RESEARCH ARTICLE

Implementing Power-to-Gas to provide green hydrogen to a bitumen upgrader

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SUMMARY

Hydrogen is an important commodity in the processing of intermediate bitumen products into a finished petroleum product and for upgrading bitumen into synthetic crude. With the continued extraction of bitumen-rich material from Alberta's oil sands project, there is an opportunity to reduce the greenhouse gas emissions of upgrading and refining operations by using electrolytically produced hydrogen in place of hydrogen produced by steam methane reformation. Recently, a bitumen upgrading facility had been proposed for the city of Sarnia, Ontario because of its pre-existing petroleum processing infrastructure. Using the Ontario electrical system, which has a lower emissions factor than Alberta, the use of electrolytic hydrogen could result in a significant reduction of greenhouse gasses. In this paper, the objective is to determine an optimal system configuration for reducing greenhouse gas emissions while maintaining a low system cost. The analysis is performed with General Algebraic Modelling System tool, a mixed-integer linear optimization in addition to a simple model in Visual Basic. For each case, an economic and environmental analysis is performed including the use of cap-and-trade values for the price of carbon emissions, which are applied to determine the overall economic impact of the emissions reductions. Copyright © 2016 John Wiley & Sons, Ltd.

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1. INTRODUCTION

The extraction and production of petroleum is a cornerstone of the western economy, especially in Alberta, Canada. Due to society's reliance on petroleum for energy, and the location of the world's most accessible reserves in politically unstable locations, it has become important to invest in the domestic extraction and production of oil. Canada, long known to have reserves that can be accessed by through conventional and non-conventional means, has one of the most significant petroleum reserves in the world. The majority of Canada's accessible oil reserves are located in Alberta, with 170 billion of the 173 billion barrels of recoverable oil being located in the province. Of those 170 billion barrels of Albertan oil, nearly all of it, 168 billion barrels, exist as oil sands [1]. The nature of oil sands petroleum necessitates specialized extraction and pre-treatment techniques in order to produce a useable

end product. To this end, the Canadian government expects capital investment in the oil sands region to add up to $207bn by 2022 [2]. However, development in the oil sands region is tempered by governmental regulations designed to limit the amount of greenhouse gasses released and limits on the environmental footprint of the bitumen extraction sites. Due to this regulatory pressure, there is a need for energy companies to develop cleaner and more efficient methods of extracting and refining their oil sands products. By producing petroleum with less CO_2 emissions, it is possible to make the extraction and use of oil sands fuel more sustainable [3].

The expanding focus on American shale development coupled with rock-bottom international oil prices is resulting in a reduction of demand for Canadian petroleum from the USA [4]. Of even greater concern for the Canadian oil industry is the cancelation of the Keystone XL pipeline, a planned pipeline that would have taken

Canadian dilbit to the United States for upgrading and refining. The pipeline, which was to pass through the American countryside, on a more direct route than the pre-existing Keystone sections, carrying diluted bitumen and synthetic crude, was canceled by President Obama in November of 2015 after years of consideration [5]. The potential acceptance of the Keystone project became a political issue in the United States, with environmental groups concerned about dangerous heavy oil leaks in American soil [6]. With the perception of Canadian oil sands products as being an environmentally unfriendly energy option, it is essential that ways be found to reduce lifecycle emissions and the potential for harmful spills.

The bitumen found in Canadian oil sands is extracted as a thick, tar-like semi-solid, which cannot be transported by pipeline as is. To lower the viscosity of the bitumen so that it can be transported, the bitumen is mixed with diluents composed mainly of naphtha or natural gas condensate, to produce a fluid known as diluted bitumen or dilbit [7]. Dilbit cannot be processed at a refinery because of its high density and sulfur, nitrogen, and heavy metal content. Thus, the dilbit must first be upgraded to synthetic crude oil before it can be refined in the same manner as conventional crude oil. Currently, about half of the bitumen produced by the oil sands development is upgraded in Canadian facilities located in Alberta or Saskatchewan while the rest is sold as dilbit to primarily American consumers [8]. The practice of selling significant amounts of unprocessed dilbit to American companies creates a single buyer market and places the fate of the Canadian oil sands industry primarily in the hands of American interest. By upgrading more domestically extracted bitumen to synthetic crude oil, Canada can gain greater energy independence and better control the sale of oil sands' products.

There are six bitumen upgraders currently operating in Canada, the five largest of which are located in Alberta. These Albertan upgraders have a combined capacity of more than 1.3 million barrels of bitumen processed per day [9]. Most of the upgrading infrastructure is located in Alberta where the bitumen is converted to synthetic crude oil before being piped to refineries. However, as Alberta's energy sources are high in CO_2 emissions, a net greenhouse gas emissions reduction can be achieved by moving operations to Ontario where the electrical grid produces significantly less CO_2 emissions [10].

