the most promising pathways for Power-to-Gas technology by applying multiple criteria decision analysis via the fuzzy analytic hierarchy process [9]. In essence key criteria important to the success of each Power-to-X technology were identified including technology prevalence, emission reduction and capital cost. These criteria were then assigned a specific weight through stochastic methods and expert opinion that indicates the relative impact on efficacy. Each technology was ranked accordingly to each criteria and the best pathway for future investment was determined. As the importance of profit and emission reduction was varied Power to gas to mobility and power to gas to power were shown as the most viable. This empowers our work to choose viable pathways but provides the opportunity to identify which methods can best be coupled to achieve the highest return.

Furthermore, Maroufmashat et. al. takes a more qualitative approach to highlight the key technologies, benefits and disadvantages of the market ready power-to-X pathways [10]. In their work they identify a significant positive trend in the general efficiency for all hydrogen technologies indicating that the payback will continue to grow. They also indicate the criticality that power-to-gas has over other energy storage technologies since the shift away from conventional carbon intense baseline generation methods, such as natural gas, will likely take place in phases over multiple years. Natural gas bridges the gap in Ontario's supply between intermittent renewables which are difficult to match supply with demand and the core nuclear power production and constitutes over 30% of the province's production. Because of its low cost and abundant supply Maroufmashat states that it will play a critical role at least in the medium term, however Power-to-gas provides an immediate pathway to start reducing the carbon content of that specific energy vector. Recently Enbridge gas has demonstrated its effectiveness with an $5.2M utility scale hydrogen production and storage facility in Markham.

Al-Zakwani et al. further expanded on their work by attempting to quantify the optimal distribution of hydrogen technologies across four of the most promising pathways, including Power to transportation, industrial use, enrichment of natural gas and methanation [11]. This study looks at the broader Provincial scale to first identify the production available from the surplus baseload and then proceeds to analyze 5 individual scenarios, which include a distribution across all pathways based on Ontario's Long-Term Energy Plans as well as 100% allocation to each of the aforementioned pathways.

In this study they develop a correlation between a fixed capital cost for a Power-to-Gas installation based on studies that relate dollar value to capacity and utilize a correlation factor to determine operational expenditure. This methodology will be further expanded on in the second paper presented in this work by corroborating a number of similar type models. They then assume the revenue earned from the sale of hydrogen to be fixed based on a predicted value for each end use. This is different from our work, since we know the manufacturer's exact expenses, we can determine the precise monetary gain from each hydrogen revenue stream.

They then analyzed three potential scenarios based on the province's electricity price, considering operation of the system in the bottom 67%, 80% and 96% of the price range to be fixed as the potential production amount. The result shows that as a stand-alone pathway, hydrogen for transportation is the most profitable in terms of simple payback and internal rate of return. They also note that there are diminishing returns once the decision is made to allocate the full production amount to a single pathway due to the necessary development of infrastructure. We will attempt to challenge the results of this study on the scale of a single energy hub. By utilizing a single system to provide multiple pathways one avoids the significant capital cost associated with providing hydrogen un dissimilar industries. Furthermore, we will attempt to generate effective models through mixed integer linear programming and constraint programming to determine exactly when it is profitable to purchase electricity for generation purposes versus fixing the buy condition.

Mukherjee et al. take a much more stochastic approach for modeling the profitability and payback of various pathways [12]. Instead of considering fixed variables such as hourly energy price, grid emission factors, hydrogen demand and curtailed amounts they develop probability distribution curves for each of these and analyze a layered combination of power to transportation, natural gas enrichment and energy arbitrage. Utilizing the EasyFIT XL software they determine parameters for a log-logistic distribution to model the changing energy price in each of the four seasons by correlating 10 years of historical data. They then utilize a model from the National Renewable Energy Laboratory that normalizing refuelling activity throughout a 24-hour period, this is then multiplied by expected daily demand based on 3 potential scenarios to form a sensitivity analysis around hydrogen demand.

Then applying a mixed integer linear programming model, they analyze 5 scenarios based on projected demand and energy price to optimize potential payback. The results show the value of the stochastic solution as the difference between the expected result utilizing a deterministic solution and the recourse problem solution which comes from the two-stage stochastic approach as an almost 15% economic benefit. Their model suggests that a levelized cost of $3.145 per kilogram of hydrogen is attainable which is not only equivalent to a $0.86 per liter gasoline price, but also shows that a near 3-year payback is achievable. On a side note, separate article written in The Businesswire identified that future advancements in hydrogen technology could see $1.5/kilogram by 2030 [13]. We attempt to further expand on these results in our model by applying a similar methodology that incorporates a stochastic approach to not only predicting hourly electricity price, but the manufacturer’s demand for other utilities such as heating and cooling.

Furthermore, we can utilize well recorded industrial data to formulate highly accurate models for things such as fuel cell demand and blending rates. We hope to combine strong analysis with strong safety analysis to demonstrate the effectiveness of this technology.

Since hydrogen technology is still maturing, current manufacturing rates have not seen an entire economy of scale. As such high capital costs can extend payback periods into areas that are not economically feasible for companies operating in a competitive marketplace. Since prior articles have shown that energy storage is a necessity for achieving a carbon neutral Ontario it is valuable to analyze how a policy driven pricing mechanism can incentivize Power-to-Gas installations. Furthermore, there are several local market incentives for green technology as well as an increasing federal decarbonization incentive. Mukherjee et. al. analyzes a 2MW hydrogen generation system using a mixed integer nonlinear programming model over 52 weeks of data providing ancillary services, enrichment of natural gas and supplying a local transportation hub of at least 100kg [14]. They incrementally increased the size of the transportation hub to 650 kg per day at which the electrolyzer could no longer keep up. Once they had determined the optimal operating regime of the system, they were able to show that a net present value at a 20-year operating life would be negative except under either a premium pricing structure or through incentivization. In this case they calculated the amortized capital cost under multiple project lifetimes which gave the necessary annual revenue to achieve break even NPV. This amount equates to the incentive necessary to bridge the gap which in summary meant either and 81% increase in demand response incentives, an 83% increase in hydrogen sale price from their benchmark $3.665/kg or a local carbon tax of $27 per tonne. Based on current market conditions of these three options the most feasible option for improving Power-to-Gas payback is carbon taxation. Given that it is currently $40/tCO2e and will increase to $50/tCO2e by April 2022 these numbers are very reasonable. We will further expand on the sensitivity analysis for the manufacturing case study of a hydrogen microgrid. However, in comparison to the work carried out by Mukherjee the technology price will be left fluid and considered as part of the optimization to determine what size system is necessary to achieve optimal payback in an industrial setting.

Al-Subaie, et. al. does perform an analysis of the implementation of Power-to-Gas in an industrial setting via the oil and gas industry [15]. This market sector holds significant potential in the provinces' southwest region due to the direct process requirement for hydrogen gas. Traditionally, hydrogen has been produced for this sector via way of steam methane reforming, which is incredibly carbon intensive. They discuss how the petroleum industry in general is facing pressure from both sides in that the requirement for lower sulphur content in manufactured products requires greater hydrogen consumption, while government policy mandates lower carbon production rates. Furthermore, a federal Clean Fuel Standard has been implemented requiring liquid fuel suppliers to reduce the carbon intensity of their products by 13% by 2030 [16].

They first simulated an oil refinery in Aspen HYSYS given a typical production rate to approximate hydrogen demand. Then, as presented in previous works, a mixed integer linear programming model was used to optimize a 1 MW polymer electrolyte membrane electrolyzer for 5 scenarios varying the carbon content of the hydrogen. The objective function was to minimize the sum of operating expenses, capital associated with storage and compression equipment and the purchase of electricity given input variables of demand, grid carbon content and hourly electricity price.

While they did not present the estimated payback, in summary they showed that under the current regulatory environment steam methane reforming was still the most cost-effective option due to low natural gas prices and was capable of producing hydrogen at $1.1 per kilogram, versus the second lowest rate of $1.8/kg for a 50% mix with electrolytic hydrogen and a $2.5/kg rate for full electrolysis. They did note that the emission reduction however was significant and equated to nearly 35,000 vehicles being taken off the road for implementation at a single production facility. Based on these results it would be valuable to revisit this study in future years given an increased carbon tax, and increased requirement of renewable content compared to the date of initial investigation. Furthermore, this highlights once again the importance of stacking additional revenue streams and the value of this analysis in manufacturing environments.

One pathway that has not yet been discussed but presents an important aspect of Hydrogen's versatility is the opportunity for long duration energy storage. This also sets a precedent for the applications described by the articles contained in this thesis as long-term storage is critical to flexible balancing of low-cost renewable electricity and peak consumption. Dowling et. al. compares hydrogen energy storage of wind and solar generation for periods exceeding 10 hours with conventional renewable to battery systems, a technology which seems to have had a more active uptake in Ontario than Power-to-Gas and make up 88% of new storage projects globally [17]. Battery technology while highly efficient and relatively inexpensive on a power capacity basis, remain pricy when looking at large energy storage. They performed least-cost optimization over 38 years data looking at how specifically battery and power-to-gas integrate to balance weather dependent renewables. In general, they showed that systems containing power-to-gas in conjunction with batteries achieved the lowest system cost of $0.12/kWH which is in comparison to $0.04 /kWh to average grid generation prices. Furthermore, they also demonstrated that the economics of power-to-gas were more than twice as sensitive to changing capital costs when compared to batteries, with the potential for technological advances to bring about $0.07/kWh energy storage.

While most of the discussion to this point has focused on the feasibility and economics of a hydrogen economy and in particular Power-to-Gas, there has been one key component we have yet to discuss and that is safety. A good primer for this discussion is the 2014 suspension of Canadian Tire's Bolton hydrogen project. This was initially reported by The Toronto Star which stated, "A residents' group in Bolton, is outraged over being kept in the dark about the plan, which involved [Hydrogen] a hazardous material." [18] This scenario emphasizes the need for governance of well-established safety regulations, public awareness of associated risk factors and most importantly inherently safe system designs that account for all potential failure modes and effects.

Kurmayer, N. states that in 2021 the European Commission identified clean hydrogen as a critical component in decarbonising heavy industry and achieving 2050 targets and emphasized the requirement for high safety standards to be established [19]. As a result, they tasked the Fuel Cells and Hydrogen Joint Undertaking with establishing an expert panel to both address hydrogen safety policy and disseminate knowledge to the public. As part of that activity, they reviewed 600 significant safety events and utilized that data to establish a list of potential failure methods and countermeasures. In the Canadian market there already exists established legislature to govern in installation of hydrogen systems including the Canadian Hydrogen Installation Code and NFPA 2 Hydrogen Technologies Code. As part of the first paper presented in this thesis, we propose an installation providing Power-to-X pathways at an industrial manufacturer and attempt to apply learning points from these relevant codes to highlight potential safety risks, perform and FMEA and propose countermeasures to mitigate probability and impact.

In many operations hydrogen is already being generated in mass quantities using methane steam reforming, and as a reactant in hydrogenation processes at elevated temperature and pressure. As such there is a mature precedent for implementing hydrogen into industrial settings. An intelligent design first begins with inherently safer design principles and passive mitigation techniques. Conventional chemical industries use hydrogen as a reactant in continuous processes, thus minimizing the amount 'stored' in the pipes significantly (hydrogen is only produced as it is used). This inherently safer design approach is entirely infeasible for the use of hydrogen as an energy storage medium, and thus cannot be applied to the proposed energy storage and distribution systems. This does not mean that inherently safer and passive design principles cannot be applied. In fact, it is crucial to consider the impact that materials of construction and equipment design can have on the likelihood of hydrogen release. Consider that hydrogen-containing equipment under pressure is particularly susceptible to hydrogen embrittlement. This process can proceed through a variety of mechanisms, and affects most common materials of construction (e.g. iron, steel). By selecting materials and design strategies to minimize the risk of equipment failure, the likelihood of release is significantly decreased.

3.0 Layered Analysis of Multiple Revenue Streams at a Southern Ontario Automotive Manufacturer

The following section is based on previously published work "*How can the integration of renewable energy and power-to-gas benefit industrial facilities? From techno-economic, policy, and environmental assessment"* by Preston, et. al. and is reproduced by permission Elsevier. This thesis author's specific contribution to this paper was to: support information gathering and the mathematical development of the model, analyze the output of the model and interpret the results, author, edit and proofread the final material

Keywords:

Power-to-Gas, Hydrogen economy, Operational and design optimization, Solar energy.

3.1 Introduction

This paper details the Second-Place design submitted to the Hydrogen Education Foundation's 2018 Hydrogen Student Design Contest, for which the results were announced at a session of the U.S.A. Department of Energy's (DOE) Annual Merit Review (AMR) in Washington, DC in June 2018. The team was tasked with developing a design for a Power-to-Gas system that uses electricity to produce hydrogen for cross market uses, such as energy storage, ancillary services and transportation fuel. The student team consisted of 5 undergraduate students, 2 graduate students and was mentored by both a post-doctoral fellow and faculty members, all of which are listed as co-authors on this article. The team focused their efforts on developing a practical business case for a large-scale automotive manufacturer, motivated by the idea that showing that the economic and environmental merits of Power-to-Gas are immediately realizable is critical to the development of a Hydrogen Economy.

3.1.1 Significance of Power-to-Gas

Ontario's energy utilities are faced with the challenge of meeting provincial demand while continuing to address the environmental concerns surrounding climate change [20]. With the share of intermittent renewables poised to double by 2032, there is an increasing mismatch between supply and demand, which results in the curtailment and discounted exportation of low carbon electricity [21, 22, 23]. There is a necessity for large-scale energy storage in these transitioning electricity systems and Power-to-Gas is one of the most promising solutions. Already European countries are beginning to realize concrete short-term investment opportunities for industrial and mobility scale Power-to-Hydrogen and Hydrogen-to-End Use technologies with more than 30 projects already in service [24, 25]. In Canada, however, there has been significantly less proactive development of hydrogen infrastructure despite the Federal government seeking to implement a carbon tax and a clean fuels standard, making it difficult for industrial emitters to adopt a business as usual approach and remain profitable [26,27].

Power-to-Gas (P2G) is defined as the process of using electrical energy to convert water into hydrogen that can be stored and later redistributed, generating revenue through multiple pathways. P2G has a higher energy storage density than competing technologies and is suitable for short term and long-term storage. As a result of these unique capabilities, it is set to play a key role in managing the province's energy system as intermittent power sources reach unprecedented levels of overproduction and short-term lows in the electricity price appear more frequently [27,28]. Business cases for Power-to-Gas are becoming realizable at the microgrid scale as industrial emitters seek out ways to improve profitability while managing their carbon footprint [30]. Not only is electrolyzer technology useful for reducing microgrid curtailment and managing off-peak baseload power, but it has the capacity to provide grid stability services such as, demand response, frequency regulation, spinning reserves, and ramping services [31]. Electrolyser operators are also likely to receive partial exemptions from grid fees, taxes and levies, further improving the economics of P2G systems. Furthermore, the versatility of P2G allows access to several profit streams, which can be combined to generate a strong business case for Hydrogen technology. Pathways such as gas grid injection can act as an instrument to de-risk primary applications, such as emission free transport [29].

Wang et al. [34] present the modelling and optimization of a CHP based district heating system incorporating renewable energy production and storage. They were successful in showing the effectiveness of efficient energy dispatch and storage scheduling on the economics of a microgrid system. In particular they demonstrated how a mixed integer linear programming model can be applied to an integrated industrialized microgrid system. However, they were modelling a fixed system of solar thermal generation and storage with design variables fixed. A second source [23] presented the thermal design of a solar hydrogen plant where they were able to identify the necessary design parameters of a solar thermal system to produce clean hydrogen. This work focused more on the technical requirements to initiate thermal water splitting and the sizing required to meet varying demand. They did not however perform any cost and environmental analysis, nor did they present the possible safety and control procedures needed to manage such a design. Garcia Clua et al. [36] optimally sized a grid assisted wind-hydrogen system that implemented electrolysis technology. This took into the account the stochastic nature of renewables to determine the theoretical optimal electrolyzer size given the nominal renewable power. No analysis was performed in regard to financials and emission offset which differs from this work which will identify key financial metrics in system design. Furthermore, their work could be expanded for the case undefined renewable size by incorporating capital costs, electricity costs, hydrogen demand and geographical parameters, all of which are considered in this work when implementing the solar hydrogen system. Anastasiadis et al. [37] investigated the economic and environmental aspects of hydrogen technology within microgrids, where they implement multi-objective optimization to balance both cost and emissions with the presence of renewable technology. For a given case study, they implemented the harmony search algorithm showing a 36% reduction in operating costs with a maximum CO_2 reduction of 300 tonne annually. For a given case study they were able to realize significant reductions in operating cost and greenhouse gas emissions but considered fixed capacities of individual components which differs from this work in that the optimum number and size of components is determined by the model. Lastly, Mukherjee et al. [38] present a holistic assessment of a hydrogen power community incorporating mixed-integer programming to minimize the annual operating costs by selecting the optimal configuration of new hydrogen technologies. While the process simulation and design procedures presented in this paper are similar, this work is novel in that its primary focus is to realize financial and environmental returns for an industrial microgrid. On the other hand, the objective of Mukherjee [30] was simply to provide a community backup power when disconnected from the grid, with the environmental assessment serving only to gain perspective on the opportunity to improve the capital-intensive nature of installing hydrogen technology. Their optimal solution was deemed non-economically feasible from the perspective of a rural community, a result we hope to improve on here.

