Design optimization of an electrolytic hydrogen for the Sarnia-Lambton upgrader

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Abstract

The proposed bitumen upgrader in the Sarnia-Lambton region refine diluted bitumen into naphtha, diesel and heavy gas oil. A key step in this process is hydrotreating, in which the fed hydrocarbons are saturated with hydrogen, and impurities such as nitrogen and sulfur are removed. According to the Canadian Nuclear Society, in Ontario, approximately 60% of the power generated comes from nuclear energy, the remainder is composed of hydro, gas, wind, solar and biofuels. However, due to the inflexibility in nuclear and wind productions, and the increased efficiency of appliances and equipment, Ontario is left with an excess base load of electricity. The aim of this study is to evaluate the techno-economic feasibility of an electrolytic-hydrogen production plant that utilizes this excess electricity with the goal of minimizing total cost and emissions. Load-shifting using compressed storage is considered, and total cost compared with conventional methods, namely steam methane reforming. A total of five control algorithms are developed and compared to one another. From these, optimal performance in cost and CO_2 reduction is observed when historical electricity price data is directly used.

Keywords
Upgrading hydrogen, optimization, electrolysis

1. Introduction and background

Unrefined diluted bitumen is exported to the USA from Alberta, motivating major oil companies and Canada to propose the construction of a bitumen upgrader in the Sarnia-Lambton region. This upgrader will allow Canada to export naphtha, diesel and heavy gas oil directly to the USA, increasing the value of Canada's energy exports. Hydrotreaters are critical to the upgrading process. Hydrotreaters saturate the diluted bitumen with hydrogen and remove impurities, such as nitrogen and sulphur. Therefore, hydrogen must be supplied to the upgrader meeting the demands of the hydrotreaters. A simplified schematic in Figure 1 shows where the hydrogen is required in the upgrading process.

The most commonly used hydrogen production method is steam methane reforming (SMR) which emits the second highest amount of CO_2 out of all hydrogen production methods. Therefore, the goal of this project is to design and optimize an industrial scale hydrogen production system that will meet the upgrader demands while reducing total emissions. Special attention will also be given to energy efficiency and cost. The optimization of the proposed system will be accomplished by running various simulations in MATLAB. Based on this information a set of design objectives were developed. These objectives of this study is to design a hydrogen production system that will: 1) supply the required amount of hydrogen to the upgrader at all times, 2) reduce CO_2 emissions associated with the hydrogen production, 3) incorporate renewable resources, either directly in hydrogen production, or indirectly to supply energy to the process, 4) maximize energy efficiency, and 5) minimize cost.
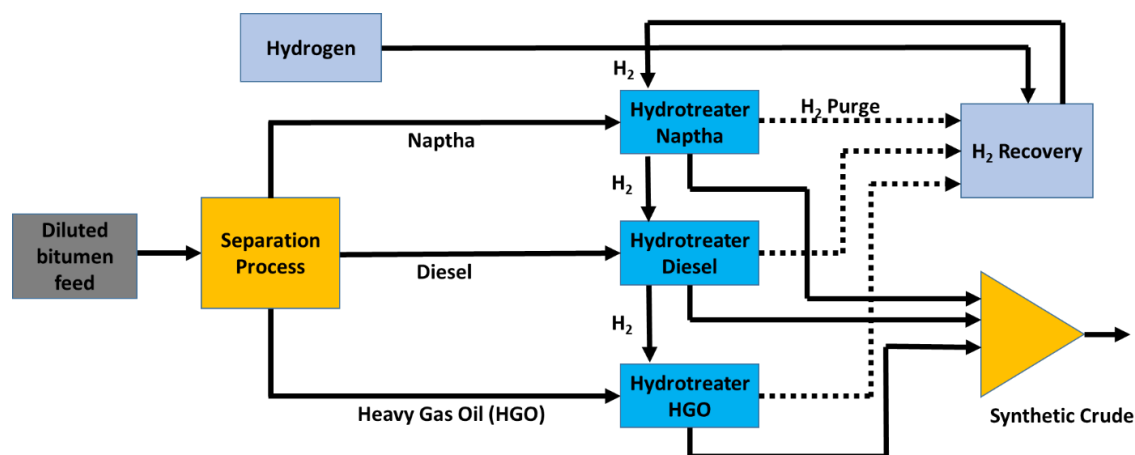
Figure 1. Section of the upgrader considered in this study

The suitable hydrogen production process chosen is electrolysis, the details of this selection process is outlined in the report. The project deliverables include an optimized model of hydrogen production plant design, that determines when hydrogen will be sent directly to the bitumen upgrader plant or when it will be stored. The general plant design is shown in Figure where the electrolyzer, compressor and storage options are highlighted. The plant design is composed of two parts: the optimal operating conditions which is a function of the carbon dioxide emissions and the economic analysis. Finally, a risk assessment & life cycle analysis is provided for the optimal design of the hydrogen production plant. The oxygen by-product is also considered as a lucrative asset and either sold as a commodity, or to other companies in the Sarnia-Lambton region.