The Canadian Academy of Engineers, in a recent report, proposes that a new bitumen upgrader be built in Sarnia, Ontario [11]. Sarnia, which is already home to three oil refineries and many industrial facilities, is able to handle the excess production of synthetic crude, and an upgrader facility fits with the desires of the population and business community. Due to the pre-existing fuel production facilities, the majority of the industrial infrastructure for a new upgrader in Sarnia, Ontario already exists. Sarnia is also near the Canada–US border, the city of Detroit, Michigan, and the St. Lawrence Seaway, which means domestic and international transportation of the synthetic crude is viable. Lastly, Ontario's power generation mix produces

significantly less carbon emissions than Alberta's, which is made up predominantly of coal, which accounts for 55% of the energy mix, and natural gas, which makes up 35% [10]. By comparison, Ontario's electricity producers emit almost nine times less carbon emissions, per kilowatt-hour of electricity [12]. Ontario's reliance on nuclear energy, which accounts for 56% of the electricity produced in the province, is another incentive for building a future bitumen upgrader in Ontario [13]. Due to the round-the-clock operation of nuclear facilities, there is excess off-peak base-load energy, which causes electricity prices to drop significantly because of the lack of demand. Thus, if energy arbitrage is used, significant operations savings can be claimed for an upgrader facility using electrolysis.

Nearly all refineries operating today use steam methane reforming (SMR) as their primary means of hydrogen production. The hydrogen is used to remove undesirable components like sulfur and nitrogen and to increase the hydrogen to carbon ratio [14]. Heavy oil upgrading is a hydrogen intensive process because of the bitumen's density and high sulfur and nitrogen content. In some cases, heavy oil may contain 10 times more sulfur and nitrogen than conventional crude [15]. Although SMR is the industry's standard for hydrogen production because of its reliability, accessible feedstock, and long-serving technology, it has several drawbacks, including the release of greenhouse gasses and a high methane consumption rate [16]. Because methane is a fuel that can be used to provide heat or electricity, the use of methane to produce hydrogen for fuel processing has energy loss associated with it. This energy loss is referred to as the feedstock energy. Although electrolyzers provide a reliable source of carbon-free hydrogen, their use is largely ignored by petroleum refiners because of the prevalence of SMR.

One standard cubic meter of hydrogen produced by electrolysis can take between 4 and 7 kWh of electricity to produce [17]. With estimated capital costs of $1000 per kilowatt, the cost of producing hydrogen on the scale required for an upgrader or refinery will take a significant capital investment [18].

To reduce the greenhouse gas emissions tied to producing hydrogen by SMR, a number of technologies may be considered. If SMR is used as the hydrogen production method, carbon capture and sequestration can be used to reduce the CO_2 emissions [19]. Alternately, thermo-catalytic decomposition can also be used to produce the needed hydrogen [20,21].

In light of the high demand for industrial hydrogen, substituting electrolytic hydrogen for hydrogen for the more commonly used SMR for bitumen upgrading is an opportunity to reduce greenhouse gas emissions considering current hydrogen use pathways. When, a grid mixture dominated by nuclear energy is used to produce electrolytic hydrogen, the emissions factor is approximately 3 kg CO_2e per kg H2, while SMR produces about 9–15 kg CO_2e per kg H2 [22]. Suleman et al. [23], for example, find that SMR releases approximately

$11 \, \text{kg} \, CO_2$e per $\text{kg} \, H2$ while electrolysis from renewable sources including wind, solar, and hydroelectricity releases less than $400 \, \text{g} \, CO_2$e per $\text{kg} \, H2$ on a lifecycle basis. El Emam et al. [24] provide an economic analysis of different hydrogen production methods.

Hydrogen produced via Power-to-Gas technology can be considered as a 'green' fuel as it is making use of excess power of which the intermittent renewable sources, such as wind and solar, are significant contributors as these sources are not dispatchable. Although the thermochemical production of hydrogen from CuCl water splitting can also provide low emission hydrogen, the use of electrolysis technology is a more likely solution in the short-term [25].

In this unique study, the authors investigate the use of an electrolyzer plant, powered by off-peak power in place of an SMR system, to provide hydrogen for a bitumen upgrader facility. Similar models, developed to determine the viability of producing hydrogen by electrolysis for oil sands operations, and other applications, are proposed by a number of authors [26–29]. Olateju et al. [26], for example, propose and optimize an electrolyzer system powered by wind energy for a large-scale upgrader refinery in Alberta. In a second study, Olateju et al. [27] examine the expansion of the wind farm for powering the electrolyzer system. Shannon develops a model for small-scale integrated upgraders, which uses electrolytic hydrogen in the Lloydminster and Cold Lake regions [28]. Previous examinations of refinery operations also focus on creating a more sustainable operation and reducing overall CO_2 emissions. Alhajji and Demirel [29], for example, examine the reduction of overall greenhouse gas emissions in an oil refinery by employing a thermodynamic analysis, which indicate irreversible heat losses throughout the refining process.