While significant efforts have been made to model the integration of hybrid renewable energy storage systems into pre-existing microgrid networks [39,40], few demonstrate positive financial and environmental returns when the number of technologies is variable. Even more pressing is the need for these business cases to be developed within a Canadian market which has seen little development of Power-to-Gas. It is also critical to note that because of the inherent risks associated with hydrogen a full enquiry into the safety of any new installation is paramount in validating the design. As such the following milestones have been developed throughout the course of this work:

- Develop a mixed integer linear programming-based model to overlay Power-to-Gas technology in a manner that minimizes annual cost,
- Consult with industry leaders to size and cost market ready, locally available Power-to-Gas equipment in alignment with the results of the model
- Perform capital costing to generate budgetary predictions for the automotive manufacturer and apply the economic and environmental results to predict financial metrics important in determining project feasibility,
- Analyze greenhouse gas emission and urban pollutant offset resulting from the use of hydrogen cars and fuel cell forklifts in industrial energy systems
- And, carry out a policy note regarding the challenges of implementing Power to gas in Ontario.

3.1.2 Problem Definition

In an effort to reduce the impact of anthropocentric climate change, Canada has implemented a Sustainable Development Strategy to decrease CO_2 emissions by 30% (2005 values) [41]. Since Ontario scrapped their previously planned Cap-and-Trade system, the federal carbon pollution pricing system will be implemented [42]. Under this system, it is predicted that carbon prices will range between \$50 per tonne CO_2 emitted and \$140 per tonne CO_2 emitted by 2040 [43]. Further, COP21 has ensured our nation has global accountability [44]. There will continue to be incentives for sustainable businesses and penalties for non-sustainable ones; the only potential uncertainty is their long-term values.

In the face of more stringent government regulations industrial manufacturers are exploring new ways to optimize their own energy systems and capitalize on the use of green energy. One innovative, long-term solution is to introduce Power-to-Gas (P2G) technology which takes inexpensive, curtailed renewable energy and stores it in the form of hydrogen gas for redistribution. To take advantage of this cost saving technology, businesses must implement energy system designs that capture multiple P2G revenue streams and integrate new equipment into the existing infrastructure in a way that optimizes the current energy management strategy [45].

The objective of this work is to develop a strong business case of Power-to-Gas system that utilizes electrical energy to generate hydrogen for multiple market uses. It does so by incorporating and optimizing the operation of a Power-to-Gas energy hub in tandem with existing equipment at an automotive manufacturing plant. An assessment of the economic feasibility and environmental benefits of proposing such a system will be performed. The project only assesses the potential savings available while continuing to meet the facility's existing electrical and heat demand, as well as any future demand for hydrogen from fuel cell vehicles and forklifts.

The flowchart shown in Figure 1 provides a highly simplified, but very useful representation of the manufacturer's energy system, incorporating the proposed key revenue streams for hydrogen technology. It shows the components of the total heat demand of the facility, consisting of the paint booth, the plastics shop and additional facility comfort and process heating. In its current state the plant has no form of renewable energy and meets the demand for electricity by either purchasing it at wholesale prices directly from the grid or by generating it through two natural gas turbines. The entire heat demand of the plant is met through the use of direct burn natural gas boilers or by heat recover steam generation (HRSG).

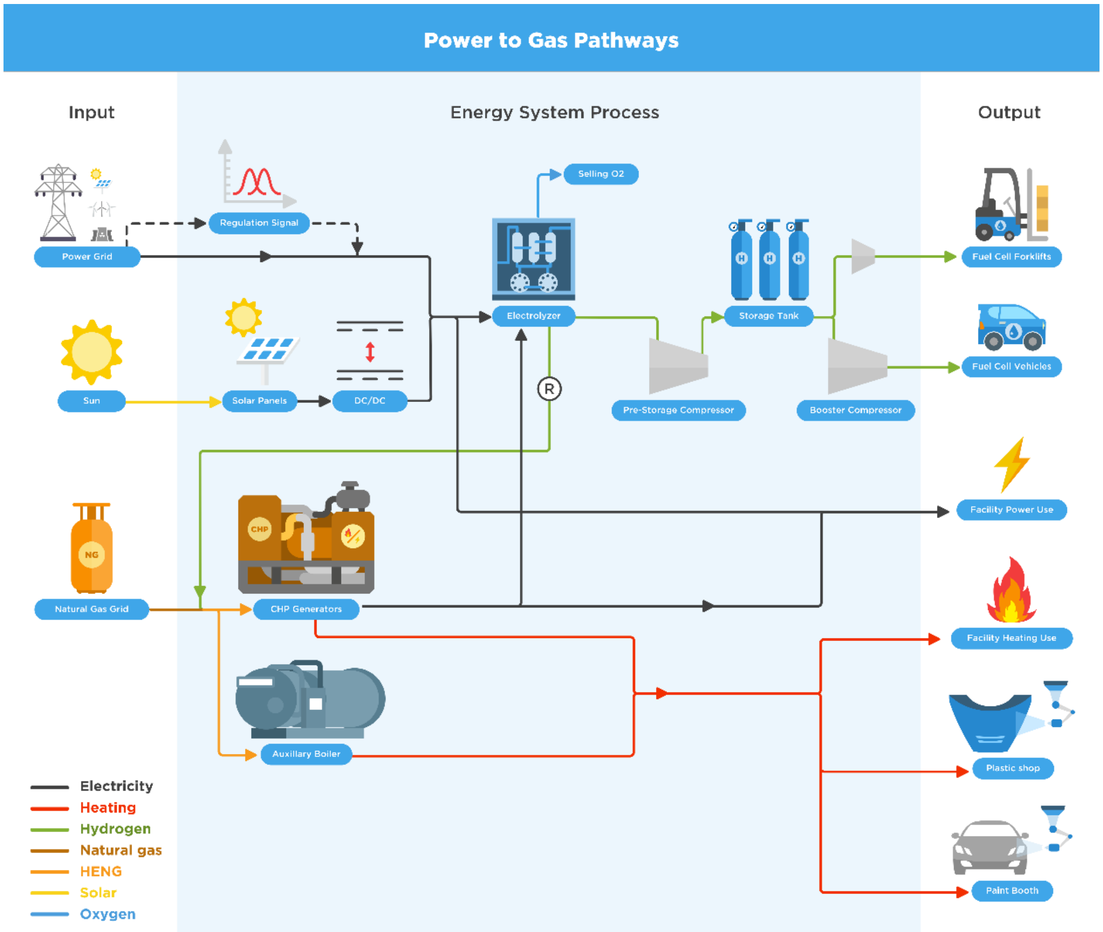


Figure 1: Process flow diagram of the automotive manufacturer incorporating pathways for Power-to-Gas technology.

Figure 1 details the suggested configuration, where a combination of electricity from the power grid, solar panels, and CHP units can be used to meet the facilities electricity demand. The objective of installing a CHP generator was to reduce the manufacturer's dependency on the grid. However, the plant has had problems with effectively scheduling the CHP units. In order to alleviate these issues, electrolyzers can ramp up and down consumption to allow the CHP units to be effectively utilized. Through a communication interface between the electrolyzers and the provincial power grid operator, the Power-to-Gas system schedules itself to provide ancillary services. In this study, the electrolyzers were used provide a demand response capacity to ramp up consumption during hours of surplus electricity generation in the provincial power grid. Furthermore, Figure 1 shows that hydrogen generated by the electrolyzers can either be compressed for storage, sent directly to end use applications or blended with natural gas to add renewable content, while the decision was made to sell oxygen generated by electrolysis.

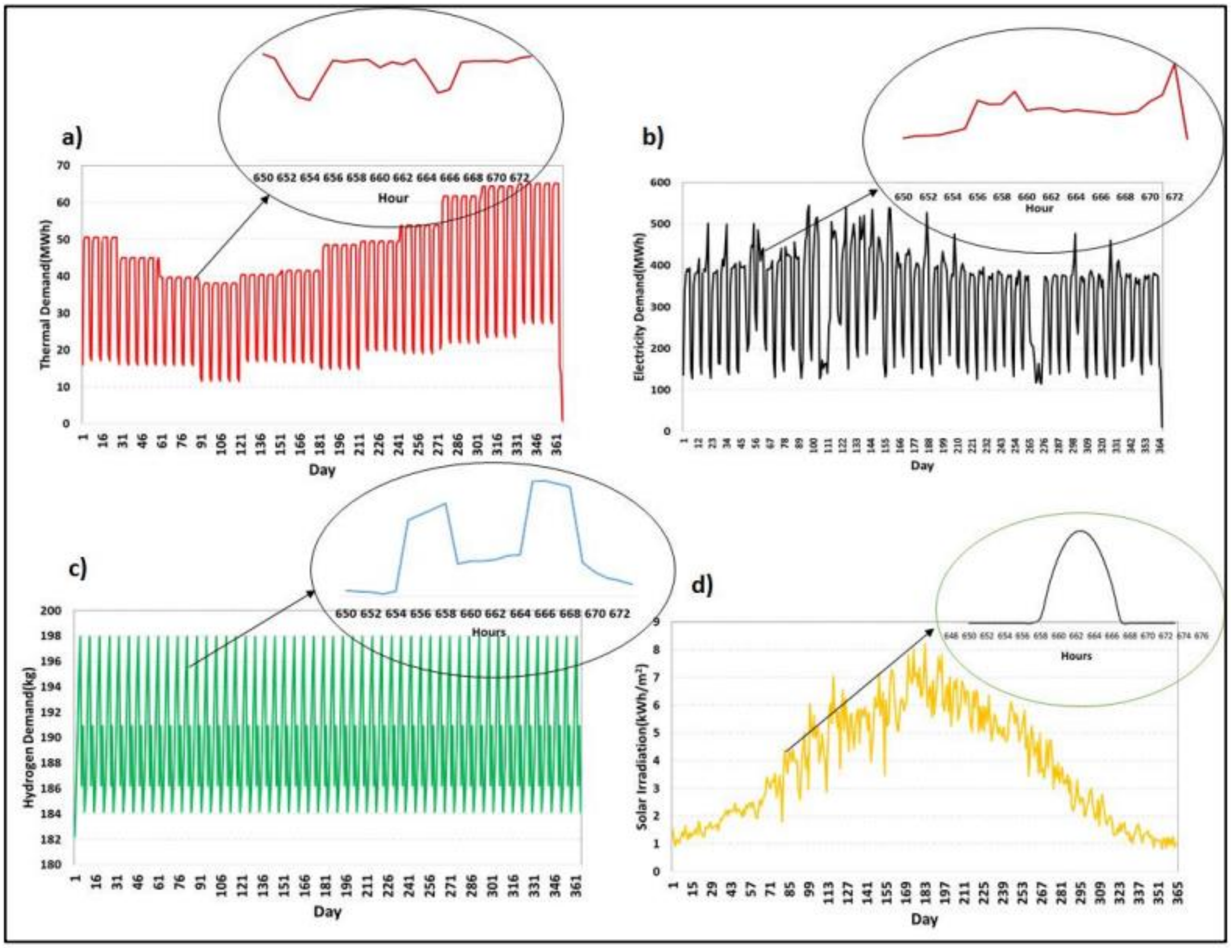


Figure 2: Primary demand profiles of the automotive manufacturer including thermal, electrical, hydrogen as well as the available solar irradiation.

To develop a mathematical model that describes the Power-to-Gas system, it is critical to define the input parameters to the system as well as the hydrogen and energy demands of the system. These hydrogen and energy demands include facility demands, such as thermal loads and electricity demands, but also external facility demands such as fueling fuel cell vehicles in the community or providing demand response services and constitute the primary MILP constraints. Figure 2 shows the four most important parametric data sets considered in the modeling study across the Company's fiscal year. The thermal demand increases during the cold Winter months and decreases during the summer months. In comparison the electrical demand has less significant annual variation since it is more directly influenced by the process load itself. The decrease in electricity demand observed in figure 2.b can be attributed to the plant equipment going under routine maintenance checks. Figure 2.c highlights the demand profile of the proposed refueling station capable of refueling 100 forklifts and 40 fuel cell vehicles (FCVs). The solar irradiation data for southern Ontario has been taken from climate data available from Natural Resources Canada's website [46]. An obvious trend that can be pointed out in figure 2.d is the increase in the solar irradiation (kWh/m^2) values during the summer months.

3.2. Model Description

In this work we institute a framework to model a Power-to-Gas installation that incorporates hydrogen as an energy vector into an existing energy network subject to demand and equipment constraints. Optimization problems of this type are best solved using a mixed-integer linear programming model (MILP) [47]. The need for mixed integer variables in our problem originates from the fact that an optimal solution will contain binary decision variables indicating whether a particular unit should operate since minimum loads are a considerable factor. The objective function of this model is the hourly summation of natural gas price, fixed electricity cost and variable electricity cost, and will be solved subject to the process material and energy balances, the capacities and efficiencies of individual components, regional temperature profiles, binary variable constraints and the known or predicted need of electricity, and heating demand.

MILP is a mature and well-established technique that has been commonly used in the field of energy system research to optimize dispatch strategies. For example, Anastasiadis et al. investigate the economic and environmental effects of hydrogen technology within microgrids, where they implement multi-objective optimization to balance both cost and emissions with the presence of renewable technology [37]. For their case study they show a potential 36% reduction in operating costs with a maximum CO_2 reduction of 300 tons; however, they considered fixed capacities of individual components which differs from this work in that the optimum number and size of components is determined by the model. Similar work is presented by Maroufmashat et al. who use a MILP approach for the optimal planning of a smart urban energy network [45]. Their work focuses on the energy management of an entire community connecting multiple energy hubs and develops operation strategies for a variety of equipment sizes. In our work however, we will focus on a single, yet more complex energy microgrid and identify the optimal new equipment sizes that minimize the annual operation, maintenance and capital cost. One final example of MILP is presented by Mukherjee et al who modify the objective function to accept equipment size as an input, optimally sizing an electrolytic hydrogen production system for a natural gas distribution system [48]. This work shows the importance of electrolytic hydrogen for reducing the carbon intensity of Ontario's utilities and the power of MILP in handling complex model formulations but does not analyze the energy dispatch itself.

This mixed integer linear programming model is run for multiple time periods and can be optimized according to the different objectives and decision variables. The result is the optimal configuration and operational schedule of energy conversion, generation and storage technologies. This model will be developed in MATLAB and a similar model will be constructed in the General Algebraic Modeling System (GAMS), which is a high-level modeling system for mathematical programming and optimization. MATLAB is well suited to a system operation model, while GAMS is more suitable for the optimization of component sizing and interaction between solar, wind and electrical grid profiles and is tailored for complex, large scale modeling applications. This integrated modelling strategy allows for the construction of large maintainable models that can be adapted to various scenarios. In general, the model's design methodology can be divided into three phases, modelling, optimization and post process analysis.

Modeling Phase: A mathematical model will be developed to simulate the energy hub that considers all its interactions on an hourly basis to determine which energy vectors are produced, stored, and consumed. In order to develop the model, it is important to well define the system, including system demand, hydrogen requirements and technical specifications for all of the energy hub components, including a CHP generation system, steam boilers, and solar photovoltaics. This framework will include logic that ensures the foremost priority is to supply fixed plant demand, with excess energy being diverted to the electrolyzer.

Optimization Phase: Design and operational variables will be optimized based on the desired objective function. This objective function incorporates the total cost of system operation, plant environmental emissions, and revenues from the sale of carbon allowances and hydrogen fuel. The size and number of energy hub components is determined by the individual design variables while equipment dispatch is calculated by the operational variables. The result of this optimization is a cost-effective operation plan, the optimal design of the energy hub, and an estimate of greenhouse gas emission and urban pollutant offset.

Post Processing Analysis: Based on the results of the optimized simulation, there are several avenues of post process analysis. The first is an economic sensitivity analysis, in which the effect of manipulating model parameters, such as market value of Hydrogen, on the net present value and payback period of the project is examined. Additionally, an economic benefits cash-flow analysis is also conducted as well as environmental emissions analysis. The potential policy initiatives that could help in financing the purchase of Power-to-Gas components will also be investigated. With one potential area of analysis being the management of surplus baseload generation.