Thermal methods of hydrogen production make use of a hydrocarbon feedstock, which is decomposed to liberate free hydrogen by the application of high temperatures. Currently, fossil fuel sources account for approximately 96% of global hydrogen production (Keller & Gregoire Padro, 2014). Various fuel sources can be used, although coal and natural gas, specifically methane, are the main research focus (Riis, Hagen, Vie, & Ulleberg, 2006). Hydrogen can be generated from coal by gasification (Riis, Hagen, Vie, & Ulleberg, 2006), while it can be generated from natural gas by one of two processes: steam reforming and partial oxidation. Most fossil fuel systems in commercial applications make use of steam reforming, because it is considered the most cost-effective method (Acar & Dincer, 2013), and it can achieve energy efficiencies of over 80 % (Abbas & Daud, 2010). Steam reforming makes use of the endothermic reaction between methane and, which occurs at high temperatures (650 – 1450 °C) and elevated pressures (3 – 25 bar) in the presence of a catalyst, most commonly nickel (Acar & Dincer, 2013), (Riis, Hagen, Vie, & Ulleberg, 2006). It should be noted that similar reactions can be conducted using a wide variety of other feedstocks including ethane, methanol, ethanol, and acetone, however, these are often less preferred due to byproduct formation and higher cost (LeValley, Richard, & Fan, 2014). Additional hydrogen can be recovered by the use of the exothermic water gas shift reaction, which is conducted at somewhat lower temperatures (400-625°C) (Keller & Gregoire Padro, 2014). Partial oxidation is the other main way in which hydrogen can be produced from methane. This exothermic reaction combines methane with oxygen, in a ratio richer than that needed for complete combustion (Riis, Hagen, Vie, & Ulleberg, 2006). Note that it is possible to combine steam reforming and partial oxidation of methane into a single process, in what is called auto thermal reforming. The goal of such a combination is to balance the highly endothermic steam reforming with the exothermic partial oxidation reaction.

While both partial oxidation and autothermal reforming allow for the use of simpler equipment than steam reforming because no external heating is needed (Riis, Hagen, Vie, & Ulleberg, 2006), the overall energy efficiency is slightly lower, at 70-80%, and hydrogen cost is usually slightly higher (Abbas & Daud, 2010). Coal gasification uses the reaction between coal, water, and sometimes oxygen at high temperatures to generate hydrogen (Acar & Dincer, 2013), (Riis, Hagen, Vie, & Ulleberg, 2006). While coal gasification uses a naturally abundant and inexpensive feedstock, it produces more carbon dioxide per unit of hydrogen (Acar & Dincer, 2013). Coal gasification is a less developed and well-defined technology than steam reforming (Stiegel & Ramezan, 2006), and tends to have higher capital costs, but may also offer lower operating costs (Acar & Dincer, 2013). All of these reactions produce products that must be separated to produce pure hydrogen, which may add significantly to the cost of the process (Riis, Hagen, Vie, & Ulleberg, 2006). They also all produce large amounts of CO2, which is an undesirable greenhouse gas. However, as previously mentioned, it is their high efficiency and low cost that make them leading technologies, and

a standard to which competitors must inevitably be compared. With impact mitigating technologies such as carbon capture and storage, it may be possible to make environmentally friendly hydrogen by these methods.