Overall emissions optimizations of bitumen upgraders also take into account the emissions from hydrogen production. Ordorica-Garcia et al. [30] optimize the greenhouse gas emissions of the oil sands industry as a whole, and also examine the use of SMR and its impact on lifecycle emissions. A lifecycle analysis performed by Nimana et al. [31] also examines the emissions from generating hydrogen for hydrocracking by SMR. As the emissions from Canada's oil sands need to reduce by 38%, the reduction of emissions from hydrogen production is one step of a holistic approach that can be taken [32]

Mukherjee et al. [33] propose an Ontario-based model for a Power-to-Gas system that uses off-peak electricity to produce electrolytic hydrogen to meet industrial purposes with reduced greenhouse gas emissions. In this paper, a number of different approaches, including a mixed-integer linear programming (MILP) optimization, are used to find an ideal operating setup to reduce emissions in the operation of the upgrader. Previously, such optimizations have been used in the analysis of energy systems. Middleton [34], for example, examines the integration of renewable energy with carbon capture and storage using a mixed linear integer programming optimization.

2. METHODOLOGY

In this paper, the objective is to develop and configure electrolyzer plant to produce hydrogen for a future bitumen upgrading facility in Sarnia, Ontario using a mixed integer linear optimization and simple controller models. Due to a shift in provincial environmental policy toward cap-and-trade and the use of Power-to-Gas to provide hydrogen for a bitumen upgrader facility would meet the goals of the provincial government and may be more economically sound. To this end, a combination of process simulation and MILP calculations are used to evaluate the economic feasibility and environmental performance of using a train of electrolyzers to supply hydrogen to bitumen upgrader facility. The hydrogen demand is determined using an Aspen HYSYS (Aspen Technology, Inc., Bedford, MA, USA) [35] simulation of the upgrader refinery, which consists of an atmospheric distillation unit (ADU), a vacuum distillation unit, a delayed coker unit (DCU), and three hydrotreaters. The simulated upgrader also includes a hydrogen recovery unit to recover hydrogen from the hydrotreater purge gas. The hydrogen demand is correlated to the dilbit input flowrate to the upgrader using a sixth-order polynomial. This equation is used to estimate the hydrogen input demand based on seasonal expected dilbit flowrates [36]. Once the extrapolated hydrogen demand curve with seasonal variation is established, a second simulation for the proposed electrolyzer train is performed. Generalized algebraic modeling system (GAMS) and Visual Basic are used to simulate the electrolyzer plant for year-round operation. The electrolyzer modeled in the simulation consumes $4.5 \, \text{kWh}$ per $Nm^3 \, H_2$ and has approximate installation cost of $1m per megawatt hour of installed capacity [17]. Based on this data, four cases are developed for hydrogen production:

Case 1 Base case: an SMR system is used to meet hydrogen demand, with a fixed emission factor of $9 \, \text{kg} \, CO_2$e per $\text{kg} \, H_2$ produced [16,37];

Case 2 Alternative model: a minimum number of electrolyzers produce hydrogen by following the hourly demand using electricity that is consumed at a variable emission factor;

Case 3 Alternative model: a minimum number of electrolyzers operate with a simple controller that produces hydrogen when the variable emissions factor for the power used is below a selected emissions factor in a system that utilizes hydrogen storage; and

Case 4 Alternative model: an optimized electrolyzer system reduces emissions to the minimum level possible through the use of hydrogen storage tanks with a variable emissions factor applied to the electricity consumed by the system.

The four cases are analyzed and compared over the expected 20-year lifecycle of a hydrogen production facility. For economic evaluations, constant cap-and-trade

values are applied to the constant emissions reductions. Hydrogen storage is also determined for those cases where it is needed, with tanks sized to reduce lifecycle costs. To optimize the application of electrolyzers, it is necessary to manipulate the operating times, number of units, and storage sizing. In each of the four cases, the upgrader model consists of two independent model formulations working in series. In Figure 1, below the two models: 'Upgrader Refinery Model' and 'Electrolyzer Plant Optimization Model' are illustrated within the logic of the experimental methodology. First, the expected monthly bitumen load is inputted to the Upgrader Refinery Model. From this first model, the necessary hydrogen demand is generated. Next, this hydrogen demand is fed, along with technical parameters of electrolysis and hydrogen storage to the electrolyzer model. This second model is used to generate the hydrogen production conditions including: number of electrolyzers, number of tanks, total emissions, and cost. There are three approaches to the modeling of the electrolyzer systems. In Cases 1 and 2, the electrolyzers produce just enough hydrogen to meet demand. In Case 3, the electrolyzer uses a simple controller coupled with hydrogen storage, as discussed in Section 2.2. In Case 4, a full system optimization, including hydrogen storage, is performed as discussed in Section 2.3.