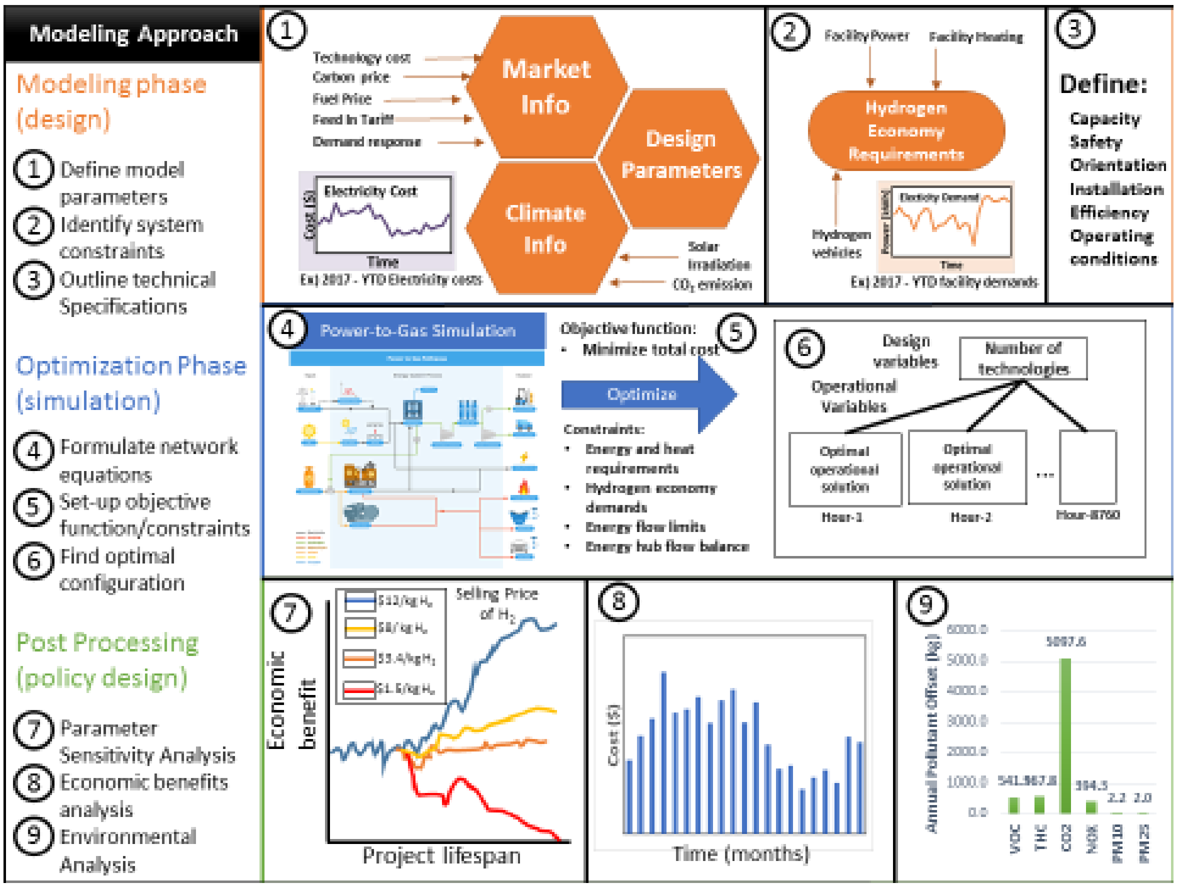


Figure 3: Summary of the analysis approach segmented into three sections; modelling phase, optimization phase and post processing.

3.3 Design Technology Screening

When installing a Power-to-Gas system it is important to recognize that the design, sizing, control strategy, and the integration of hydrogen technology all influence the overall efficiency, reliability, and financial feasibility of the plant. As such, it is critical to screen individual manufacturers and select the most appropriately sized components for the installation while subsequently arranging them in an intelligent manner. These decisions ultimately affect the modeling phase by acting as constraints to the mass and energy balance and influence both the economic and environmental feasibility. This section outlines the methodology used in selecting each component and integrating them atop the existing energy framework in a way that maximizes safety while achieving optimal profitability.

3.3.1 Hydrogen Generation Module

In the context of a Power-to-Gas system, selected key electrolyzer module specifications were, conversion efficiency, the nameplate capacity (DC electricity supplied to the electrolyzer at full-load operation), output pressures of Hydrogen and overall gas purity. In addition to other specifications, these key factors will be used as the decision-making criteria when rating different electrolyzer modules. Currently in the market there are two types of electrolyzers utilized. These two types are PEM and Alkaline electrolyzers which differ in the feed solution as well as the membrane technology. Of the different suppliers of hydrogen electrolyzers, Hydrogenics was chosen as the supplier for this study. Due to their vast array of electrolyzer options, they have the highest potential to offer fully integrated and comprehensive electrolyzers to meet the client’s demands and extensive years of experience.

Of the different electrolyzers offered by Hydrogenics, two were selected and compared based on the decision-making criteria. The first was the HySTAT60, which is an outdoor unit that produces 10 Bar hydrogen at an efficiency of 68.3% and with a nameplate capacity of 312 kW. The second is an equivalent PEM electrolyzer with the same nameplate capacity but a higher efficiency of 78%. Additionally, the output pressure of the PEM electrolyzer is higher (30 bar) leading to lower compressor requirements when storing produced Hydrogen. Another advantage of the PEM electrolyzer is its ability to ramp up and down power consumption quickly. According to a ramping test done by Eichman et al [49], it was shown that a polymer electrolyte membrane (PEM) electrolyzer takes less than ½ a second to complete almost all of a 25% ramp down from its maximum operating level to a lower operating level. When ramping the electrolyzer back up, it was shown that it takes ½ a second for the PEM electrolyzer to complete a 75% ramp up from when the electrolyzer was turned off and restarted again in a quick succession. This is an added value for the ancillary service market for demand response. A possible downside is a lower serviceable life and higher maintenance costs due to stack refurbishments [50]. However, these drawbacks are outweighed by the cost savings in efficiency and compressions which is why the PEM electrolyzer is chosen for this design.

3.3.2 Tank Storage Units

To effectively balance fluctuating energy prices and provide ancillary grid services once the electricity has been converted to hydrogen it must be stored. Due to the maturity of the technology tank storage was selected as the preferred method for this system. Factors affecting the cost of hydrogen storage include the storage capacity of hydrogen and the holding pressure. The International Energy Agency has done analyses on the technology used to store hydrogen and found the energy requirement to compress hydrogen from 1 to 200 bar to be only 7% of the energy that the hydrogen can provide [51]. Moreover, it was concluded that 70% of the energy from the hydrogen could be recovered when the gas decompresses to its original state at atmospheric pressure. As a result, the total electricity used to compress the hydrogen is only 2.1% of the gas's potential energy [52].

In terms of end use applications, gas turbine generators will require a storage pressure of 30 bar, forklifts a pressure of 250 bar, and fuel cell vehicles, which store hydrogen at 700 bar, require tank storage to be between 800 and 850 bar as recommended by the National Renewable Energy Laboratory (NREL). The additional over pressurization results from the significant pressure drop at the dispenser nozzle. To mitigate this and reduce compression costs, a booster compressor should be installed following the storage vessel. The booster compressor will provide one-directional flow of readily compressed gas and only discharges once the pressure of the outlet drops below the pressure within the system.

A storage vessel with greater capacity at 89 kg and an operating pressure of 172 bar is chosen as the most feasible option for the bulk hydrogen storage [53]. This tank is an American Society of Mechanical Engineers (ASME) steel vessel which proves to be the best investment for our requirements. Ultimately, there will be one pre-storage compressor transferring hydrogen from the electrolyzer and two post-storage compressors supplying forklifts and FCVs.

3.3.3 Compressors

The hydrogen must be compressed prior to storage in any vessel and must be passed through a booster compressor before end-use application. A storage vessel with a capacity of 89 kg and a compression pressure of 172 bar was selected for tank storage and as such a pre-storage compressor will be responsible for raising hydrogen to this pressure from the 30 bar at the outlet of the electrolyzer. On the other hand, the post-storage booster compressors will have to achieve a pressure of 250 bar for hydrogen forklifts and 825 bar for fuel cell vehicles respectively.

The pre-storage compressor will be a Greenfield reciprocating compressor with a maximum flow capacity of 87 kg/hr and an inlet pressure of 20 bar [51]. This compressor is capable of achieving a maximum outlet pressure of 413 bar, which exceeds the necessary 172 bar required for tank storage. The forklift refueling system will also implement a greenfield reciprocating compressor with a maximum flow rate of 42 kg/hr, a suction pressure of 2.4 bar and a maximum discharge pressure of 310 bar [52]. The HydroPac C15-40X-EXT/SS-H2 piston compressor has been chosen as the most suitable compressor for the fuel cell vehicle refueling station [55]. This booster compressor is capable of compressing gas from 70 to 897 bar which can fulfill the requirements presented by NREL. This booster compressor has a power rating of 40 HP and is capable of maintaining this power rating during fluctuations in the inlet to the compressor.The inlet flow can vary between 70 to 414 bar and the operating capacity will vary accordingly between 11 to 30 kg per hr [53].

To verify that the compressors could meet the hydrogen demand it was necessary to estimate the total amount required by end use applications. Refueling the 100 forklifts operating in the plant is a priority. As such, this constrains the total number of fuel cell vehicles considered for deployment to a value of 40. A study performed by NREL states that the average consumption for FCV refueling is 2.64 kg/day [54]. The forklifts have a daily hydrogen consumption of 0.9 kg/day, so the daily hydrogen demand for transportation will amount to an estimated 222 kg/day [55]. The remaining hydrogen generated by the electrolyzer will be sent in the form of hydrogen enriched natural gas to the CHP and to end use heating applications, reducing the carbon footprint of these operations.

3.3.6 Renewable Energy Source

In addition to the Power-to-Gas system components, the potential utilization of rooftop area available for solar panel installation has also been accounted for. The implementation of a dual axis solar tracking module in southern Ontario (Canada) can generate an average of 1 kWh/m^2/day, while a stationary configuration with an optimal south-facing latitudinal tilt can generate 0.73 kWh/m2/day [63,64]. The automotive manufacturer has 160 000 m^2 of unshaded available roof space for solar arrays, potentially generating a daily energy output between 117 and 160 MWh. Canadian Solar's Dymond CS6X-340 double glass solar generation modules were selected based on their power output capacity, weight, durable operating range and favorable economics. The solar modules are designed to withstand Canadian weather conditions with a safe operating range of -40°C to +85°C and a snow pressure rating of 5400 Pa [65]. All infrastructure will adhere to best practices for rooftop solar installations as outlined by the Canadian Standards Association (CSA) in article SPE-900-13[66].

3.3.4 Refueling Station and Dispensers

The Power-to-Gas plant will plan to provide for hydrogen for 140 hydrogen powered vehicles. The provincial government of Ontario supports the direction of this project as there has been an Electric Vehicle Incentive Program (EVIP) in place since 2010. The program is continuously updated to promote Ontario's Climate Change Action Plan to reduce greenhouse gas emissions by making green energy sources more feasible. There are different streams of incentives depending on whether the vehicle is leased or owned, but base incentives of $6,000 to $10,000 are available depending on capacity [56]. Additional incentives of $3,000 become eligible for more expensive vehicles with an MSRP from $75,000 to $150,000 [57].

The type of dispensers used for the Power-to-Gas system have briefly been mentioned already based on the NREL study, but it must be determined how many will be available. H2A provides a formula to determine the number of required dispensers based on the daily capacity of the refueling station:

$$Dispensers = \frac{Daily\ Capacity}{305.85 * Daily\ Capacity^{0.0763}} \qquad (1)$$

The equation is based on data from Chevron about the amount of time that each hose is occupied during peak times. These dispensers are applicable to the 250 bar and 700 bar fills necessary for the FCV and forklifts, respectively [58]. For 700 bar tanks on-board the vehicles, codes from SAE J2601 indicate that the dispensing stations must keep the hydrogen fuel between -17°C and 40°C when entering the FCV tank to avoid any risk of overheating [38]. Since the compressor raises the pressure to 825 bar, the temperature will be slightly higher when leaving the discharge, however, cooling water between the process units will be used to maintain these specified temperatures. By using the above equation, the refueling station requires a single 2 hose dispenser system with for meeting a maximum daily dispensing capacity of 222 kg/day. The model simulation accounts for the cooling cost using an energy consumption value of 0.26 kWh per kg of hydrogen cooled, which is used by the Argonne National Laboratory in their Hydrogen Refueling Station Analysis Model [39].

3.3.5 Blending System

Due to the sensitivity of pre-existing components in the manufacturer's energy distribution system it is necessary to install an effective blending system that controls the amount of hydrogen injected into the natural gas pipeline. Such a system consists of two primary components, a gas regulator and a blending control system that can be managed from the centralized HMI. The facility requires fuel be injected into the gas turbines at a pressure of 220 psig (15.1 barg) [61]. As such dual stage 1009 series regulator supplied by Praxair was selected to reduce the pressure from the 30 bar storage to the 15.1 bar injection pressure. As for the control system an Environics 3000 series low-cost gas mixing system was selected. The system offers two controls, the mass flow rate exiting the mixer using Precision Mass Flow Controllers (MFCs) as well as the concentration of hydrogen using PLC logic. The system has repeatability up to 0.05% as well as a series of I/O modules to connect the controls to a central HMI [62].

3.3.7 Ancillary Services & Demand Response System

Another important consideration is to ensure that the system has the ability to perform ancillary services in order to generate external revenue streams. As mentioned previously, the main ancillary service being utilized will be to provide demand response services to the electricity market in Ontario. In order to provide demand response, the main criteria is to have an electrolyzer with a fast ramp up and down time, which has been proven with the PEM electrolyzer selected in section 3.1. Currently, the Independent Electricity System Operator (IESO) oversees the operation of the electricity market in Ontario. The IESO through its demand response auction program [60] procures demand response capacity or participants that can alter their electricity consumption profile. Participants of the auction program submit offers to provide their demand response capacity within 1 or more of the 10 different power zones of Ontario's power grid. For the different power zones in Ontario it is common to see surplus baseload generation and according to the IESO, surplus baseload generation occurs when the total hourly electricity produced by the wind, nuclear, and hydroelectric generators exceeds Ontario's electricity demand [67]. The automotive manufacturing plant considered in this study is located in the Southwest power zone. This power zone has a total of 14 wind farms which have a combined maximum capacity of 1653 MW. On average, the contribution of these wind farms during hours of surplus baseload generation in Ontario is ~3.12%

with the maximum value of surplus baseload generation being 201.5 MWh. The hourly generation output by fuel type and hourly demand data for Ontario have been taken from IESO's data directory to estimate the province's hourly surplus baseload generation [68].

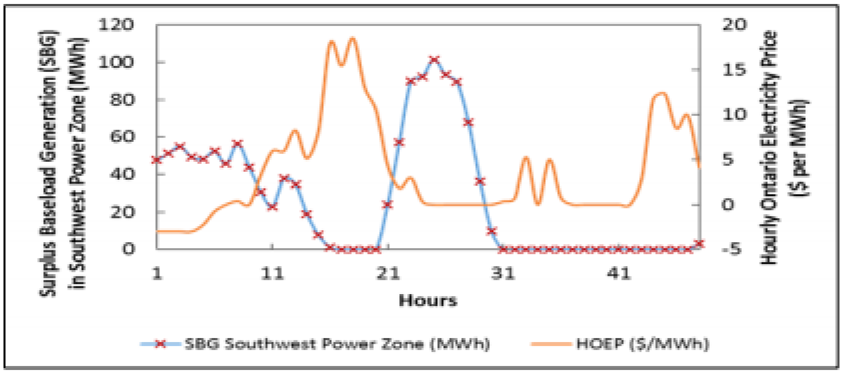


Figure 4: Comparison of hourly Ontario electricity price (HOEP, $ per MWh) values with hourly surplus baseload generation in the "Southwest" power zone (MWh).

Figure 4 shows a 48-hour plot of the hourly Ontario electricity price and the hourly surplus baseload generation in the "Southwest" power zone in Ontario. It is observed that during hours when the electricity price is close to or below zero, surplus baseload generation increases, leading to the monetary potential to provide demand response. Therefore, the Power-to-Gas system must be able to participate and bid into the demand response auction. Based on the auction market clearance price, the system must be able to predict surplus baseload generation based on projections provided by IESO. From there, the system must be able to ramp up their electricity consumption accordingly, using electricity input controls offered by the electrolyzers. These controls are connected with I/O modules to the facilities HMI.