Electrolysis is a process that uses electricity to drive a non-spontaneous reaction such as water splitting, where hydrogen is produced by passing direct electric current (DC) in water causing the evolution of hydrogen and oxygen at the cathode and anode, respectively. Currently, electrolysis of water accounts for around 4% of global hydrogen production (Ferrero, Lanzini, Santarelli, & Leone, 2013). Compared to other methods of hydrogen production, electrolysis does not have carbon or sulfur contamination, however they cost more compared to fossil fuels (Acar & Dincer, 2013). The current state of the art technologies for electrolysis can be divided into three sub categories: alkaline electrolysers, proton exchange membrane (PEM) electrolysers and high temperature electrolysis (HTE). Alkaline electrolysers generally use mixtures of sodium hydroxide and water with a concentration around 20-30 wt% as the electrolyte. Operating temperatures are between 70-90oC. Efficiencies between 64-85% and operating life times between 15-20 years have been reported in literature. In terms of cost and production, alkaline electrolysers are relatively cheaper compared to other technologies, and can produce hydrogen on the megawatt scale significantly reducing the cost of hydrogen. A drawback of this technology is that the hydrogen produced must be purified to remove water which is accomplished using integrated humidifiers (Ferrero, Lanzini, Santarelli, & Leone, 2013). PEM electrolysers use a solid polymer such as NafionTM instead of an aqueous solution as the electrolyte, thus the need for purification is not required for this pathway. Compared to alkaline electrolysers, PEM electrolysers are shown to have efficiencies around 50-60% (Fuel Cells, 2000). Higher capital costs and relatively short operational lives limit the commercial scalability to around 10kW. PEM electrolysers have operating conditions around 40-80oC but require larger current densities compared to alkaline electrolysers (Ferrero, Lanzini, Santarelli, & Leone, 2013), (Giglio, Lanzini, Santarelli, & Leone, 2015). On the other hand, HTE electrolysers are an upcoming promising technology that uses solid oxide electrolysis cells (SOEC), such as zirconia stabilized with yttria, to electrolyze high temperature steam (700-800oC). Compared to the other technologies, HTE reduces the electrical energy requirement by using the heat generated from the steam to achieve the required enthalpy of reaction and have been shown to have efficiencies up to 80% under pressure (Ferrero, Lanzini, Santarelli, & Leone, 2013), (Acar & Dincer, 2013). This method has not yet been fully commercialized in the energy sector. Recently, the Idaho National Laboratory (INL) performed a feasibility assessment using multi-stacked planar cells (15kW capacity) and a mixture of steam and hydrogen as the feed stock, where the tests results showed promise for commercial scalability (Shoots, Brien, Condie, & Hartvigsen, 2010). Additionally, current active research in industry and academia revolves around decreasing the operating temperatures for SOEC to reduce initial capital costs.

Currently, nuclear energy is a common source of clean energy (electricity) for electrolysis, however there are a number of political issues that surround the topic especially after accidents such as Fukushima disaster in 2011. Therefore, intermittent renewable energy sources such as wind, solar and concentrated solar, biomass gasification, geothermal, hydropower and tidal and wave power, are being explored as alternative resources (Acar & Dincer, 2013), (Case, 2006). From these proposed technologies one of the most economical and practical options is wind power. The current drawback in implementation is that there is an increased capital cost of equipment and the hydrogen production cost is almost 6-10 times more than fossil fuels. As of September this year, the total average installed wind capacity in Ontario is 4042 MW and with the implementation of the Feed in Tariff (FIT) program, more investors are attracted to using renewable energy sources (Ontario, n.d.).There are four main methods for production of hydrogen from biological sources: Biophotolysis of water by algae, Photodecomposition of organic material by bacteria, fermentation, and biomass gasification (Das & Veziroglu, 2001). Biological processes are generally environmentally friendly and offer opportunities to make use of waste materials. They are renewable, and do not require extreme temperatures or environmental conditions to operate (Das & Veziroglu, 2001), (Wang & Wan, 2009). However, they have not yet seen substantial development for commercial applications (Riis, Hagen, Vie, & Ulleberg, 2006), (Keller & Gregoire Padro, 2014).

Photobiological processes for hydrogen production use biological systems that have been somehow modified (either genetically, or by manipulation of environmental conditions) to favor the production of hydrogen gas instead of carbonaceous biomass. They are an area of significant research interest, however, many challenges including low hydrogen production rates, low energy efficiency, and scale-up of production systems remain to be overcome before they become commercially feasible (Riis, Hagen, Vie, & Ulleberg, 2006), (Das & Veziroglu, 2001). Fermentative hydrogen production has been considered to be more feasible at the present time than the photobiological processes, mostly since fermentative processes offer much higher production rates. It may be possible to use wastewater or other wastes as a substrate for hydrogen production (Wang & Wan, 2009). Biomass gasification uses a process similar to the gasification of coal (Riis, Hagen, Vie, & Ulleberg, 2006), although it is less energy efficient (40-50% vs. ~60%)

(Abbas 2009). Hydrogen production from biomass is generally not considered to be cost-competitive with other methods, but there is room for substantial process improvement (Keller & Gregoire Padro, 2014). Its commercial implementation is very limited.