2.1. UPGRADER SIMULATION

The data input for the simulation are derived from the projected monthly dilbit feed into the upgrader. In order to generate an accurate annual forecast for the hydrogen demand, the monthly variable bitumen input is used. The monthly dilbit feed rate is adapted to an hourly production profile based on publicly available data [36]. The dilbit feed data is then inputted to the Aspen HYSYS upgrader simulation with a delayed coker as the primary conversion method. The Aspen HYSYS simulation, based on the design of an Albertan upgrader, is laid out according to Figure 2, later.

The dilbit, known as Cold Lake Blend and consisting of a roughly 75:25 mixture of bitumen and condensate enters the process from tanks at ambient conditions [38]. Cold Lake Blend is the chosen input as it is among the most pervasive dilbit blends transported by pipeline in Canada [39]. The separation of the diluent and a portion of the light gas oil fraction are carried out at atmospheric conditions in the ADU. The atmospheric topped bitumen exits the ADU and enters the vacuum distillation unit, which enables further liquid fractions recovery while avoiding coke deposition on the furnace. Vacuum topped bitumen is produced as a residue and is fed to the Delayed Coking Unit (DCU).

Delayed coking produces valuable hydrocarbon fractions from a heavy feed at a high temperature, in a low pressure, and uncatalyzed environment. As no hydrogen is added during delayed coking, petroleum coke is produced as a by-product and must be periodically removed. Fluids from the DCU are fed to a downstream fractionator where liquid fractions, as well as a non-condensable stream, are recovered. The petroleum coke, meanwhile, may be sold to offshore markets or otherwise stored. A DCU is chosen as the vacuum residue conversion process because it is the most commonly used in industry, compared with alternative processes [15]. Other vacuum residue conversion processes can also be effective. For example, hydrocracking can increase the SCO conversion rate from 76% using a DCU to 94% [40]. Hydrocracking, however, comes with the cost of significantly higher hydrogen consumption: 1269 scf H_2 per bbl bitumen for hydrocracking versus 426 scf H_2 per bbl bitumen for delayed coking. In addition, hydrocracking releases significantly more greenhouse gasses than the DCU [41].

Following the DCU, the remaining liquid fractions are mixed and sent to one of three hydrotreatment units according to the fraction's boiling point. This is a catalyzed, high temperature, high pressure process in which hydrogen is used to saturate the hydrocarbon chains and displace any contaminants as well as to increase the hydrogen to carbon ratio. Importantly, for this analysis, this hydrotreatment process is also the only process that consumes hydrogen in the upgrader. The hydrotreaters are modeled as two or more hydroprocessor bed unit operations in series with acid gas and liquid separators and a recycle loop for the
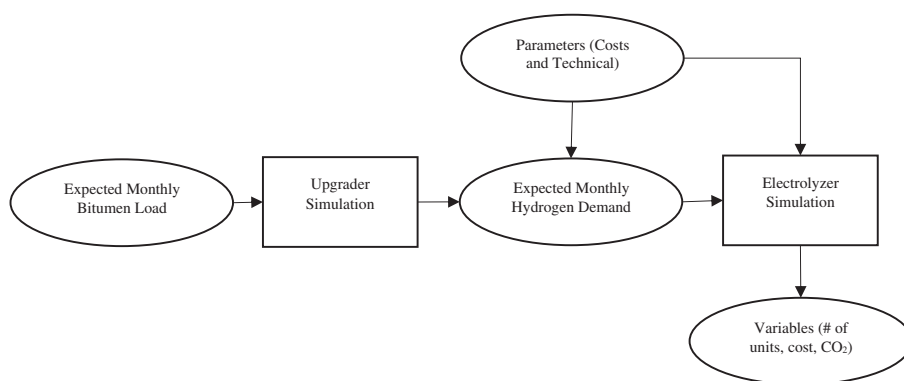

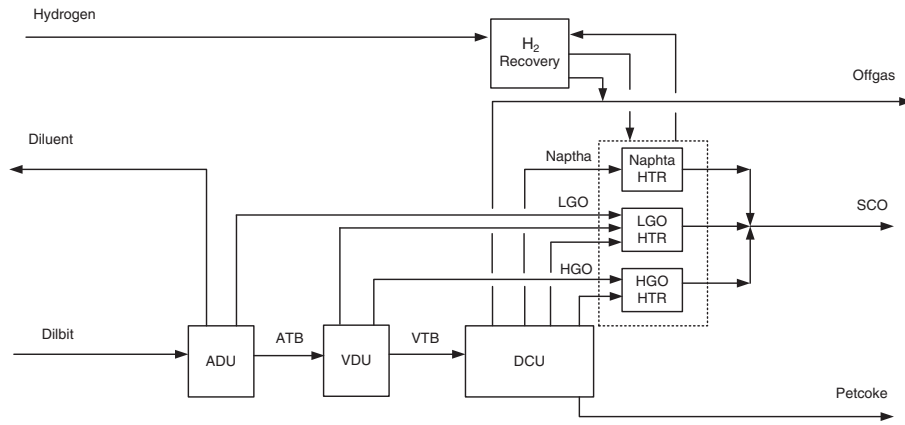**Figure 1.** Proposed experimental design.