3.4. Results: Cost, Economic & Environmental Analysis

With the objective of providing a clean, sustainable pathway to meet the automotive manufacturer's energy demands the model targeted the minimization of total cost and the reduction of annual environmental footprint. Atop the monetary benefits realized through the more efficient operation of the energy system, the automotive manufacturer's installation generates revenue through ancillary service income, environmental benefits and the economic replacement of conventional fuels. A subsequent sensitivity analysis was performed across a combination of 20 different scenarios to determine the best fit for P2G implementation. The study concluded that the model was more sensitive to a fluctuation in hydrogen price and demand response benefit than it was to variations in per tonne carbon reduction.

3.4.1 Production Income

Five primary revenue streams result from the production of hydrogen gas, including the production of hydrogen for forklifts, the production of hydrogen for fuel cell vehicles (FCVs), selling power from solar photovoltaics, the hydrogen enrichment of natural gas, and the sale of oxygen by-product. The P2G system is capable of generating 76,073 kg of hydrogen annually which given a capital recovery factor of 9.8 (considering the lifespan of 20-year with the 8% interest rate) will be produced at a levelized cost of 3.6 USD per kg. Of the total hydrogen production 32,850 kg will be supplied to a fleet of 100 forklifts that are currently using hydrogen purchased at a rate of $8 per kg. A sensitivity analysis that ranges the hydrogen price across 4 levels indicated that there is potential for a total annual economic savings on forklift hydrogen between $40,061 and $320,487. The four price points used were $1.5 (current SMR price), $3.6 (current model levelized cost), $8 (current market price), and $12 (high range value) per kilogram hydrogen. An additional 36,494 kg will be fed to fuel 40 FCVs in replacement of existing conventional combustion cars. Similarly, the sensitivity analysis predicted the annual revenue to fall between $44,504 and $356,039 for the hydrogen selling price of 1.5 to 12 USD per kilogram. Due to the energy storage capacity of the proposed system, the addition of renewable solar energy to the automotive manufacturer's existing generation becomes economically feasible. Installing 1500 solar photovoltaics on the rooftops of existing and proposed infrastructure, an additional annual generation of 473,960 kWh is realized, which equates to $94,792 per year. Using hydrogen enriched natural gas can offset 26895 m^3 annual demand of natural gas, which can save $5000 per year. The by-product of electrolysis is oxygen gas which can be sold to feed the demand of localized industrial applications. It is determined that the system will generate 608,587 kg of oxygen gas annually that if sold at a price of $0.13 per kilogram would produce an annual revenue of $64,321.

3.4.2 Ancillary Service Income

Using the PEM electrolyzer the system will take advantage of regulatory grid services through demand response. The electrolyzer will ramp up to increase the plant's demand during periods when the grid is dumping renewable wind energy at a low price and decrease as purchasing from the grid becomes more expensive. The demand response provided by the automotive manufacturer will generate an additional revenue of $522,520 annually.

3.4.3. Environmental Reduction Income

The imposition of a provincial Cap-and-Trade program generates additional revenue streams for Power-to-Gas based on a reduction of greenhouse gas (GHG) emissions. For the automotive manufacturer this reduction comes in four forms, the replacement of forty internal combustion vehicles with FCVs, the enrichment of consumable natural gas, the generation of clean solar energy, and offset of carbon rich energy with curtailed renewable wind. All revenue streams are analyzed for 2 separate carbon prices, the current Cap-and-Trade price, which is $18 per tonne CO_2, and a mid-range long term carbon price forecast of $30 per tonne CO_2.

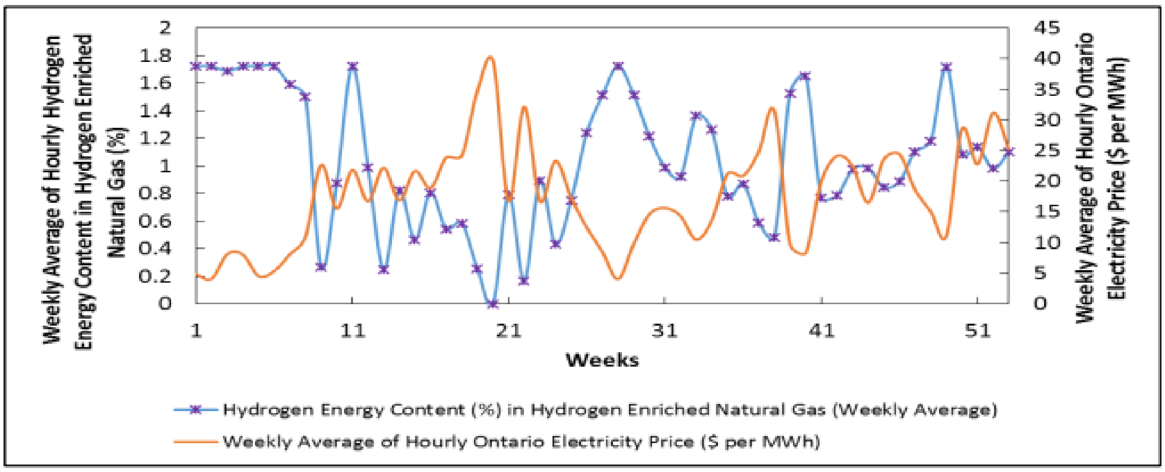


Figure 5: Variation of weekly average hydrogen energy content in hydrogen enriched natural gas (%) with weekly average of hourly Ontario electricity price ($ per MWh).

Based on current use rates replacing the 40 conventional vehicles would result in an annual offset of 170 tonnes CO_2 which corresponds to a revenue increase between $2497 and $4163. Figure 5 shows how the model chooses to blend hydrogen into the natural gas consumed by the CHP and boiler units. The hydrogen content, which is optimized for each hour, was averaged over each week and compared to the corresponding weekly HOEP average. As such a general trend becomes clear, with the model choosing to increase hydrogen production and subsequently blending during periods of low electricity price. Blending hydrogen into the natural gas pipeline entering the manufacturer can offset 65 tonnes of CO_2 per year which corresponds to $894-$1626 of revenue. The addition of solar panels to the existing infrastructure would potentially generate enough electricity to offset 24 tonnes of CO_2 equating to annual savings of \$425-\$700. Lastly, an offset of 2100 tonnes of CO_2 could be achieved by using the electrolyzer to provide demand response to the grid, increasing the consumption of curtailed renewable power by 42250 MWh. Given the sensitivity analysis this equates to a predicted revenue increase between \$37,816 and \$63,027.

3.4.4. Equipment Cost & Payback Analysis

With the objective of providing a clean, sustainable pathway to meet the automotive manufacturer's energy demands the model targeted the minimization of total cost and the reduction of annual environmental footprint. The design of this Power-to-gas system included predicting the ideal number of fixed-sized components, such that the heat, electrical and hydrogen demands could be met with minimal capital, operation and maintenance cost. This section summarizes the capital and operating costs for each Power-to-Gas component identified in technology screening. This information was combined with the results of the model to determine several financial parameters useful in evaluating the project's feasibility. However, the objective was simply to meet the automotive manufacturer's requested payback period on capital investment of 3-years. Table 1 shows the capital investment cost while Table 2 provides the maintenance and operating costs.

Table 1: Capital costing for primary components of new Power-to-Gas technologies.

Component Description	**Cost($ CAD)**
Hydrogen Compressor and Dispensing System	
HydroPac (C15-40X-EXT/SS-H2) Reciprocating Piston Booster Compressor	130,127
Greenfield Reciprocating Compressor	302,660
2 Hose Dispenser System	99,826
Pre-Cooling System	183,791
Electrolyzer, On-Site Storage, and Renewable Generation	
PEM Electrolyzer Module	1,006,398
Pressurized Storage Tank (89 kg @ 172 Bar)	95,580
Greenfield Pre-Storage Reciprocating Piston Compressor	320,619
Photovoltaic Solar Panels	439,024(293/panel)

Table 2: Operational and Maintenance costing for primary components of new Power-to-Gas installation

Operation and/or Maintenance Cost	Cost ($ CAD)
Solar Panel Annual Operating Cost	$21 per kW per year
Water Cost	$2.16 per m^3
Replacement Cost of Electrolyzer	35% of Capital Cost
Purchase Price of Electricity for Electrolysis	HOEP
Annual Operation and Maintenance of Tanks and Compressors	5% of Capital Cost
Annual Operation and Maintenance of Electrolyzer	2.5% of Capital Cost
Energy Consumption Factor: Booster Compressor for Forklift Refueling	0.93 kWh per kg of H2
Energy Consumption Factor: Pre-Storage Compressor	29 kWh per kg of H2
Energy Consumption Factor: Booster Compressor for Fuel Cell Vehicle Refueling	6.35 kWh per kg of H_2
Demand Response Auction Price	$368.5 per MW-day

Based on both capital and operating costs the net present value, return on investment and payback period can be calculated for a variety of scenarios which depend on hydrogen price, carbon trade price and which revenue streams are accessed and to what degree. The financial returns realized by each major pathway are listed alongside these metrics for 20 unique scenarios in Table 3. It is shown that the optimal model is capable of providing a desirable payback period under two circumstances. The first, which produced a payback of 2.9 years, was the case where there was no carbon trade, active demand response and a hydrogen price of $12 per kg. The second which was even more favorable operated under the same conditions but incorporated a carbon trade price of $18 per tonne CO_2 resulting in a payback of 2.8 years.

Table 3: Sensitivity of financial and environmental returns to model parameters including carbon trade and hydrogen purchase price.

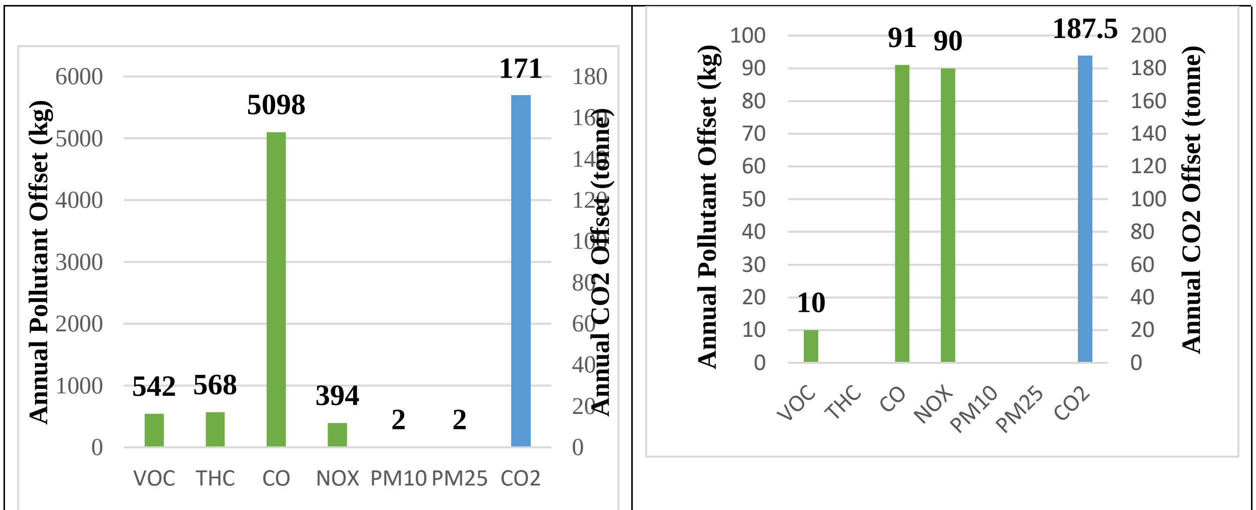
Scenario	Description	Premium Price		Production Income (USD)	Ancillary Service Income (USD)	Environmental Reduction Income (USD)	Net Present Value (USD)	Return on Investment	Payback Period
		Carbon Trade Price ($/Tonne)	Hydrogen Price ($/kg)						
1	*No Environmental Coinsiderations, No Demand Response*	N/A	$ 1.50	$ 165,568.00	$ -	$ -	$ (4,878,343.00)	-186.00%	-11.40
2		N/A	$ 3.60	$ 283,960.00	$ -	$ -	$ (3,716,042.00)	-142.00%	-23.50
3		N/A	$ 8.00	$ 532,020.00	$ -	$ -	$ (1,280,544.00)	-49.00%	19.20
4		N/A	$ 12.00	$ 757,529.00	$ -	$ -	$ 933,525.00	36.00%	7.20
5	*No Environmental Coinsiderations, Demand Response*	N/A	$ 1.50	$ 165,568.00	$ 522,520.00	$ -	$ 251,750.00	10.00%	9.00
6		N/A	$ 3.60	$ 283,960.00	$ 522,520.00	$ -	$ 1,414,142.00	54.00%	6.40
7		N/A	$ 8.00	$ 532,020.00	$ 522,520.00	$ -	$ 3,849,631.00	147.00%	4.00
8		N/A	$ 12.00	$ 757,529.00	$ 522,520.00	$ -	$ 6,063,711.00	231.00%	2.90
9	*Environmental Considerations, No Demand Response*	$ 18.00	$ 1.50	$ 165,568.00	$ -	$ 34,533.00	$ (4,539,387.00)	-173.00%	-13.40
10		$ 18.00	$ 3.60	$ 283,960.00	$ -	$ 34,533.00	$ (3,376,995.00)	-129.00%	-34.00
11		$ 18.00	$ 8.00	$ 532,020.00	$ -	$ 34,533.00	$ (941,507.00)	-36.00%	15.30
12		$ 18.00	$ 12.00	$ 757,529.00	$ -	$ 34,533.00	$ 1,272,572.00	49.00%	6.60
13	*Environmental Considerations: High Offset Benefit, No Demand Response*	$ 30.00	$ 1.50	$ 165,568.00	$ -	$ 57,544.00	$ (4,313,356.00)	-165.00%	-15.20
14		$ 30.00	$ 3.60	$ 283,960.00	$ -	$ 57,544.00	$ (3,150,963.00)	-120.00%	-48.50
15		$ 30.00	$ 8.00	$ 532,020.00	$ -	$ 57,544.00	$ (715,476.00)	-27.00%	13.50
16		$ 30.00	$ 12.00	$ 757,529.00	$ -	$ 57,544.00	$ 1,498,603.00	57.00%	6.30
17	*Environmental Considerations Demand Response*	$ 18.00	$ 1.50	$ 165,568.00	$ 522,520.00	$ 34,533.00	$ 590,798.00	23.00%	8.00
18		$ 18.00	$ 3.60	$ 283,960.00	$ 522,520.00	$ 34,533.00	$ 1,753,189.00	67.00%	5.90
19		$ 18.00	$ 8.00	$ 532,020.00	$ 522,520.00	$ 34,533.00	$ 4,188,677.00	160.00%	3.80
20		$ 18.00	$ 12.00	$ 757,529.00	$ 522,520.00	$ 34,533.00	$ 6,402,758.00	244.00%	2.80

These scenarios explored the sensitivity of payback to carbon emission ($ per tonne) and hydrogen sale price ($ per kg). It is concluded that the carbon emission allowance price is still not high enough to drive a significant improvement payback period and return on investment. The selling price of hydrogen and the demand response service incentive are seen to be the major factors in improving the project's economic feasibility. The cost of carbon emission will have to be higher in order to drive innovation from large-scale industrial polluters.

3.4.5. Environmental Analysis

A primary concern in the design of a Power-to-gas (P2G) system is its potential to limit the release of environmental impacts on the local residents. In the interest of reducing their contribution to global warming and avoiding the hefty fees associated with ta carbon tax, the automotive manufacturer developed a mandate to eliminate carbon emissions by the year 2050. A lifecycle analysis of the Power-to-gas systems has been performed and implemented in the modeling phase in alignment with the company's strategic goals. Environmental benefits including in terms of emission allowance trade was explained in details in the results section, which include environmental revenue from generating power by solar PVs, using Ontario's surplus power, using hydrogen for vehicle, offsetting natural gas usage.

Analysis of the Power-to-Transport pathway determined that an average daily production of 200 kg H2 is required. By balancing the emissions generated by from producing hydrogen with the benefit of offsetting conventional fuels the net annual reduction is calculated and presented in Figure 6(a).



(a) (b)

Figure 6: Annual emission offset (a) by the Replacement of 40 Conventional Vehicles, (b) By using HENG

For the purpose of downstream applications, the enrichment of natural gas is limited to 5 vol. % hydrogen [69]. The model maintained the total energy delivered to end use processes given individual equipment efficiencies and the higher heating value of the gas blend. Given the per volume emission benefit associated with blending, the total annual greenhouse gas emissions and pollution offsets are shown in Figure 6(b).