Conventional hydrogen production methods such as steam reforming (SMR) and coal gasification were compared to alternative technologies that are considered to be green such as electrolysis and biochemical. The selection of a hydrogen production technology depends on criteria such as reduction in greenhouse gas emissions, specifically carbon dioxide, capital cost, maturity of technology, efficiency and hydrogen purity. Electrolysis was considered as the method of hydrogen production in this study, as it is a comparable alternative to hydrogen production methods which use non-renewable resources. In addition, unlike biochemical methods, there are large facilities which use electrolysis as a main source for hydrogen production. In this case, there is an excessive base load of electricity available in Ontario due to the inflexible production from nuclear and wind energy, thus electrolysis would be an ideal sink to alleviate this issue.

2. Case study

2.1 Process description

The proposed process using electrolysis will draw electricity from the grid, and water from local sources. These will be preprocessed (rectification for the electricity, deionization for the water), and fed to the electrolyzer system. Hydrogen and oxygen products will be collected and purified, with the main purification requirement being removal of water. Hydrogen will then be either sent directly to the upgrader, or compressed and stored for later use. A block flow diagram for the process is shown below.

Figure 2. Proposed block flow diagram of electrolyzer system

Electrolysis is a technology platform that is primarily divided into three sub-technologies which are alkaline, proton exchange membrane (PEM) and solid oxide electrolysis cells (SOEC). SOEC was immediately excluded as a feasible option due to the lack of technological maturity and commercial availability of SOECs. On the other hand, alkaline electrolyzers have been used in large scale facilities for the past 30 years and more recently the scale up of PEM electrolyzers have been tested (NREL, 2009). Furthermore, both alkaline and PEM electrolyzers from companies such as Hydrogenics, Siemens, IHT, ITM, Proton-on-Site and Nel we compared. Criteria that has been considered is production capacity, efficiency, ramp rates, operating pressures and available storage. Table below compares different electrolyzers, and showcases a general criteria range for both PEM and alkaline electrolyzers. These electrolyzers are screened from a number of commercially available and demo phase electrolyzers based on their ability to meet the hydrogen demand for the upgrader.

Table 1. General criteria range for both PEM and alkaline electrolyzers.

Type	Alkaline	PEM

Company	Hydro genics	Nel	McPhy	IHT	Proton On Site	ITM	Siemens	Hydro genics
Product	Hystat 60	Nel A485	Mclyz er	S-556	M series	HGas series	Silyzer 200	HYG 5MW
Production (Nm^3/h)	24-60	301-485	8-60	760	200 - 400	12-216	225	1100
Outlet Pressure (barg)	10	250	12	32	30	20-80	35	30
Energy efficiency (kWh/Nm^3)	4.9	3.8-4.4	4.1	4.3-4.6	5.6	4.8-5.8	5.56	4.5

There are a number of large-scale hydrogen production plants based on alkaline electrolyzers, the commercial PEM electrolyzers are comparable in terms of the performance criteria outlined in Table . In addition, the electrolyte used in alkaline electrolyzers is a basic solution, which requires additional processing equipment to prepare, and poses greater hazards, compared to using deionized-distilled water which is used in PEM. Thus, the shortlist of commercial products was reduced to PEM electrolyzers. The information presented in Table was used to perform a design analysis to finalize the commercial PEM electrolyzer which would be used to design and model the hydrogen production plant. The HYG 5MW electrolyzer from Hydrogenics was chosen as the commercial PEM electrolyzer. The specifications, including cost were obtained for the electrolyzer and are presented in Table below. These specifactions were directly obtain from Hydrogenics.