Figure 2. Ontario Upgrader flowsheet.

gas stream. The use of the hydroprocessor bed unit in the simulation effectively models the reactions rather than relying on correlated data to determine the yields, as has been explored previously [42].

Pure hydrogen is fed to each high temperature reactor from the hydrogen recovery section of the upgrader. The reactor is a pressure swing adsorber unit that separates hydrogen from the high temperature reactor purge gas with a 90% efficiency and with 100% hydrogen selectivity [42]. Makeup hydrogen, supplied by the electrolysis plant, is fed into the process to balance out the hydrogen losses in the system. The pressure swing adsorber exhaust gasses are combined with the DCU off-gas and are used as refinery fuel and for steam generation [41,42]. The model is evaluated for 21 different diluted bitumen flow rates ranging from 100,000 to 300,000 bbl per day, including the seasonal variations of feed.

To determine the hydrogen demand from the bitumen feed rates, a sixth-order polynomial regression using MATLAB (MathWorks, Inc, Natick, MA, USA) is carried out, based on the relationship illustrated in Figure 3. The sixth-order regression accurately accommodates for the number of inflections in the plot and provides statistical significance. The sixth-order polynomial equation has the form:

$$Q_{Hydrogen} = \sum_{k=0}^{6} a_k (Q_{Dilbit})^k \tag{1}$$

where $Q_{Hydrogen}$ represents the volumetric flowrate for hydrogen, in million standard cubic feet per day; Q_{Dilbit} is the quantity of dilbit processed, in mbbl per day; and a is the regression coefficient for the given dimension k.
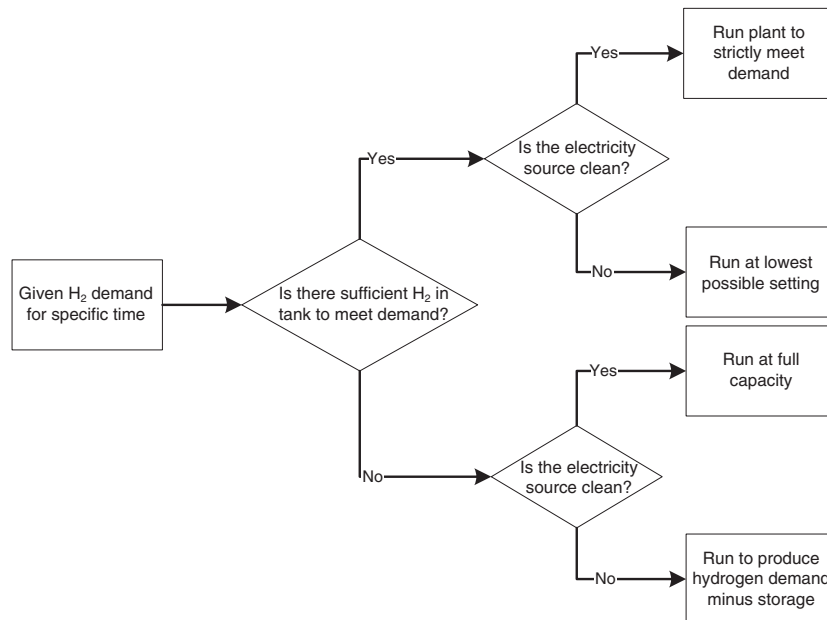

Figure 3. Control logic for electrolyzer plant sizing model in Case 3.

2.2. ELECTROLYZER CONTROLLER MODEL

Equation (1) is used to predict the monthly hydrogen demand for the upgrader. These data are then fed to the second model to optimize the hydrogen plant in Case 4. In Case 1, it is assumed that an SMR unit meets the calculated hydrogen demand. In Case 2, the minimum number of electrolyzers that can meet the maximum required hydrogen output is used to follow the demand for hydrogen without storage. The model used for the simulation in Case 3 consists of two logic switches that control and modulate the level of electrolyzer activation. The switches control for the following: the level of hydrogen currently stored in tanks and CO_2 emissions factor for electricity used.

An initial stored volume of hydrogen of 0, at time 0, is set for the tank. An hourly difference is taken among the sum of hydrogen produced per hour, the hydrogen stored, in the previous hour, and the hydrogen consumed by the process during the given hour. The described relationship between the amount of hydrogen in the tank and the production and consumption of hydrogen is illustrated in Equation (2).

$$H_2^{Surplus,hour\ 2} = H_2^{Surplus,\ hour\ 1} + H_2^{Produced,\ hour\ 2} - H_2^{Consumed,hour\ 2} \tag{2}$$

The maximum value of $H_2^{Surplus}$ over the 20-year life cycle is taken to be the tank size. The CO_2 emissions factor, measured in units of $kg\ CO_2/MW$-h, determines the time of day in which the electrolyzer is operating. The logic for the controller program that is utilized in Case 3 is demonstrated later in Figure 3.