3.5 Policy Analysis

There are three types of obstacles for the large-scale deployment of Power-to-Gas systems which are technology-related, policy-related and problems related to public acceptance. In regard to technology the primary concern is the ability to inject hydrogen into natural gas pipelines. This practice is uncommon, and most pipelines are not prepared to handle high concentrations without experiencing leakage and embrittlement. To address this, there would have to be a compatibility analysis before injection to deem if the pipeline is suitable for the transport of hydrogen. Standards and codes regarding the gas quality (i.e., upper hydrogen concentration) in natural gas pipelines still have yet to be proposed in North America and are needed to better control risks associated with failures. Harmonized standards are necessary for the safe, efficacious global distribution of hydrogen gas. Operating pressures, pipeline materials, upper hydrogen concentrations, and other factors such as temperature must be analyzed to determine proper safety standards for operation.

From policy perspective the development of Power-to-Gas systems in Ontario is lacking incentives for the industrial and transportation sectors. Incentivizing the use of renewable energy in the industry and transportation sector is more beneficial for Ontario compared to incentivizing the development of renewable energy for electricity generation. This is because the electricity generated in Ontario is already more than 90% emission-free, making it very difficult for new renewable generation capacity to reduce GHG emissions. The transportation, industry, and building sector in Ontario are mainly dependent on fossil fuels, and thus hydrogen has the noticeable potential to replace them and reduce emissions. At the same time, a Power-to-Gas system provides the option to take that renewable energy from the electricity sector to other sectors and benefit from the already-made investment there.

Public acceptance issues also plague the development of Power-to-Gas systems. A higher acceptance subsequently leads to higher penetration of hydrogen into the entire energy system. While the safety issues of using hydrogen have already been addressed from the technical side, there is a safety concern among the public about explosions at end-use appliances. Public understanding of hydrogen technology can be increased with educational projects or by funding pilot Power-to-Gas projects for public institutions, such as municipalities and post-secondary institutions.

4.0 Profit Sensitivity to Policy Condition and Technological Safety Analysis

The following section is based on previously published work "*An Economic, Environmental and Safety Analysis of Using Hydrogen Enriched Natural Gas (HENG) in Industrial Facilities"* by Preston, et. al. and is reproduced by permission from Elsevier. This thesis author's specific contribution to this paper was to: support data collection and preparation, develop the costing models for each component, support the development and simulation of the mathematical model, interpret the results, and support both editing and proofreading

Keywords:

hydrogen enriched natural gas; combined heat and power unit (CHPs), power-to-gas; hydrogen economy; failure modes and effects analysis

4.1. Introduction

The development of renewable energy infrastructure within the province of Ontario has resulted in a mismatch between supply and demand, with the Independent Electricity System Operator (IESO) dumping terawatts of clean, low carbon electricity each year at very low cost [70,71]. With a significant federal carbon tax on the horizon, there is a need for strong, robust business cases for microgrid systems that incorporate large-scale, efficient energy storage systems [72 ,73, 74]. One of the most promising technologies available on a commercial scale is power-to-gas, an energy storage concept where low price, curtailed renewable energy is used to transform water into hydrogen gas that can be later redistributed through various revenue streams [75].

Of the many revenue streams available to power-to-gas, the enrichment of natural gas with electrolytic hydrogen has garnered significant interest given its ability to reduce operating costs while increasing renewable content [77, 78]. This is particularly important in the context of Ontario's utility market, given Environment and Climate Change Canada's 2016 proposal of a nationwide clean fuels standard that will include commercial and residential natural gas [79]. The production of hydrogen enriched natural gas (HENG) in Ontario is already occurring on the utility scale; however, based on global research, there is potential to realize significant financial and environmental returns through local industrialized implementation as well [80]. It is important to recognize that these economically favorable and robust business cases exist today and that hydrogen enrichment through power-to-gas is a technology of the present rather than of the future [74]. As such, this work will evaluate the economic and environmental feasibility of introducing electrolyzer-based hydrogen production to enrich the natural gas feed stream of a combined heat and power plant at an automotive manufacturer in southern Ontario as a case study for broader provincial development.

A computational model will be developed for the 2018 calendar year, simulating the hourly production, storage and injection of hydrogen, subject to system capacity, plant demand and end-use constraints [81,82]. Subsequently, a sensitivity analysis will be performed to evaluate how changing carbon price and government capital incentives affects the investment's financial metrics. In each scenario, the optimal system performance is identified, given storage and production parameters decided by facility operators. This information can be further used to suggest key component sizing and predict overall capital and operating costs for a projected scenario. This analysis forms the basis for preliminary design development and illustrates what metrics policy makers should target to improve adoptability of technologies focused on the decarbonization of the industrial sector.

This work is novel in that it simulates hydrogen enrichment in a real system separately from other pathways, suggesting design features unique to a CHP-based industrial energy system. In addition, it is valuable in that it identifies policy issues specifically for these types of preliminary business cases, given features of Ontario's energy system. The economics presented are unique to the provincial market, and they stand to demonstrate that simple systems without complex stacking of revenue pathways can still obtain profitability given the appropriate incentives. Yeong et al. verified the capability of such power-to-gas technologies to be implemented within the Canadian energy system, noting that given appropriate evaluation, the existing infrastructure would possibly withstand hydrogen blending up to 5% by volume without substantial level-up to avoid failure related to hydrogen embrittlement [83]. While this work provides excellent insight into the flexibility of the natural gas transportation framework to accept hydrogen, it does not extend into an economic analysis for practical business cases. In a study on early business cases for hydrogen by Tractebel Engineering, distinct concrete business cases were developed for power-to-gas, which include hydrogen blending into the gas grid [74]. While these business cases are shown to be profitable in a European context where renewable content within the energy supply chain is high, they need to be extended to the Canadian energy grid and to cases where alternative revenue streams such as hydrogen for mobility and grid ancillary services are not currently practical. Mukherjee et al. [84] performed a techno-economic and environmental assessment of a hydrogen-powered community within the Ontario market, estimating capital expenditure, economic returns and identifying key safety parameters required for an effective design [85]. This paper will extend on this work by considering hydrogen-enriched natural gas as a potential pathway and by incorporating suggestions for an inherently safer design. Further studies have recognized the need for power-to-gas and have made attempts to analyze the technical feasibility of blending hydrogen into CHP feed streams. Work by Lo Basso (2015) and Whidden (2010) both verified the capacity of HENG to be produced and blended into combined heat and power feed streams without significant detriment to system performance [86, 87]. These studies were successful in identifying the potential greenhouse gas reductions obtained with blended plants, and they motivate an investigation into the practical economic feasibility of these pathways in industrial plants, particularly within the Canadian economy.

Another report that provides considerable insight into the usefulness of hydrogen in reducing the carbon intensity of fossil fuels was published by the International Energy Agency. While they concluded that a grid-wide introduction of hydrogen generated from fossil fuels is not as economically favorable as alternative abatement options, they were able to show that the introduction would incur little costs outside those associated with production up to 3% vol. and that options exist to scale blending as high as 25% [88]. They go on to recommend further work in this area because hydrogen technology acts as a necessary bridge between fossil fuel systems and stable renewable infrastructure. The simulations presented in this report attempt to demonstrate the value of pathway optimization in the context of industrial microgrids and how electrolytic hydrogen in particular can overcome infrastructure transition costs.

By developing this simulation, we are demonstrating that not only is hydrogen blending a safe technology, but it is also readily implementable on the industrial scale. Furthermore, we are demonstrating that there are economic and environmental benefits available from exploiting a single power-to-gas pathway given the appropriate government incentives. As such, the following milestones outline the objectives of this work:

Developing a mathematical methodology for the storage and injection of hydrogen-enriched natural gas at an industrial manufacturer's microgrid;

Performing a technology assessment of the key components of the power-to-gas system, highlighting proposed suppliers, capital and operating costs;

Analyzing key project environment and economic return indicators to assess the feasibility of the capital expenditure

Validating the results of this methodology by performing a failure modes and effects analysis to identify potential risks to plant safety.

4.2. Simulation Approach

This paper investigates the economic and environmental feasibility associated with the operation of a power to gas system integrated within an industrial manufacturer's energy system.

Under current operation the heating demand of the facility is met entirely by the steam output of two combined heat and power (CHP) units, which when supplemented by the provincial energy grid also meet the company's electricity demand. By introducing power-to-gas, the manufacturer can take advantage of fluctuations in the Hourly Ontario Energy Price. When this price drops sufficiently low due to a surplus of available grid energy, not only is it favorable to pull more from the grid than the CHPs, but this energy can also be used to generate hydrogen gas. As electricity prices climb, such that CHP generation is favorable, this hydrogen can then be mixed with natural gas to feed CHP units. Through this, one can decarbonize the heating and electricity demand for industrial facilities, bringing about significant energy savings and emission offsets. The challenge that is the focus of this paper is determining when to produce and store hydrogen and in what amounts.

As shown in Figure 1, electricity from the grid, for which the wholesale price fluctuates, will be fed to the electrolyzer. This hydrogen is either sent directly to the natural gas pipeline or to temporary storage. The decision regarding when to produce hydrogen is made by fixing an upper limit on the grid electricity price, above which no production occurs, for an entire year of analysis, then varying this limit across a broad range to determine the optimal financial performance for the given incentive structure. Similarly, the decision to store hydrogen is made by varying the storage coefficient, which is a ratio of the production demand to the amount stored.

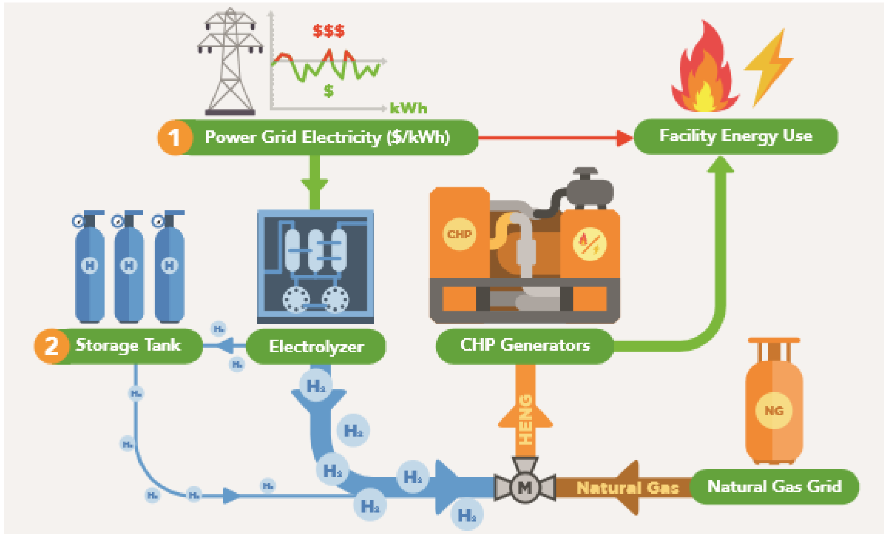


Figure 7: Simplified schematic of the industrial manufacturer's energy system including applicable hydrogen technologies.

A model is developed to simulate the blending of hydrogen into the CHP's natural gas stream while considering both the demand of the manufacturer for steam and electricity as well as the cost and carbon content of the energy grid to determine the optimal system sizing and operating conditions [80, 81]. In order to develop the model, it is important to define key system parameters including historical demand and pricing data, technical specifications of key hydrogen technologies as well as limitations of the existing energy hub components. One notable constraint is that the proposed configuration should provide the CHP with energy in the form of hydrogen-enriched natural gas (HENG) equivalent to the existing natural gas consumption. Moreover, hydrogen cannot be injected into the existing natural gas pipeline or consumed by end-use application (i.e., gas turbines) at a volumetric fraction of more than 5% without significant retrofitting of existing infrastructure [82].

Because the provincial grid imposes a lesser carbon footprint than that of gas turbines, any offset of natural gas by hydrogen reduces the carbon intensity of the system. This offset results in additional revenue, the amount of which depends on the carbon tax imposed by relevant governments and on the price below which the company decides to generate hydrogen. Once the energy system of the client is clearly defined, we construct the model with the objective of meeting the hourly electricity and heating demand of the facility while maximizing total revenue generated from a potential Cap and Trade or carbon tax market and natural gas consumption savings. The result is a system sized for optimal blending and an answer to the question of when to produce and store hydrogen. Based on this, we estimate the potential offset of greenhouse gas emissions and key financial metrics. This process will be repeated across a range of carbon prices and government-based capital grants with their effect on the net present value and internal rate of return of the project being investigated. Given projections developed for the province of Ontario's previous Cap and Trade program, we will vary the carbon price between $30 per ton and $100 per ton [4]. Regarding capital grants, investigating the effect of the integration of renewable energy and power-to-gas benefit industrial facilities [88, 89].

The logical flowchart for this mathematical methodology is outlined in Figure 2. The model is simulated over an entire year, and key performance indicators of the model such as total revenue generated and emissions offset are tabulated in the computational software MATLAB. Furthermore, to determine the optimal design conditions, two main operational variables, the storage coefficient and electrolyzer price threshold are manipulated. The price threshold is a logical condition in which past a certain hourly electricity price, the electrolyzer is not run and stored hydrogen is used to meet facility energy demand. Based on the distribution of electricity prices throughout the course of a year, this leads to opportunity for optimization. Secondly, there is the storage coefficient which is an operational variable which dictates the fraction of produced hydrogen stored versus sent to the CHP unit.

As previously mentioned, the simulation incrementally increases the limit on the electricity price, under which the decision is made to generate hydrogen. Deciding on a fixed price limit effectively prevents the simulation from achieving a global optimum while avoiding the necessity for tedious hourly optimization that would be costly to implement in practice for the company. If the Hourly Ontario Electricity Price (HOEP) falls below this value for a given time increment, no hydrogen will be sent from tank storage to the CHP unit; instead, it is sent directly from the electrolyzer to the CHP and to storage. In this case, the percent blending of hydrogen into natural gas is determined by taking the minimum of the infrastructure limit of 5% and the blending limit required to maintain the necessary power output from the CHP. Because hydrogen has a lower energy content than natural gas, as the percent blended at a fixed volumetric flowrate increases the total thermal and electrical energy produced decreases. As such, the total gas consumption must increase in order to meet the required industrial demand; however, it is constrained by the maximum flowrate that the turbine is rated for. As such, this constrains the allowable blending, the maximum of which is calculated in Equation (1), where E_{dem} represents the total required energy input to the turbine unit and the maximum flow of natural gas which for the system in question is 1700 m^3/h:

$$X(k)_{\mathrm{blend,power}} = \frac{E_{\mathrm{dem}}(k) - \frac{F_{\mathrm{max}}}{G_{\mathrm{NG}}}}{F_{\mathrm{max}}(\frac{1}{G_{H_2}} - \frac{1}{G_{\mathrm{NG}}})} \quad (2)$$

In this simulation a decision variable known as the storage coefficient, relates the total hydrogen generation to the amount sent to the CHP during periods of low electricity price. This is varied to determine the optimal storage rate balancing between the cost of storage capacity and the potential future savings as the HOEP climbs. It may seem surprising that not 100% of the hydrogen generated during low price scenarios is sent to storage and that some would be consumed in the CHP. This is because it is theoretically more efficient from both a cost and environmental perspective to directly replace CHP generation with grid electricity, as opposed to converting electricity to hydrogen and hydrogen back to electricity. However, this is not necessarily the case for two reasons; the CHP must always be operating in order to meet the steam demand and the capability of the equipment to ramp is highly constricted by a stark drop in efficiency, as well as costly wear on the machine. Therefore, if environmental incentives are in place, it remains a potentially viable solution to offset the significant footprint of burning natural gas. It was found that at a storage coefficient greater than 0.5, the amount of stockpiled hydrogen produced would often go unused, which would lead to unfavorable economics of the project. As such, in order to condense the scope of study the storage coefficient was ranged from 0 to 0.5. In the case where the amount of hydrogen sent to tank storage exceeds the inventory carrying capacity, production is scaled back to send only the maximum allowable amount, curtailing electrolyzer load.