Table 2. HYG 5MW PEM electrolyzer specifications used in design and modelling

Specification	Value
Capacity (MW)	5
Electrical consumption (kWh/Nm^3)	4.5
System efficiency (HHV, %)	78
H_2 flowrate (Nm^3/h)	1100
H_2 outlet pressure (bar)	30
H_2 purity (dry basis, %)	99.998
O_2 flowrate (Nm^3/h)	570
O_2 purity (wet basis, %)	99.5
Inlet water flowrate (L/Nm^3 H_2)	2
Capital cost (Million USD/MW)	1
Annual operating & maintenance cost (% capital cost)	2.5
System availability (excluding maintenance) (%)	98

2.2 Technical constraints

As previously mentioned, the hydrogen produced by the hydrogen plant will be used in the hydrotreater units in the upgrader, thus the hydrogen plant should be able to sustain the minimum amount of hydrogen required by the upgrader at all times. Using seasonal diluted bitumen production data and the results from the bitumen upgrader analysis, the

required annual hydrogen demand was determined. The analysis performed in this study assumed that there was no change in the annual hydrogen demand.
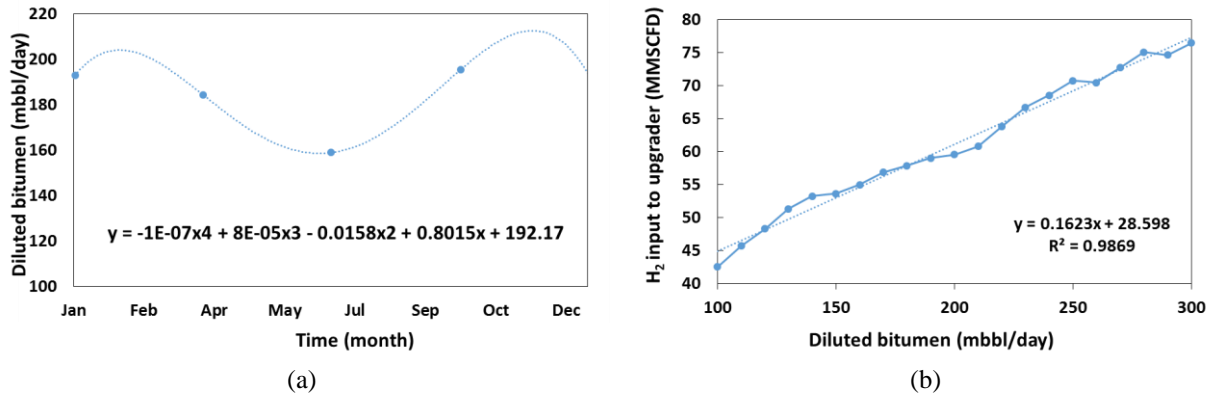

(a)

(b)

Figure 3. (a) The seasonal diluted bitumen production obtained from Suncor and (b) the correlation between hydrogen demand and diluted bitumen production was used to determine the annual hydrogen demand

The annual hydrogen demand is determined and shown in Figure . Based on the fitted data points the daily hydrogen requirement can be determined. However, in reality there will be variations in annual hydrogen demand based on the supply and demand of the diluted bitumen. The power required to run the electrolyzers come directly from grid electricity and due to the fluctuations in hydrogen demand and electricity prices there is an apparent need for temporary hydrogen storage arises. Ideally, the model designed should be producing hydrogen at times of low electricity cost and storing it for use at times of high electricity cost offers significant economic benefits.
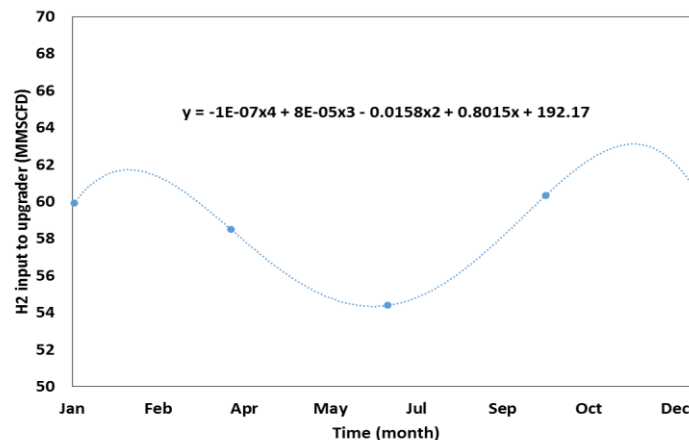
Figure 4. Annual hydrogen demand required for upgrader

3. Design & Modelling

3.1 Control Objectives

The largest operating cost for the proposed process is electricity. However, varying output to utilize off-peak power can potentially reduce operating cost (Bartels, 2010), and may also provide environmental benefits. Integrating such variability into the system design requires a control system to determine when extra hydrogen should be produced, and when it should be drawn from storage. Besides minimizing electricity cost, the control algorithm must also ensure that:

- Enough hydrogen will be available, from either storage or production, to supply upgrader demand at all times.
- Produced hydrogen must fill the storage tanks during electricity off-peak prices, and drain during on-peak prices in order to minimize the overall electricity cost per year.
- Hydrogen supply and demand are balanced overall