2.3. Electrolyzer optimizer model

In Case 4, the electrolyzer is optimized to determine the configuration and operating conditions for the hydrogen production system of the bitumen upgrader. In this case, the objective function is the summation of the emissions produced by all operations, as given in Equation (3). The goal of the optimization is to minimize the emissions in Equation (3) while providing enough hydrogen to meet demand through the use of electrolysis and hydrogen storage.

$$Emissions = \sum_n E(n) \tag{3}$$

The source of emissions for the optimized system includes the electricity for the production of hydrogen, calculated from the variable emissions factor and for the compression needed to store the hydrogen on-site. In this application, the compression required in approximately 300 barg [35]. Thus, the objective function can be rewritten according to Equation (4).

$$Min\left(\sum_n E(n) = \sum_i E(electrolyzer_i) + \sum_j E(compressor_j)\right) \tag{4}$$

where $E(electrolyzer_i)$ is the amount of emissions produced by electrolyzer i and $E(compressor_j)$ is the amount of emissions produced by compressor j. Each of these terms is calculated as illustrated in Equations (5) and (6).

$$E(electrolyzer_i) = \sum_t EF_t \ x \ P_t \tag{5}$$

where EF_t is the emissions factor of the grid at hour t, in $kg\ CO_2e$ per kWh at time t, and $P_{i,t}$ is the power used to generate hydrogen using electrolyzer i during hour t.

$$E(compressor_j) = \sum_t EF_t \ x \ P_{j,t} \tag{6}$$

where EF_t is the emissions factor of the grid in $kg\ CO_2e$ per kWh at time t, and $P_{j,t}$ is the power used to compress hydrogen with compressor j during hour t.

The MILP model is subjected to the inequality constraint shown in Equation (7), where the power supplied to the electrolyzers cannot violate the minimum and maximum operating levels of the entire hydrogen production system.

$$N_{electrolyzer} \times P_{Min,Ele} \leq P_t \leq N_{electrolyzer} \times P_{Max,Ele} \tag{7}$$

Equation (7) implies that all of the electrolyzers will be operating at the same power level at a particular time point. The hydrogen produced in a particular hour t is expressed by Equation (8) as a function of the power bought in that hour.

$$H2_t = P_t \times 0.01462517 \tag{8}$$

where H_{2t} is the amount of hydrogen, in kilogram, produced during hour t, and P_t is the total amount of power supplied to the electrolyzers, in killowatt, during hour t.

2.4. Variable emissions factor

For each hour of operation over the life of the hydrogen production facility, the electricity generation profile is taken from the corresponding day and hour over the period from 2012 to 2014. The hourly emissions factor for the Ontario grid is calculated by dividing the total CO_2 emission for that hour, calculated by multiplying the electricity source by associated generation technology emissions parameters as shown in Table I, by the amount of energy generated in that hours. This results in a range of emissions factors from $22\ kg\ CO_2e$ per MWh to $225\ kg\ CO_2e$ per MWh. The emissions intensity of the energy at that

Table I. Emissions factors for different sources of electricity.

	Nuclear	Natural Gas	Hydroelectricity	Wind	Biofuels	Coal
gCO per MWh	11.0	297.5	0.0	0.0	1,425.0	152.7
gNO$_X$ per MWh	22.8	1.1	0.0	0.0	104.4	1,275.8
gVOC per MWh	2.8	70.3	0.0	0.0	13.9	83.5
kg CO$_2$ per MWh	12.0	487.4	0.0	0.0	177.0	1,001.1
gSO$_X$ per MWh	26.5	118.2	0.0	0.0	1.2	3,268.1
LH$_2$O per MWh	31,960	—	69,077.3	1.0	1,617.9	—
gCH$_4$ per MWh	26.1	1,531.7	—	—	569.0	1,469.8

particular time is then determined by evaluating whether that emissions factor is above or below a threshold value. The program would then proceed with the logic given in Figure 3.

As shown in Table I, nuclear and hydroelectricity are two of the cleaner sources of energy available to grid. In Ontario, these two sources represent a large portion of the electrical grid, meaning that energy users can expect a low CO$_2$ emissions factor. The cyclical nature of the emissions factor is illustrated in Figure 2 later. During the middle of the day, when energy demand increases, the emissions factor increases. This increase is due to the ramping up of natural gas energy production to meet the growing demand. During off-peak periods, the energy mix is made up mostly of nuclear energy and hydroelectricity, resulting in a reduction of emissions. Due to the elimination of coal-powered energy generators in Ontario, the overall emissions factor has visibly dropped between 2012 and 2014, as illustrated in Figure 4.