For a case where electricity price exceeds the internal limit, the electrolyzer will consume no electricity and will produce zero hydrogen. Instead, all hydrogen injection into the CHP natural gas line comes from tank storage. The hydrogen blending percentage is taken to be the minimum of the infrastructure limit; the blending limit required to maintain power and the percentage were the entire inventory to be emptied due to injection as calculated in Equation (4).

$$X(k)_{blend,inventory} = \frac{I(k-1)}{F_{NG_{eq}}(k) + I(k-1)G_{NG}(\frac{1}{G_{NG}} - \frac{1}{G_{H_2}})} \quad (3)$$

Based on the determined blending percentage, the new overall and individual gas flowrates sent to the CHP are calculated as shown in Equations (3) through (5). The total hydrogen production is the sum of the blended amount and the amount sent to storage.

$$F_{T-CHP}(k) = \frac{F_{NG_{eq}}(k)G_{NG}}{(G_{comb})} = \frac{F_{NG_{eq}}(k)G_{NG}}{\left(X_{blend}(k)G_{H_2} + (1 - X_{blend}(k))G_{NG}\right)} \quad (4)$$

$$F_{NG-CHP}(k) = \frac{(1 - X_{blend}(k))F_{NG_{eq}}(k)}{\left(\frac{G_{H_2}}{G_{NG}} - 1\right)X_{blend}(k) + 1} \quad (5)$$

$$F_{H_2-CHP}(k) = \frac{X_{blend}(k)F_{NG_{eq}}(k)}{\left(\frac{G_{H_2}}{G_{NG}} - 1\right)X_{blend}(k) + 1} \quad (6)$$

Based on correspondence with the manufacturer a fixed value of \$0.19 per m^3 is set for the volumetric cost of purchasing natural gas. Applying emission factors for natural gas and for the electrical grid as listed by the Independent Electricity System Operator, the emission offset can be determined. While producing hydrogen will see an increase in electrical utility expenditure, it is also necessary to account for the increased consumption of water at the municipality's industrial rate. Based on the emission and natural gas offsets, the system's environmental and economic savings and expenses can be determined using the following formulae for any individual combination of production limit and storage parameters (Equations (6) and (7)).

$$\text{Revenue} = \sum_{k=1}^{8760} C_{Cap\&Trade}(EF_{NG}\Delta NG(k) + EF_{grid}\Delta E_{grid}(k)) + \sum_{k=1}^{8760} C(k)_{NG}\Delta NG(k) \quad (7)$$

$$\text{Expenses} = \sum_{k=1}^{8760} C_{grid}\Delta E_{grid}(k) + \sum_{k=1}^{8760} C_{H_2O}\Delta H_2O(k) \quad (8)$$

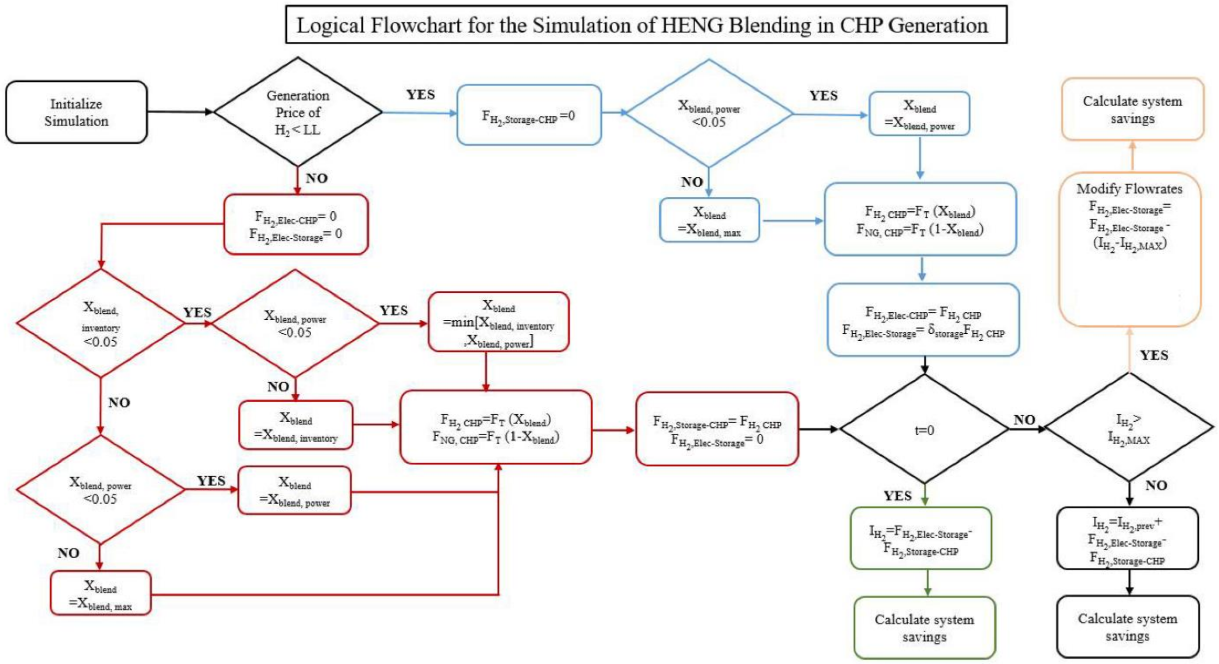


Figure 8: Outline of the simulation logic determining the amount of hydrogen to generate, produce and store within the power-to-gas system.

Before running the simulation across a range of operating parameters, the model was first tested on a select two weeks of data with a fixed price limit and storage coefficient in an effort to validate the effectiveness of the above equations. The following graph shows the resulting breakdown between energy generated by hydrogen and natural gas combustion, wherein the model continues to meet the total requirement for electricity and heating demand. While actual demand figures are shown only in percent form per the company's request, the hydrogen blending as indicated by the grey line is effectively modulated between 0–5%. The model chooses to supply the full 5% when possible to achieve the maximum emissions offset and return on investment, except for when the energy requirement reaches 96.5% of the system's maximum capacity. At this point, the hydrogen blending must be reduced in order to achieve the required output. The yellow portion of this line indicates when the model is calling for hydrogen to be released by the storage unit into the CHP. To demonstrate that the model is choosing these times effectively, the HOEP was overlaid to show this clearing corresponds to peaks in the local electricity price. As the amount of hydrogen blending increases, subsequently so does the total gas usage; however, there remains a net decrease in natural gas consumption of 1.6% over the two-week period (Figure 3).

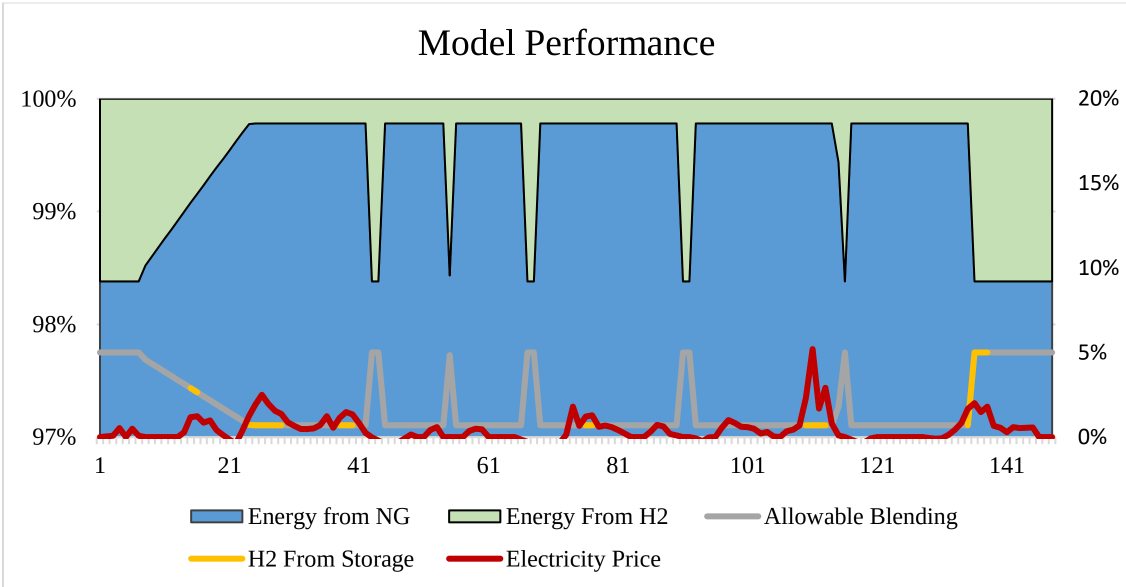


Figure 9: Two-week period of the model's operation, showing ability to select the appropriate blending percentage, as well as when to utilize stored vs. generated hydrogen based on the overlay of HOEP.

4.3 Technology Screening

In our simulation, we varied two parameters: the storage coefficient and the operational limit or minimum electricity cost required to run the electrolyzer. At each increment of these parameters, the economic and environmental benefit was calculated. Because the condition of the two decision variables impacted equipment size, we needed effective models relating capacity to capital to determine return on investment. In a P2G system of this type, there are three primary components: a hydrogen generation module, storage unit and compressor. In addition to this, considerations must be made regarding the piping, electrical, controls, and blending unit. For the purpose of this paper the focus will be directed toward the key P2G components as the remaining equipment is mature and similar to other compressed gas generation or consumption processes. For our purposes, these auxiliary installation costs will be built into the capital estimate of the electrolyzer.

4.3.1. Hydrogen Generation Module

Currently there are two types of electrolyzers widely available within the manufacturer's market for P2G applications: alkaline and Polymer Electrolyte Membrance (PEM). While alkaline does pose advantages in maturity and operating range, we will not consider this as a viable option due to the required ramp rates being on the order of hours [90]. This is simply not aggressive enough to effectively respond to changes in the Hourly Ontario Energy Price [91]. Instead, we select a

PEM system which, while not as mature, is widely available in the local market from suppliers such as Siemens, Proton Onsite and Hydrogenics. These systems offer increased purity, higher output pressures—but perhaps most important in reference to our application is the rapid ramp rate of up to 100%/s [92].

We determine the cost of the electrolyzer unit by applying a correlation presented by Saur [91] as expressed in the equation below. As the model determines the nominal hydrogen flowrate required for given system parameters, we can calculate the capital cost. It was also important to account for the electrolyzer's operation and maintenance costs as well as a single stack replacement halfway through the operational life equaling 35% of the capital cost as recommended through direct communication with the supplier. In terms of operating costs, it is considered that water will be consumed at a rate of 4.45 L per kg of hydrogen produced and will cost $2.16 per m3 with an annual upkeep of 2.5% capital cost [92].

$$C_{elec} = \$224{,}490(\dot{q}_{H_2})^{0.6156} \tag{9}$$

While the form of this equation is valuable, there has been significant work done in recent years to economize the electrolyzer. Because Saur presented this equation in 2008, we verify the accuracy by comparison with today's numbers. Mayyas, A., et al. performed a bottom-up cost analysis for this electrolyzer type and estimated a range of 500$/kW and 1100$/kW for a megawatt scale PEM dependent on global manufacturing rates [93]. Based on recent production figures reported by the International Energy Agency and assuming a 78% stack efficiency or 44.7 kWh per kg of H_2, we generate the following recalibrated formula [94-97]:

$$C_{elec} = \$88{,}568(\dot{q}_{H_2})^{0.6156} \tag{10}$$

4.3.2. Hydrogen Storage Units

The next significant component in the P2G system is the storage unit, which will be directly impacted by the model's selected storage coefficient, a fixed variable relating the production rate of hydrogen to the amount stored for later use at elevated prices. The total volume of the storage technology greatly impacts the system's capability to support grid ancillary services and offset the electricity consumption of the industrial manufacturer.

There are many potential options available for hydrogen storage which, for the most part, can be divided into three main categories: physical-based, material-based and underground storage [98]. Material-based chemical or physical sorption technologies are still in their infancy, and while they offer promising solutions to many of the problems associated with conventional methods, their storage density remains low, contributing to commercial unavailability. Bulk storage refers primarily to the pressurization of hydrogen in natural forming underground caverns, which must be sufficiently tight as to avoid permeability and be void of minerals rich in sulphite, carbonate or sulfates, so as to avoid acidification [99]. The specificity, combined with the required infrastructure modifications, lends itself to a very high capital cost for this option. As such, this leaves physical based storage methods—particularly compressed gas storage due to safety benefits we will detail later—as the preferred choice. Not only is compressed storage a mature technology, but it is widely commercially available, relatively inexpensive and capable of achieving storage volumes and pressures required for this installation.

The pressure requirement of the CHP unit is a relatively low 15.1 bar, and as such, the capability of the pressure vessel is influenced by the consideration of an inherently safe design, the cost of the pressure unit itself and the cost of the compressor. While significant research lead by organizations such as the Department of Energy looks towards more lightweight, higher density designs servicing the automotive sector, commercial tanks are readily available to handle pressures of up to a maximum 500 bar [100]. A study by James, B. D., et al. investigated in detail the cost of Type IV 250 bar compressed gas pressure vessels [101]. Based on an annual production of 10,000 systems per year in 2016, the estimated cost of an installed storage system is $5221(2007) per unit with each unit capable of storing 5.6 kg H2, which, after adjusting to 2020 values, gives $6580. We will calculate the volumetric storage of hydrogen by cumulatively adding the product of the storage coefficient and the hydrogen injected into the natural gas stream. The maximum point will determine the number of 5.6 kg storage units required by our system and thus the capital cost. In addition, we will account for an annual maintenance fee of 5% of the total.

4.3.3. Compressors

A compressor is required to take the hydrogen from the 20-bar outlet typical of PEM electrolyzers and bring it to the 250 bar for storage. Regarding efficiency, it is widely known that the two-stage double-acting reciprocating compressor has superior energy efficiency for high level gas compression [102]. In 2014, NREL, as part of work to design a hydrogen refueling station, surveyed several vendors and, based off this work, selected a two-stage diaphragm compressor of this type to increase hydrogen from 20 to 250 bar [103]. At that time, their particular system was designed to handle 33 kg/h of hydrogen. Furthermore, research is ongoing to improve the operation of diaphragm compressors specifically for the application of hydrogen, enabling low cost and long-life solutions for the unique challenges this gas presents.

From a costing perspective, there is not substantial literature that relates hydrogen specific compression capital to desired operating parameters. However, there are well established correlations for determining reciprocating compressors in general. One such graphical correlation was selected from Chemical Engineering Economics [104]. As per this publication, additional cost multipliers need to be accounted for, including a 1.25 times pressure-based correction factor, a 2.5 times stainless steel correction factor, a 1.49 installation factor and a 2.6 module factor.

4.4. Results and Discussion

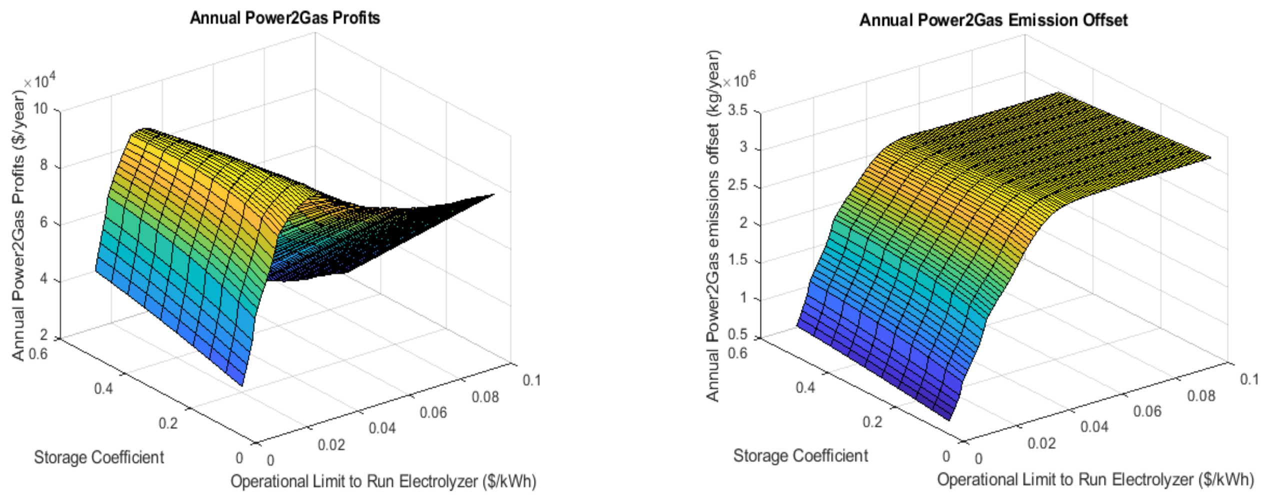
4.4.1. Economic and Environmental Analysis

The simulation is implemented across an entire year for each combination of generation price limit and storage coefficient. The result is a surface plot that shows the impact of storage coefficient and generation limit on the annual profit and emission offset of the proposed installation. For each parameter setting in the simulation, the maximum required hydrogen production rate and the maximum required tank storage capacity can be determined and used to estimate the system's capital and operating costs. Using this information, the net present value (NPV) and internal rate of return (IRR) for each scenario can be determined, and the optimal configuration can be selected for a fixed carbon price and capital grant incentive.