Three data inputs were deemed necessary and sufficient for each model to make production decisions: electricity price as a function of time, hydrogen demand, and maximum electrolyzer production capacity. Two outputs were required

for later cost estimation: total electricity cost for a year of production, and total storage capacity. An additional pair of input and output were then added for environmental calculations: CO_2 emissions as a function of time, and total CO_2 emissions for a year of production. These did not factor in production decisions, but were tracked for use in the impact assessment. Also taken as inputs was the specific energy requirement to produce H_2 with the Hydrogenics electrolyzer (MWh/kg), and the specific compressor energy requirement (kWh/kg) for a compressor operating at 80% efficiency, a performance compatible with literature values (Parks, 2014(NREL)). Potentially storage capacity could have been regarded as an input, and electricity cost determined by allowing the control algorithms to operate with all equipment specified. It was determined that this would not be a suitable course of action because it would introduce two independent variables (production capacity and storage capacity), while making algorithm design much more complex. Also supporting the treatment of storage capacity as an output were preliminary calculations indicating storage cost would be small compared with other costs of the system. Allowing it to vary freely would thus not significantly skew results.

3.2 Control Algorithm Descriptions

All control algorithms were implemented in MATLAB. MATLAB was chosen because the team was familiar with its workings, and because its capabilities were well-suited to the logical programming and graphing functions that would be required. Electricity price and CO_2 emission data were provided as an Excel spreadsheet of hourly Ontario wholesale price ($/MWh) and carbon emission (kg CO_2/MWh) figures. Upgrader H_2 demand was obtained as a daily value using the polynomial fit developed previously. Five control algorithms were developed. They are described below, identified by both descriptive name ("Constant", "Threshold", "Derivative", "Historical", and "Current"), and number (I-V). The algorithms are represented visually in Figure 5.

- Model I – Constant: Model I assumes constant production such that the hydrogen produced matches the upgrader demands at any given time. Production is not affected in any way by electricity price.

- Model II – Threshold: Model II follows a fixed threshold, where hydrogen production is maximized at off-peak (defined by comparison with a predetermined threshold) electricity prices and minimized at on-peak times. The available tank size and electrolyzer production are set based upon the outputs of model V. This simplistic model does not consider past or future price, only current values.

- Model III – Derivative: Model III is a derivative model, where hydrogen production is maximized when the second derivative of price is increasing and the tank is drained when decreasing. Backward finite difference approximations are used to accomplish the differentiation, considering past and current price values.

- Model IV – Historical: Model IV is a predictive model that uses an average of hourly prices from the last 10 days to predict the hourly prices of the current day. From the given electrolyzer size and the upgrader H_2 demand, the number of hours per day for which hydrogen can be drawn entirely from storage, assuming it is produced at maximum rate at all other times, is determined. The predicted prices are then sorted from high to low, and the hours with the highest expected price are chosen to receive H_2 from storage. If a fractional number of hours' supply is available, it is assigned to the lowest of these high price hours.

- Model V – Current: Model V uses the same sorting method as Model IV, but instead of using averaged price data from previous days, it uses actual price data from the current day, representing the ideal case where price is known exactly, or nearly exactly, in advance. This model achieves fully optimal performance over each day.
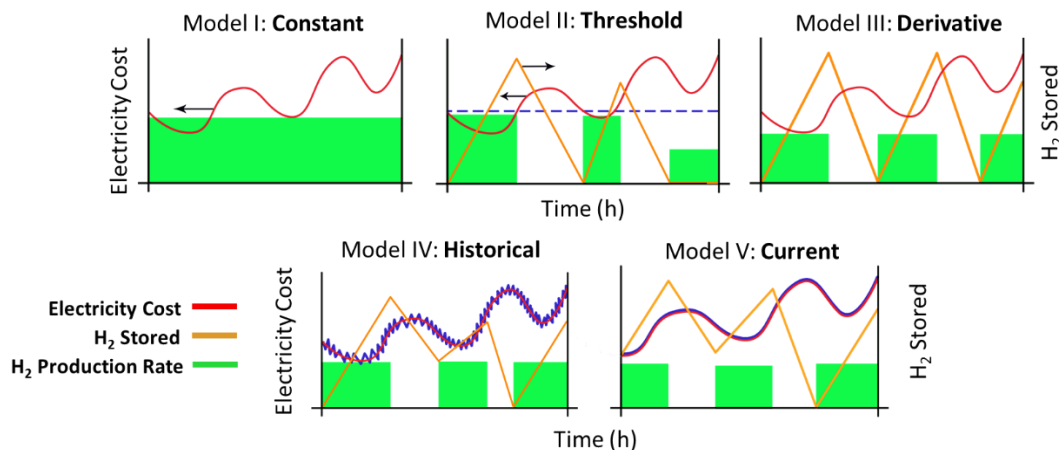
Figure 5. Illustration of control algorithm operation