Case 1, described in the Introduction, does not use the logic described in Figure 3 to produce results as neither case uses energy storage at all. Rather, Case 1 uses and specifies a capital cost and calculates emissions reduction based on a static emissions factor for the production of hydrogen by SMR. In Case 2, an electrolyzer is used to produce enough hydrogen to meet demand with a varying emissions factor. In Case 3, on the other hand, the logic in Figure 3 is used to determine the optimal operation of the facility, with static cap and trade values. A simplifying
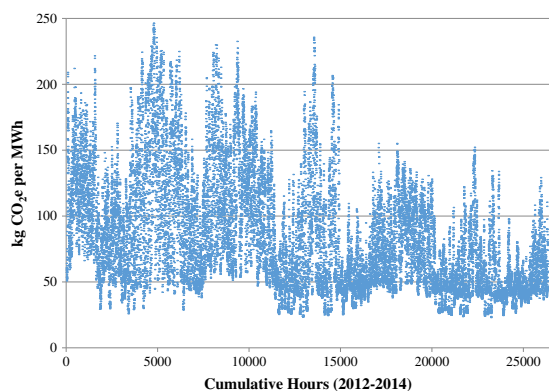
assumption in this model is that modulation of electrolyzer load is carried equally by all units. In Case 4, an MILP approach is used to optimize the system. This optimization is carried out using the GAMS, which determines the amount of tanks, electrolyzers, and the operating level that will produce the minimum amount of emissions. Thus, the result of the GAMS model, although not adhering to controller logic, represents the best performance possible.

3. RESULTS

Each of the simulation cases described previously is run, and Cases 2, 3, and 4 are compared with the base case, Case 1, which uses SMR for hydrogen production. In each of these simulations, the performance of the upgrader itself, which is modeled in Aspen HYSYS, remains constant. The parameters used for the upgrader simulation can be found in Appendix 1 at the end of this paper. In the upgrader simulation, there is a significant reduction in the emissions produced when electrolysis is used to produce hydrogen in place of SMR. In Table II later, the emission results for all four cases are given. In each of the three cases when the electrolyzer is used, there is a noticeable reduction in greenhouse gas emissions. For example, when the electrolyzer is merely follows the demand for hydrogen, it is possible to provide a 102,075 tonne reduction in CO$_2$e.

An even more effective method is to optimize the use of low-cost, low-emission energy by using on-site storage tanks to facilitate greater production of hydrogen when the emissions factor for energy is lower. To do this, a simple controller is used, which ramps up the electrolyzer when the emissions factor passes a threshold. The results of running the electrolyzer system using energy storage with this simple controller are compared with the production of hydrogen through SMR in Table II previously. Here, the hydrogen production system utilizing the simple controller can create greater emissions reductions than previous, with a single year reduction of 118,501 tonnes. The optimal annual CO$_2$e emissions reduction, based on the GAMS method described in Section 2, is 144,925 tonnes of CO$_2$e in a single year. Over the course of 20 years, it is possible to save between 2 and 2.8 million tonnes of CO$_2$e. If such a system, installed in Ontario for example, was able to use carbon credits at a market value of $30 per tonne of carbon, the value of these greenhouse gas emissions would be between $60m and $84m.

Figure 4. Overall emissions factor for the Ontario Electrical Grid, 2012–2014.

Table II. Single-year and 20-year simulation results for all four cases.

H$_2$ production scheme	Number of electrolyzer	One-year emissions (t CO$_2$e)	One-year emissions reduction (t CO$_2$e)	20-year emissions reduction (t CO$_2$e)	kg CO$_2$e per kg H$_2$	Number of 616 kg H$_2$ tank
Case 1: steam methane reforming	N/A	230,255	—	—	11	
Case 2: electrolyzer: produce to meet demand	299	128,180	102,075	2,041,496	5	
Case 3: electrolyzer simple controller, optimized	299	111,752	118,501	2,370,025	4.8	2,350
Case 4: electrolyzers, full MILP optimization	966	85,330	144,926	2,898,497	3.3	9,442

MILP, mixed-integer linear programming.

Table III. Capital and operating costs for all four cases – electrolyzers with storage tanks.

H$_2$ production scheme	Capital cost ($ × 10^6)	Operating cost ($ per kg H$_2$)	Carbon credit cost ($ per kg H$_2$)	Yearly costs ($ × 10^6)	Present value of yearly costs ($ × 10^6)	Total 20-year cost ($ × 10^6)
Case 1: steam methane reforming	82	3.84	0.54–0.64	117	2,115	2,198
Case 2: electrolyzer: produce to meet demand	0.3	2.51	0.30	71.9	1,298	1,298
Case 3: electrolyzer simple controller, optimized	651	2.53	0.30	72.4	1,307	1,958
Case 4: electrolyzers, full MILP optimization	2,611	1.98	0.20	55.8	1,007	3,617

MILP, mixed-integer linear programming.