Figure 4 shows one example of a surface plot for the annual simulation with a carbon price of 30$/ton CO_{2e}. The maximum annual power-to-gas profit occurs at a storage coefficient of 0.15 and a price limit $0.031/kWh and is equal to $95,973 per year. As the carbon price is varied from 30$/ton CO_{2e} to 100$/ton CO_{2e}, the storage coefficient and price limit of the electrolyzer change; however, they remain unaffected by changes in the capital grant because it simply scales the price for the entire range of system sizes. In particular, the model will choose to store a higher amount of hydrogen at higher carbon prices, which intuitively makes sense given that the higher natural gas price will motivate the desire to offset a greater volume. Similarly, the general trend is to increase the operational limit to run the electrolyzer from 0.031$/kWh in the case of the lowest carbon tax up to 0.051$/kWh in the case of the 100$/ton CO_{2e}.

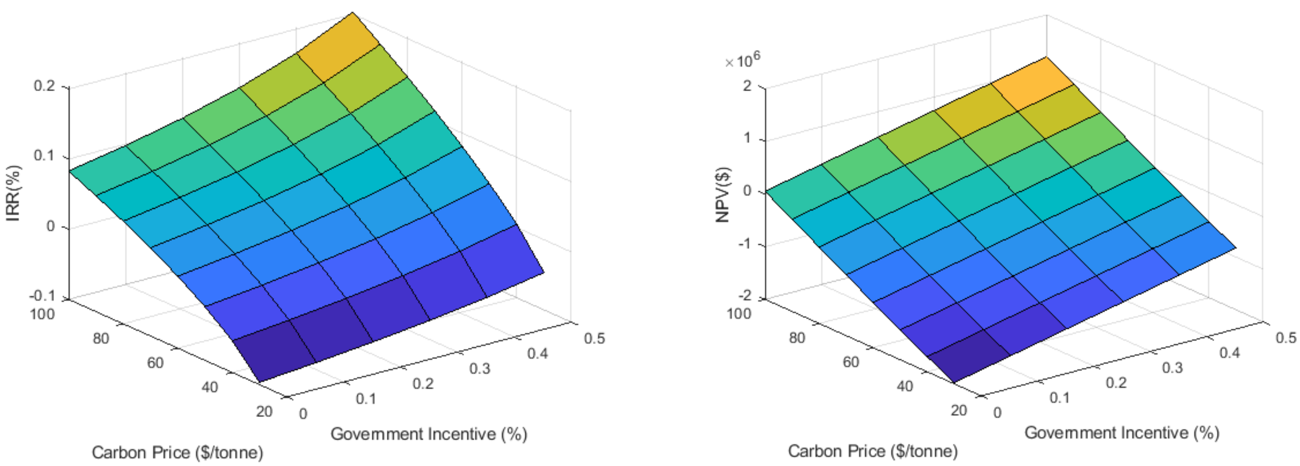
The environmental emission offset follows a similar pattern in regard to carbon price; however, is less sensitive than the profit (Figure 4 b). The surface plot shows that the environmental offset is fairly unaffected by the storage coefficient which can be derived from the fact that the actual amount of hydrogen blended into the system is not heavily dependent on this parameter, which is more likely to actually affect the cost of the hydrogen produced. The amount of carbon abated increases rapidly with a change in the electrolyzer's operation limit, similar to that of the power-to-gas profits. This asymptote indicates the point where the maximum amount of hydrogen blending is achieved. This also explains why the system profits reach a maximum at this point: as the amount of hydrogen generated may increase the cost, no more can be used to offset natural gas. For the $30 per ton case, a total CO_{2e} offset of 2630 tons was realizable. In cases where the maximum available revenue and desired emission offset, either internal decision makers are tasked with weighing the tradeoff or the problem must be transferred to a multi-objective optimization problem.

Because electrolyzer size was not considered a constraint in the model, the range and frequency of hydrogen production values were recorded and used to suggest a nominal capacity. Correlations published by Mukherjee et al. [83] agree with regional market data (NextHydrogen. Personal communication, December 2018) collected from a local supplier on the per installed kilogram price of electrolytic hydrogen systems [105]. Using this information, 48 separate possible incentive schemes are analyzed, incrementing carbon price by 10$/ton CO_{2e} from 30$/ton CO_{2e} to 100$/ton CO_{2e} and capital incentive by 10% of initial cost from 0% to 50%. The IRR and NPV for the entire range of data is presented in Figure 5.



(a) (b)

Figure 10: Surface plots illustrating the effect of changes in the storage coefficient and the operational limit on the electrolyzer on the annual power-to-gas profits (a) and emissions offsets (b).



(a) (b)

Figure 11: Surface plots illustrating the effect of changes in the carbon price and the government capital incentive on the annual Internal Rate of Return (a) and Net Present Value (b).

Based on the criteria of a positive NPV at the Company's 8% hurdle rate and suggested 25-year lifespan and an IRR greater than that of the hurdle rate, 16 scenarios prove to be economically viable. These 16 scenarios define the feasible region of Figure 4 and show that as the capital grant increases from 0–50%, the carbon price necessary to guarantee profitable returns decreases from 100$/ton CO_{2e} to 60$/ton CO_{2e} assuming discrete 10$ increments (Table 1). While certain scenarios do achieve profitability, the net present value may not be significant enough to incentivize the organization to undertake such a development. An example of this occurs when the capital incentive is fixed at 0% with a 100$/ton CO_{2e} carbon price and a NPV of $53,240 results. In such a project, the importance of power-to-gas must be argued on grounds of non-economic means. That is the importance of an environmental offset (which in this case would be approximately 3073 ton CO_2/year) above and beyond that of direct financial remuneration should be taken into account. In this case, the company in question has set a net-zero reduction target by the year 2050; as such, this problem should be converted to a multi-objective optimization, a topic for future work [85,106].

In the best case, we see a potential return of $1,207,477, a significant amount given the capital investment of $1,152,348. This results in a simple payback of 3.8 years, well within the company's requirements for projects of this scale. However, this scenario will require a capital grant incentive of 50% with a carbon price of 100 $/ton CO_2. It is important to note that while capital incentives have a significant and direct effect on the project's IRR, favorable NPVs can still be realized at lower capital incentives, so long as the carbon price remains sufficiently high. The most promising perhaps is the $745,782 NPV available at 100$/ton CO_{2e} and 30% capital incentive. Such capital incentives are immediately realizable through organizations such as the Low Carbon Economy Fund which offers to cover 25% of the capital investment made by large businesses in projects that reduce CO_2 while stimulating the economy [107].

From an environmental standpoint, the amount of carbon offset by the model falls within a range of 3046 ton CO_2/year to 3073 ton CO_2/year and increases with the corresponding carbon price at a rate less than that seen by the financial metrics. Based on this analysis, in order for the project to be economically profitable, a $60/ton CO_{2e} tax must be implemented.

Table 1. Feasible solutions (shown in green) to the simulation showing favorable economics under carbon prices greater than 60$/ton CO_{2e}.CAD-Canadian Dollars.

Capital Grant Incentive	Carbon Price ($/ton CO_{2e})	Overall Capital Cost	Internal Rate of Return	Net Present Value(CAD)	Annual Profit (CAD)	Environmental Offset (ton CO_{2e})
30%	100	1,613,287	13.76%	745,782	302,890	3073
40%	70	1,382,817	8.74%	77,021	211,263	3046
40%	80	1,382,817	11.48%	376,126	241,728	3046
40%	90	1,382,817	14.06%	675,232	272,192	3046
40%	100	1,382,817	16.56%	976,629	302,890	3073
50%	60	1,152,348	8.12%	9917	180,916	3020
50%	70	1,152,348	11.42%	307,868	211,263	3046
50%	80	1,152,348	14.51%	606,974	241,728	3046
50%	90	1,152,348	17.45%	906,079	272,192	3046
50%	100	1,152,348	20.33%	1,207,477	302,890	3073

4.4.2. Results: Safety Analysis

Any review of the potential applications of power-to-gas and the hydrogen economy is incomplete without some discussion regarding the potential mitigation of potential safety risks. Recent local industrial installations have sparked controversy regarding the potential hazard to local communities; therefore, it is necessary to address this even in the design phase.[111] By identifying these risks, the appropriate safeguards can be implemented to mitigate the likelihood of failure, prioritizing the safety of all stakeholders and easing community concerns. The proposed design, while implementing relatively mature technology, is novel within the regional market and, because it involves blending highly flammable substances, must be treated with particular attention to global as well as local best practices and standards.

While hydrogen's applications are promising, a significant hurdle to widespread use is the lack of well-established codes for stationary storage and its integration to our existing energy distribution framework [113]. Hydrogen is a very reactive chemical that poses significant fire and explosion hazards. Further, systems for hydrogen storage and transport require special materials of construction to prevent the escape of the very small molecule from its container; this is made even more challenging by the fact that hydrogen must be stored at high pressure to be sufficiently energy dense for practical purposes. Additionally, unlike hydrocarbon-based gaseous fuels (such as natural gas), chemical tracers cannot be used to make leaks more detectable to humans (either visually or through odor), as they cannot diffuse as fast as hydrogen [114].

Considering this, any hydrogen storage and distribution systems installed during this period of time (while the technology is not common-place) must be subject to stringent safety analyses to ensure that unexpected and unforeseen hazards can be mitigated and that public safety is not endangered.

4.4.2.1. Failure Modes Effects and Analysis

The first aspects to examine are inherently safer design principles and passive mitigation techniques. Conventional chemical industries use hydrogen as a reactant in continuous processes, thus minimizing the amount "stored" in the pipes significantly (hydrogen is only produced as it is used) [115].. This inherently safer design approach is entirely infeasible for the use of hydrogen as an energy storage medium, and thus it cannot be applied to the proposed energy storage and distribution systems.

This does not mean that inherently safer and passive design principles cannot be applied. In fact, it is crucial to consider the impact that materials of construction and equipment design can have on the likelihood of hydrogen release. Consider that hydrogen-containing equipment under pressure is particularly susceptible to hydrogen embrittlement. This process can proceed through a variety of mechanisms and affects most common materials of construction (e.g., iron, steel) [117]. By selecting materials and design strategies to minimize the risk of equipment failure, the likelihood of release is significantly decreased.

One aspect of passive equipment design that is often overlooked is the connections between process equipment and piping systems. Flanges in particular are a "weak spot" in many piping systems; if there is a leak of hydrogen from high temperature and pressure line, a jet fire often results [118]. This can heat the flange bolts and cause them to lengthen (this effect is exacerbated if it is a long-bolt flange), resulting in a larger leak and larger jet fire. Thus, welded connections should be considered whenever possible, and precautions should be taken in flange size and gasket selection to avoid jet fire occurrence.

While passive design principles are often the method of choice, active safeguards are an integral part of any successful design. The most common active safeguard in hydrogen systems is the pressure relief valve (PRV or PSV). These are devices with a carefully calibrated spring set to open at a specific pressure so as to avoid overpressuring the equipment. The valve can be directed to discharge to a flare header or to another safe location to control the venting of flammable materials [119].

While passive design principles and pressure relief equipment help minimize the risk of leaks, they do not eliminate it entirely; as such, it is important to have equipment that can detect leaks or fire and alarm to alert operators of the loss of containment. Infrared detection and other explosion monitoring sensors (e.g., Lower Explosive Limit (LEL) detectors) can be used near hydrogen generation, storage, and transport equipment to reduce the severity of such loss of containment events [119].

The last line of defense for industrial hydrogen safety is procedural safeguards. The most common ones employed in industry are facility-siting regulations and hot-work permitting systems.

Facility siting, often combined with required industrial electrical classification determinations, is used to provide guidance as to where certain types of equipment can be used. It is common to ban non-intrinsically safe devices and internal combustion engines (or anything else that could inadvertently ignite a hydrogen leak) from process areas where hydrogen is used.

Hot-work permitting systems are used to stringently regulate where, when, and how “hot work” (work that can generate sparks or other ignition sources) is performed on an industrial site. These permitting systems are often accompanied by gas testing procedures, grounding requirements for electrical equipment, and spark watch/fire watch requirements for any work that could result in the ignition of flammable substances.

If all of these planned safeguards fail, emergency response is used to mitigate the effects of the event once it has started. This involves having appropriate hydrogen emergency response training for plant operators as well as regular communication with local authorities to coordinate emergency response efforts. Because the required training and communication is heavily dependent on facility location and the specifics of the chemical process, a more detailed discussion will not be presented.

NFPA 2, the Hydrogen Technologies Code, can be relied on for most regulatory direction and safety requirements for these systems. As such, it will be the main resource for the work that follows. All standards referenced in this paper can be found listed in Appendix A. The following standards, some of which are referenced by NFPA 2, will also be consulted:

NFPA 68 (Standard on Explosion Protection by Deflagration Venting)

NFPA 69 (Standard on Explosion Prevention Systems)

NFPA 70 (National Electrical Code)

CGA G-5.5 (Hydrogen Vent Systems).

4.2.2. Power-to-Gas Design Considerations

To mitigate the failure of individual technologies within the power-to-gas system, it is necessary to develop an inherently safer design. In this section, we will highlight some of the more important features in the safe design of a hydrogen enrichment system.

Safety for Compressors and Storage: Compression and processing equipment for gaseous hydrogen is regulated under sections 7.1.15, 7.1.20, and 7.1.21 of NFPA 2. As a baseline for structural protection, the equipment foundations must be engineered to prevent frost heaving, and the equipment must be protected from vehicle damage. The compressors themselves are also subject to stringent pressure protection; each compressor must have discharge pressure monitoring and must be equipped with check valves at the outlet to avoid over pressurizing weaker equipment upstream in the event of backflow. Further, each compressor must be outfitted with valves so that each compressor can be easily isolated from the system for maintenance. Each compressor must also be outfitted with pressure protection that has appropriate relieving capacity for abnormal operating conditions. All equipment used in the system must be specified for hydrogen service. Finally, because the equipment will operate unattended, it must be outfitted with a high discharge and a low suction pressure automatic shutdown control.

Pressure protection must be provided throughout the system; NFPA 2 specifies that the pressure relief device discharge must be compliant with CGA G-5.5. This provides specific information on the required length-to-diameter ratio of the discharge piping, as well as guidelines to prevent pluggage or obstruction of the vent. Pressure relief valves or rupture discs should be installed on the compressor, electrolyzer, storage tanks and in areas of the piping network where there is potential to have isolated spikes in pressure. All piping, fittings, and components should contain a CRN number and the design must be registered and assigned a P# via the Technical Standards and Safety Authority. Next, pressure and temperature indicators must be installed in and around the process units, always providing workers the operating conditions of the systems.

Whether or not the quantity of gas meets the conditions for a bulk system (more than 3.96 m^3 of hydrogen), installing the system in a gas room or a detached building will be the safest storage method. The building or room must be built of noncombustible or limited-combustible materials and must be outfitted with mechanical ventilation at a rate of at least 1 scf/min per square foot of floor area in the storage space. The vents must be installed within 0.3 m of the ceiling (because hydrogen is much lighter than air) and the ventilation system must operate continuously [116].

Explosion control must also be provided, either by means of explosion prevention in compliance with NFPA 69 or deflagration venting in compliance with NFPA 68. Vessel construction must adhere to relevant pressure vessel codes and must have a suitable method of pressure relief [116].

The room will be subject to electrical requirements specified in Article 501 for Class 1, Division 2 areas according to NFPA 70, and heating must be provided by steam, hot water, or other indirect means. The space should be secured against unauthorized entry [116].

Safety for Electrolyzer: The process of water electrolysis is hazardous mostly due to its products and the amount of energy that must be put into the process. Electrical hazards can be mitigated by following NFPA 70 for all high-voltage lines and equipment. Ensuring that the oxygen and hydrogen are collected separately will reduce the risk of hydrogen ignition, and installing leak detection systems as well as automatic shut-down interlocks should reduce the risk of oxygen or hydrogen gas build-up [116]. Intensive separation equipment is not required because the oxygen and hydrogen are already separated at their collection points. However, the pure oxygen that forms can be very hazardous because it can create a flammable atmosphere. To prevent an oxygen-rich atmosphere from forming near the electrolyzer, the oxygen should be vented outside, and gas monitors should be installed near the electrolyzer to detect leaks of either O_2 (any concentration exceeding 23.5% oxygen being unacceptable) or H_2 (any amount exceeding 25% of the Lower

Explosive Limit being unacceptable). The unit must also contain constant monitoring of key process parameters including flowrates, pressure and temperature to avoid damage to the membrane causing mechanical failure and the release of explosive gas. It is also important that the system is monitored and interlocked to the water level to avoid running dry.