4. Results and discussion

It can be seen from Figure that the "current" model V achieves minimum yearly electricity cost, and minimum CO_2 emissions. Compared with constant production, a cost reduction of about 40% can be realized. Note that the 20000 kg H_2/h plant capacity is arbitrary, but the same trend is visible over all possible plant sizes. Increasing plant capacity tends to accentuate the difference between the models, while lowering yearly cost in all cases except the "constant" Model I, which is not affected by electrolyzer size. Because the "current" Model V has the best performance, it was selected for use in the overall economic optimization. The model was used to generate yearly electricity cost as a function of plant capacity over a range from the minimum possible (8900 kg/h), up to 40000 kg/h, a figure expected to be much greater than the optimum.
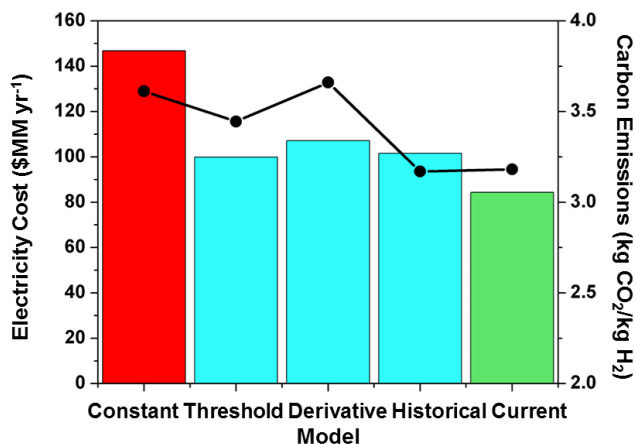
Figure 6. Comparison of model performance
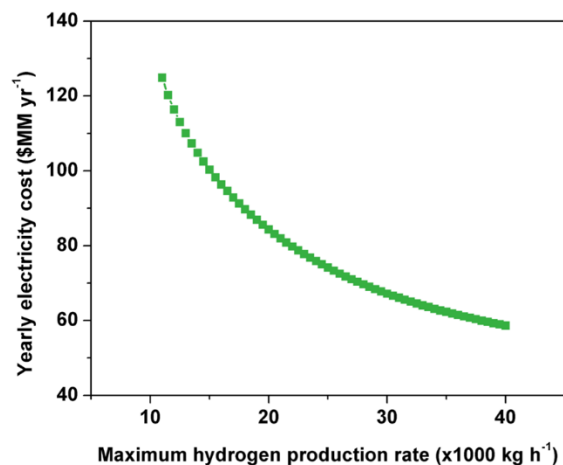
Figure 7. Electricity cost vs. plant size, "Current" model V

Using the "current" Model V results, enough information was available to compute both operating and capital cost for any size plant. A MATLAB cost calculation code was constructed, accounting for the following factors: 1) Electricity costs for electrolyzers and compressors, 2) Water utility cost, 3) Electrolyzer O&M, 4) Oxygen sales, 5) CO_2 credits, 6) Electrolyzer capital cost, 7) Compressor capital cost, 8) Tank capital cost, and 9) Building capital cost. Water utility costs used municipal rates for the Sarnia-Lambton region, oxygen sales were for wholesale oxygen as used in Basic Oxygen Steelmaking (BOS). Each 340 kg H_2 storage tank was priced at $202640, and each 42 kg/h H_2 compressor at $192000, based on data obtained from faculty advisors. Standard installation factors were used for all equipment. Building cost was sourced from a commercial real estate guide (AltusGroup, 2014). The optimum plant parameters obtained are summarized in Table 3.The H_2 price computed for this design is comparable to the cost of H_2 produced by SMR. Emissions of pollutants are considerably reduced (Bartels, 2014).
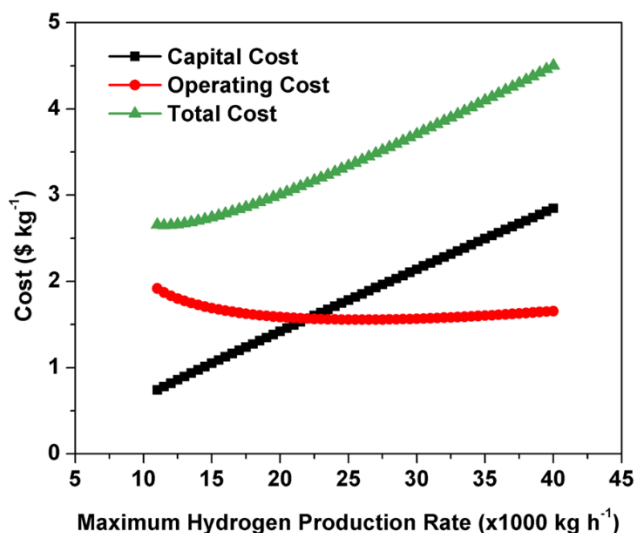
Figure 8: Capital cost, operating cost, and total cost of H_2 production vs. plant capacity