An important element of assessment is to compare the overall cost of installing and producing hydrogen. The capital cost of an SMR facility of the size studied here is $30m for the equipment and $82m if one includes the necessary catalysts and materials needed for initial setup [43]. Based on the cost of purchasing natural gas to produce the hydrogen, the operating cost is approximately $0.83 per kg H$_2$. In Table III, the costs of operating the electrolysis scenarios are illustrated. The cost of the electrolyzers is approximately $1000 per MW capacity while the tanks are $277,000 each [44].

From Table III, previously, it can be seen that the operating costs of hydrogen produced through electrolysis are competitive with SMR in all modes of operation. For the assumed 20-year lifecycle of the equipment the biggest cost element is the yearly expenditure on electricity, water, and carbon. For the SMR setup, the costs are similarly for electricity, natural gas, and carbon.

4. CONCLUSIONS

To reduce the greenhouse gas emissions from the production of petroleum via bitumen, the use of electrolytic hydrogen for the hydrocracking step in the upgrading of dilbit is an excellent alternative to using hydrogen produced from steam

methane reformation. Electrolysis is a cleaner alternative to SMR and is also competitive economically. Over the expected 20-year lifespan of the hydrogen producing facility, electrolysis costs between $1.3bn and $3.1bn, while SMR costs $2.2bn. There are three cases examined in this paper that utilize Power-to-Gas for hydrogen production: the first simply follows the demand for hydrogen by the upgrader; the second uses a simple controller to guide the operating strategy of the electrolyser based on emission factor; and the third is a detailed optimization to reduce overall life cycle emission that includes varying the operational strategy of the electrolyzer and the incorporation of hydrogen storage, which results in the greatest reduction of emissions. The most cost effective strategy is Case 2, where the electrolyzer produces enough hydrogen to meet demand, which costs $1.3bn to operate over 20 years. Due to the high cost and number of tanks required to store the gaseous hydrogen in the optimized system, the cost of Cases 3 and 4 exceed the cost of SMR and Case 2. However, the optimized systems in Cases 3 and 4 provide 2.4 and 2.9 Gt of emissions reductions, respectively, over SMR while Case 2 provides 2.0 Gt. Thus, although the optimized cases provide the most emissions reductions, the simple controller that uses a threshold emissions factor and a smaller number of hydrogen storage tanks may offer a low-fidelity solution that provides comparable emission reductions at a significantly reduced capital investment.

APPENDIX I: DESIGN PARAMETERS FOR UPGRADER.

Parameter	Unit	Value
Atmospheric Distillation Unit		
Dilbit Feed API Gravity	°	20.5
Diluent Recovery Unit Inlet Temperature	°C	193
Diluent Recovery Unit Pressure	Bar	1.37
Diluent Recovery Unit Stages/Reflux Ratio	-	14/0.25
Diluent Recovery fraction	%	24
Diluent API Gravity	°	60.8
LGO Recovery Unit Inlet Temperature	°C	369
LGO Recovery Unit Pressure	Bar	1.37
LGO Recovery Unit Stages/Reflux Ratio	-	14/0.3
Atmospheric Topped Bitumen API Gravity	°	7.6
Vacuum Distillation Unit		
Inlet Temperature	°C	415
Inlet Pressure	Bar	0.05
Condenser Temperature	°C	149
LVGO Pumparound Inlet/Outlet Temperature	°C	227/121
HVGO Pumparound Inlet/Outlet Temperature	°C	282/232
Column Stages/Reflux Ratio	-	20/10
Vacuum Topped Bitumen API Gravity	°	1.6
Delayed Coker Unit		
Delayed Coker Furnace Temperature	°C	510
Delayed Coker Furnace Pressure	Bar	3.103
Coker Steam/VTB Ratio	kg/bbl	0.75
Coker Fractionator Inlet Temperature	°C	443
Coker Fractionator Inlet Pressure	Bar	1.37
LGO Pumparound Inlet/Outlet Temperature	°C	224/176
Coker Fractionator Stages	-	16
Hydrotreaters (Naphtha/LGO/HGO)		
Number of Catalyst Bed Stages	-	2/2/3
Inlet Temperature*	°C	204/371/399
Inlet Pressure	Bar	82/103/117
Total Hydrogen/Feed Ratio[†]	MSCF/bbl	4/4/6
Reactor Diameter	m	3.05/4.88/6.71
Product Specs		
SCO API Gravity	°	31–32
SCO Sulfur Content	Wt-%	<0.1
SCO Recovery from Bitumen, Mass Basis	%	76
Offgas Lower Heating Value, Mass Basis	kJ/kg	45540

*Reactor inlet temperature is kept constant by purge gas streams on the bed outlet except for the Naphtha hydrotreater, which had a secondary heater to 399 °C.
[†]Total hydrogen includes hydrotreater recycle and feed from hydrogen recovery unit.

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