Safety for Hydrogen-Enriched Natural Gas Pipelines: Most of the hydrogen produced will be consumed in the CHP; in order to ensure that the integrity of the existing equipment will not be compromised, the hazards associated with transporting hydrogen in pipelines should be considered.

The major consideration is how the inclusion of hydrogen in the natural gas stream might affect the mechanical integrity of the piping system. Certain metals (particularly, cast iron and some kinds of steel) should not be subject to more than 5% hydrogen in the pipeline by volume, or else they risk being embrittled by the hydrogen gas; this is very undesirable considering the high temperature and pressure to which the system is subjected. However, some types of steel could handle hydrogen concentrations of up to 20% without modification [82].

The end use equipment (that is, the CHP turbine itself) is also subject to limitations in hydrogen content. It is estimated that the end-use device for this system can handle a hydrogen content of 5% at the most; if retrofitted at additional capital cost, up to 40% hydrogen could be used in the turbine. If small volumes of hydrogen are used, there should be no mechanical integrity concerns with either the piping or the CHP; if more significant amounts are to be used, then the CHP will certainly require a retrofit, and other system piping and pipe fittings may need to be upgraded.

Local regulations place a limit on the change in rate of hydrogen injection of 2%/min due to the potential of over pressurization. To mitigate this, pressure sensing devices will be connected to the regulator via the programmable logic controller's (PLC) control circuit to ensure this amount is not exceeded. To prevent risk of explosion and failure due to embrittlement, all material will be rated to schedule 80 and built according to ANSI.ASME B31.3. Furthermore, LEL monitoring should be present at all times near high-risk areas to detect potential hydrogen leaks.

It should be noted that hydrogen blending will not introduce additional electrical area classification requirements, as the area should remain classified as being a space where flammable gases are handled inside of a process but should not escape unless there is a process upset (Class 1, Division

2). However, for existing leak detection systems to be able to detect hydrogen leaks, gas detection equipment should be installed near the ceiling of the building containing the CHP. Further, existing pressure safety valve contingency studies should be revisited to ensure that blending hydrogen into the natural gas does not change the required relief capacity. A full summary of the Failure Modes and Effects Analysis of the system can be found in Table 2.

Table 2. Summary of the Failure Modes and Effects Analysis of the power-to-gas HENG system noting the potential control measures available to mitigate risk.

Process Function	**Failure Mode**	**Severity**	**Potential Effect(s) of Failure**	**Detectability**	**Potential Cause(s)/Mechanism(s) of Failure**	**Occur**	**RPN**	**Relevant Codes/Standards**	**Potential Control Measures**
Hydrogen Dispensing	Operation error	6	Leakage leading to deflagration	4	Human error	3	72	1	Periodic training for operator certifications
	Rupture of underground pipes	8	Leakage leading to deflagration	6	Corrosion due to cold temperatures	2	96	1,3,4,5,6	Apply corrosion-resistant coating. Use thicker piping (Schedule 80)
	Backflow of gas	7	Pressure buildup leading to explosion	3	Power outage	3	63	1,3,4,5,6	Back-up power storage
Storing Hydrogen	Tank level at lower limit	6	Implosion	3	Uncontrolled outlet flow or failure of control valves	3	54	1,3,5,6,7,8	Low level sensor interlocks and alarms. Preventative maintenance of valves

	Overflow	7	Release of H2 leading to deflagration	3	Uncontrolled inlet flow or failure of control valves	3	63	1,3,4,5,6,7,8	High level sensor interlocks and alarms. Preventative maintenance of valves
	Underpressure	7	Implosion	3	Decreased temperature or uncontrolled outlet flow	2	42	1,3,4,5,6,7,8	Pressure indicator interlocks and alarms. Preventative maintenance of valves
	Overpressure	7	Gas buildup leading to explosion	4	Increased temperature or uncontrolled inlet flow	2	56	1,3,4,5,6,7,8	Pressure indicator interlocks and alarms. Preventative maintenance of valves
	Fracture	7	Leakage leading to deflagration	6	Forklift collision	2	84	1,3,4,5,6,7	Safeguards and barriers implemented to protect transfer areas
	Heated storage tank	9	Pressure buildup leading to explosion	5	External fire	1	45	1,5,6,7,9,10,15,16,17,18	Instantaneous fire suppression systems. Install temperature sensors
Hydrogen Compression	Overpressure	7	Gas buildup leading to explosion	4	Failure of control valves	2	56	1,3,5,8	Pressure indicator interlocks and alarms. Preventative maintenance of valves

	Heated compressor	10	Pressure buildup leading to explosion	5	External fire	1	50	1,3,5,6	Instantaneous fire suppression systems. Install temperature sensors
	Backflow of gas	7	Leakage leading to deflagration	3	Reduced inlet pressure	2	42	1,3,5,6	Implement check valves
Electrolysis	Oxygen accumulation	7	Combustion	6	Blocked vent for oxygen gas	2	84	5,8,11	Preventative maintenance inspections. Gas detectors in place
	Gas leaks	6	Combustion	4	Failure of control valves	3	72	5,11	Gas detectors interlocked with electrolyzers
	Water purification failure	3	High levels of impurity	3	Impurity and residue build-up	3	27	5,8,11	Sensors in place to detect purity of water interlocked with shutting down electrolyzer. Preventative maintenance inspections
	Electric charge builds up	6	Potential ignition source	2	Low water levels, improper wiring	3	36	5,8,11	Level sensors for water interlocked with electrolyzers

Hydrogen Enriched Natural Gas in Pipelines	Hydrogen embrittlement	6	Gas buildup leading to combustion	7	H_2 concentration introduced too high	2	84	3,4,12,13	Apply corrosion-resistant coating. Use thicker piping (Schedule 80)
	Plugged Line	7	Pressure buildup leading to explosion	3	Manually closed valve	3	63	3,4,5,12,13,14,19	Proper lock-out & tag-out procedures
	Overshoot hydrogen injection limit	7	Pressure buildup leading to explosion	4	Increased percentage of hydrogen pipelines	3	84	3,4,12,13,14	Invest in dedicated gas engines with sophisticated control systems. Control inlet of hydrogen to be < 2% min^{-1}
	Excavation damage	9	Combustion	6	Human error	2	108	3,4,5,12,13,14,19	Safeguards and barriers implemented to protect transfer areas
Process Control Systems	Uncontrolled flows into process units	6	Pressure buildup leading to explosion	3	Control system failure	4	72	4,5	Depending on the process, the valves should be programmed to be fail-safe and open/close upon failure
	Overpressure of	6	Pressure buildup	3	Valve failure or blockage in pipe	6	108	4,5	Valves should be fail-safe. Pressure relief valves and rupture

	process units	leading to explosion			discs should be in place

4.5 Nomenclature

G_{NG} = HHV Natural Gas, G_{H2} = HHV Hydrogen, HOEP=Hourly Ontario Energy Price, LL = Limit on H2 generation price, $X_{blend,\ inventory}$ = H_2 Volume Fraction Sent to CHP After Inventory Dump, $X_{blend,\ power}$ = Maximum Volume Fraction of H_2 to Maintain Electrical Power, $X_{blend,\ max}$ = Maximum Volumetric Blending, X_{blend} = Actual Volumetric Blending, $F_{H2,Elec\text{-}CHP}$ = H_2 sent from Electrolyzer to CHP, $F_{H2,\ CHP}$ = H_2 sent to CHP, F_T = Total Gas Sent to CHP, F_{max} = Max flowrate to CHP, $F_{NG,\ CHP}$ = NG Sent to CHP, $F_{NG_{eq}}$ = Equivalent natural gas flowrate required to achieve energy demand, $F_{H2,Storage\text{-}CHP}$ = H_2 sent from Storage to CHP, $F_{H2,Elec\text{-}Storage}$ = H_2 Sent from Electrolyzer to Storage, δstorage = Storage Coefficient, t = Current Time Stamp, I_{H2} = H_2 in Inventory, $I_{H2,MAX}$ = Inventory Maximum Capacity, $I_{H2,prev}$ = Previous Hour's H_2 Inventory

4.6 Relevant Codes and Standards

Reference Number	Relevant Standard
1	OHSA 1910.103
2	SAEJ2600
3	CAN 1784-000
4	ASME B31.12
5	NFPA 2
6	NFPA 55
7	FSM Division 13.03
8	ISO-TC 58
9	FSM Division 13.02
10	FSM Division 16.06
11	ISO 22734-1:2008
12	ASME B31.3
13	ASME B31.9
14	SAE J2578
15	NFPA 70
16	NFPA 72
17	NFPA 110
18	NFPA 170
19	NFPA 52
20	NFPA 68
21	NFPA 69

5.0 Conclusions

In general, the necessity for lower carbon emissions across all sectors has prompted exponential growth of renewable energy generation. Inherent to this technology is intermittency, which proves greatly problematic when balancing grid supply and demand. As a result, there is a global demand for efficient, large, long-term energy storage solutions that capitalize on the capture of off-peak, low carbon energy. The development of Power-to-Gas, has in recent years, not only served as a solution for balancing grid inefficiencies but has provided several potential pathways to decarbonize end-use applications. While this technology is already proven on the utility side, major industrial operations can now begin to target reductions in a range of carbon intensive processes with minimal initial modifications to process equipment. Power-to-gas can support renewable curtailment all while introducing green content to transportation, hydrogenation, power generation, and natural gas, while offering many benefits over alternative storage solutions including length, capacity, size and cost.

With this said across Ontario and the rest of Canada the uptake of hydrogen technology has been relatively slow when compared to certain States in the U.S.A and across Europe. In this thesis we were successfully able to demonstrate that either through layering of hydrogen pathways or an appropriate government incentive structure there is an opportunity for payback period's less than 2 years and with substantial emissions offsets that see 2050 target reductions become relatively obtainable. We were also able to address the question of whether hydrogen could be safely implemented at the industrial scale, highlight major risk factors, and propose sound countermeasures that are in alignment with Provincial and National legislature. It is necessary to prevent these sorts of robust and versatile case studies that develop models that can be applicable to multiple industries and applications. Profitable and safe demonstration projects will lead to increased uptake which in turn leads to improved capital and operating costs of installations.

5.1 Conclusions from A Layered Analysis of Multiple Revenue Streams at a Southern Ontario Automotive Manufacturer

The primary objective of this work was to develop a safe and economically feasible design for a Power-to-Gas system that generates hydrogen for cross market uses and that is capable of supporting renewable generation and ancillary services. This design was developed for an automotive manufacturer resulting in a payback period of 2.8 years with an annual emission offset of 2359.7 tonnes CO_{2e}. This submission won the Second Place prize at the 2018 Hydrogen Student Design Contest organized by the Hydrogen Education Foundation.

Initially a mathematical model was developed to simulate the energy hub, defining important system parameters, such as demand, hydrogen requirement, and technical specifications. The energy management dispatch strategy was optimized using a mixed integer programming model in both GAMS and MATLAB, which was later adapted to incorporate Power-to-Gas storage and redistribution pathways, suggesting the ideal sizing and number of energy hub components.

The installation of the Power-to-Gas system requires a total capital investment of $2,620,448. The electrolyzer and 1500 solar panels will account for 41% and 17% of the capital costs, respectively, as they are major processes used to supply electricity and hydrogen gas. The compressors accounts for most of the operating costs which total $237,653. 76,073 kgH2 per year can be produced for all the end-use applications. Based on a sensitivity analysis, the annual revenue for selling hydrogen at $1.5 to $12 per kgH2 can sum to $54,741 to $437,928. In the modelled carbon tax program, CO2 allowances can be sold at $18 to $30 per tonneCO2 and the model predicts a CO2 offset of 2359.7 tonnes. The optimal streams of revenue include selling hydrogen at $12 per kgH2. With a combination of these optimal revenue streams the automotive manufacturer can expect a payback period of 2.8 years. Finally, the policy analysis of implementing Power-to-gas system in Ontario are investigated.

5.2 Conclusions from Profit Sensitivity to Policy Condition and Technological Safety Analysis

The use of hydrogen enriched natural gas to offset the carbon intensity of fossil fuels in industrial combined heat and power microgrids has shown favorable financial and environmental potential given a significant enough provincial or federal carbon tax. Our system used electricity from Ontario's provincial grid to convert water into hydrogen in a 345 m^3hr^{-1} PEM electrolyzer. This hydrogen was compressed to a pressure of 172 Bar using a Greenfield reciprocating compressor and either stored for later use in 89 kg tanks or sent directly to a blending system to be injected into the combined heat and power plant's natural gas stream.

Currently realizable capital incentives can see IRRs as high as 13.76% with net present values of approximately $750,000. To realize financial feasibility, the carbon price in Ontario must achieve or exceed a minimum of 60$/ton CO_{2e}. In Ontario, the carbon price is currently 20$/ton CO_{2e}; however, it is projected to increase to 50$/ton CO_{2e} by 2022. The feasible region ranged from 100$/ton CO_{2e} with 0% capital grant producing an IRR of 8.31% to 100$/ton CO_{2e} and 50% capital grant corresponding to an IRR of 20.33%. In all economically feasible, cases the system operating under an optimal storage coefficient and operational limit produced an emission offset greater than 3000-ton CO_2 per year. The system's finances were relatively sensitive to changes in the operational limit of the electrolyzer; however, they plateaued after maximum available blending was achieved. As such, improving blending tolerances could allow for significant increases in the economic viability of the project. While a 5% maximum was considered in the simulation, given a thorough assessment and modification of the infrastructure and end-use application compatibility, it would not be unreasonable to see this number increase into the range of 10–20% in the future.

Hydrogen has been a part of industrial operations for decades, and as such, there is a significant precedent for its safe use. While the proposed uses of hydrogen for this project are less well-established, existing knowledge for the safe storage and handling of flammable gases as a fuel source can be coupled with the knowledge of hydrogen-specific hazards to develop a comprehensive safety management strategy.

New generation and storage systems should be designed to state-of-the-art standards for materials of construction (to avoid hydrogen embrittlement) as well as pressure protection and leak detection; facility siting is also paramount to ensure that risk is minimized. Existing infrastructure that will now be handling hydrogen gas (i.e., CHP and associated piping) should be rated for a maximum hydrogen content to ensure that the material is not weakened by the blending of hydrogen, and advanced hydrogen detection systems should be installed near the ceiling to detect any accumulation of hydrogen in enclosed areas. Refueling stations should be designed to industry standards, including modern safety features such as automatic shutoffs and breakaway hoses. Finally, hydrogen fuel cell vehicles should be designed to minimize the quantity of hazardous materials carried on board, and rigorous preventative maintenance should be performed to ensure that all safety devices associated with the vehicles are functioning properly.

As with any other potentially hazardous chemical, the existence of the hazards does not mean that the process cannot be made safe. If appropriate steps and mitigations are taken to ensure that the system poses negligible risk to the industrial site and surrounding community, a hydrogen generation, storage, and use system can be built to optimize the energy consumption patterns for the industrial site.

While the proposed system can achieve favorable economic and environmental outlooks, given the right incentive structure, it would not be feasible if it could not be operated safely. A Failure Modes and Effects analysis was carried out that identified 22 possible failures amongst 6 critical control points. After reviewing relevant codes and standards for hydrogen-based systems in Ontario as well as applicable national standards, active safeguards were suggested to mitigate the risk associated by each failure mode. In doing so, we can conclude that a power-to-gas system implemented on the industrial scale in Ontario would not only see favorable returns given the correct regulatory climate but also would not impose any significant risk to the public or to the plant.

5.3 Recommendations

From a modeling perspective this work utilized published correlations to determine capital cost. As demonstrated by Al-Subaie et. al. and by our work focusing on government incentives the payback of Power-to-Gas is greatly tied to improvements in technology pricing. Therefore, it would be beneficial to expand this thesis to include actual quoted numbers from multiple suppliers, or update the correlations based on 2021 data. Furthermore, it is value added to investigate the relationship between the decreasing capital cost of hydrogen technologies and the increase in manufacturing rates to determine how future payback will be impacted by development rates.

Both papers presented in this thesis focused mainly on a manufacturing environment and the potential hydrogen pathways that are commonly present. However, it may be valuable to investigate case studies of niche industries, particularly those that utilize hydrogen or oxygen in end use applications. In particular hydrogen has long been considered one of the most promising options for consumer transport, however the delay in implementation can be attributed to a significant lack of refueling infrastructure and the overall cost required compared to battery electric vehicles that can be recharged using existing systems. With that said battery vehicles become less feasible when considering large load, long haul trucking where the physical space required for batteries detracts from the payload. Trucks that take similar routes in local networks could highly benefit from a few centralized hydrogen refueling stations. This becomes an attractive option for any industry that utilizes transport trucks and could pose as a significant revenue stream. Incorporating this into the model not only for a single manufacturer, but for a local network could prove to be highly profitable.

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