Table 3. Optimum plant parameters

Parameter	Value
Number of 5 MW Electrolyzers	125

Plant Capacity (MW)	625
Number of 340 kg H_2 storage tanks	140
H_2 storage capacity (kg)	47800

Table 4. Comparison of PEM electrolysis and SMR H_2 production cost

Parameter	PEM Electrolysis	SMR
H_2 cost ($/kg)	2.67	2.75
CO_2 emissions (kg CO_2/kg H_2)	3.2	11
NO_X emissions (kg NO_X/kg H_2)	0.0434	12.3

A sensitivity analysis was performed to assess how robust the price analysis was to error, and which factors had the greatest influence. A factor of ±40% (large to make differences more visible) was applied to each single item (e.g. electrolyzer O&M) individually, and the effect on total H_2 price was observed. The largest factor in H_2 price was electricity price, followed by electrolyzer capital cost. Notably, H_2 price is highly insensitive to storage costs. This suggests that perhaps a system considering long-term storage (instead of the daily storage used here) could be economical despite the much larger capacities needed.
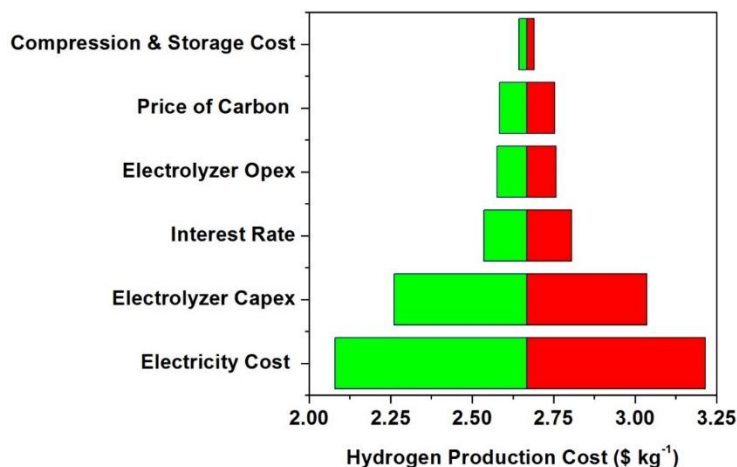

Figure 9. Tornado plot for H_2 production cost

5. Conclusions

Using PEM electrolysis is a feasible alternative to SMR for hydrogen production because it is comparable in hydrogen production cost depending on the plant size chosen. In addition, the CO_2 and NO_x emissions are significantly reduced and provide opportunities for cap & trade due to the payback from the carbon offsets. From the analysis, the most optimal controller is the Current model (Model V) which assumes that the variation in electricity prices in a day are very well known. The drawbacks to this model are that any deviation from the expected price may incur increased costs, it sets tank size instead of utilizing any available capacity, and it does not optimize the use of storage over multiple days, but rather each day individually. However, the other model results suggest that these effects are not

likely to cause a major effect on the conclusions of this study. With this in mind, future work in this area would benefit from a long-term optimization that handles tank capacity in a more sophisticated way. The optimal plant configuration uses a relatively modest excess of electrolysers – 29% above the minimum requirement – to achieve cost-shifting. The cost of compression and storage is small compared to the cost of the electrolyser units themselves. Accordingly, the total system cost is most sensitive to variations in electricity price and electrolyser capital cost.

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