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Development of a pricing mechanism for valuing ancillary, transportation and environmental services offered by a power to gas energy system

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A B S T R A C T

Power to gas is a novel energy storage concept that can help in providing energy storage and offer sustainable and efficient alternative ways to utilize the surplus electricity generated by the provincial grid of Ontario, Canada. This situation of 'surplus electricity' also exists elsewhere as there in increasing intermittent renewable power on various grids. The ability of the power to gas energy hubs to utilize the existing natural gas distribution and storage network (within the province) to distribute and store the electrolytic hydrogen produced is one of its major advantages. In this study an optimization model of a power to gas energy hub having a hydrogen production module capacity of 2 MW has been developed. The goal of the optimization study is to carry out an economic feasibility of the energy hub under existing pricing mechanisms for the three primary services that it provides, namely: 1) Offsetting CO_2 emissions at natural gas end users by providing hydrogen enriched natural gas; 2) Providing demand response when directed by the Independent Electricity System Operator of the province, and 3) Providing pure hydrogen to a fuel cell vehicle refueling station. It is observed that current pricing mechanisms are not valued high enough for the power to gas energy hub to be economically feasible and payback periods longer than the project lifetime (20 years) have been observed. Therefore, through a post-processing economic calculation, the additional monetary incentive required for the energy hub to achieve a NPV equal to zero for shorter project lifetimes of 8, 9 and 10 years have been calculated. The required additional monetary incentives (for the new project lifetimes) have then been split proportionally to the share of the revenues earned by the energy hub while providing each of the three services. Through this, the existing pricing mechanisms have been scaled up and a new pricing mechanism has been developed that highlights the monetary requirements of a power to gas energy hub to be economically feasible. It is seen that the required increase in the pricing of the three different services offered by the energy hub are reasonable and lie within the ranges proposed for them in coming years.

1. Introduction

With the ever increasing supply of electricity from green energy, many jurisdictions including the province of Ontario must balance an intermittent sources of renewable energy (wind and solar), whose generation profile at times do not match with the electricity demand profile. Furthermore, due to the current electrical system's high reliance on nuclear energy, there is a surplus of baseload power generated during certain off-peak periods. This surplus is often sold to neighboring jurisdictions at a loss in order to balance the power on the grid. One method for management of the supply and demand is to operate the renewable generation assets by making it dispatchable, as Ontario has had to do [1,2].

Research on potential implementations of large scale energy storage technologies in countries with growing renewable energy portfolio has been rigorous in the past few years. de Boer et al. [3]

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carry out a comparative analysis of the benefits of the integration of large scale energy storage systems like pumped hydro storage, compressed air energy system and power to gas energy hubs in an electricity grid with growing penetration of wind farms. In their rigorous analysis it is seen that the power to gas energy hub concept can be effective energy storage systems in countries which have existing natural gas systems that can act as a sink to store large amounts of surplus electricity.

The Independent Electricity System Operator of Ontario has been actively trying to procure energy storage technologies to help alleviate the surplus electricity generation issue that it faces during the power grids transition to a renewable energy economy. Power to gas is one of the technologies procured by the IESO [4].

Power to gas proposes to utilize surplus electricity produced by the power grid to produce hydrogen through electrolysis. The hydrogen can be injected into the existing natural gas distribution and storage system within the province and in this manner the natural gas grid is used for energy storage which helps to support renewable energy integration [5]. Linking the natural gas grid with the power grid will enable Ontario to utilize the large storage capacity offered by the existing underground natural gas reservoir. Walker et al. benchmark power to gas with respect to other existing energy storage technologies (in the context of Ontario) and highlight that the concept has a potential storage capacity that is orders of magnitude greater than competing technologies [6]. They also highlight the power to gas's ability to provide energy storage over a longer time period (weeks or seasonally). The hydrogen injected in to the natural gas grid can also find direct end use at natural gas end users. Nastasi et al. [7] analyze the benefits of linking the power and natural gas grids by suggesting an effective way of utilizing intermittent power generated by renewable energy storage systems. In their work Nastasi et al. look at the 'greening' of the natural gas grid by injecting renewable hydrogen produced via electrolyzers into the natural gas distribution network. The hydrogen enriched natural gas blend produced, helps in offsetting CO_2 emissions at the natural gas end user and is seen as a more efficient way of using hydrogen in comparison to its storage and re-use at a later time point to produce electricity. The linking of the heating and the electricity network is a potential solution for easing the transition to a renewable energy economy and forming a seamlessly interlinked energy network or a 'smarter energy network'. Collet et al. [8] carry out an environmental and techno-economic analysis on yet another potential energy recovery pathway of the power to gas energy hub concept where, hydrogen produced from both renewable and non-renewable energy sources is combined with CO_2 from biogas to produce bio-CH_4. The bio-CH_4 can then be injected in to the natural gas distribution network once it meets the specific standards set by natural gas utilities for it to be used by the end user. Maroufmashat et al. look at the feasibility of incorporating a Power to gas energy hub in an urban community and their analysis shows how different energy vectors including hydrogen can be exchanged between hubs, thus forming smart urban energy systems [9]. Although there are a number of pilot plants using power to gas globally, few of these use the injection of hydrogen into the natural gas system [10]. Only a small number of pilot plants worldwide use natural gas pipelines or underground gas storage reservoirs to distribute and store the gas. However, a power to gas plant in Falkenhagen, Germany demonstrates that this type of hydrogen injection is viable [11].

Also, the development of hydrogen generation capacity initiates a transition to a 'hydrogen economy' where zero emission transportation addresses both urban air pollution and climate change issues.

The ancillary service market can provide additional revenues for power to gas facilities with modern polymer electrolyte membrane (PEM) electrolyzers which can alter their load and output quickly in order to provide this service. To determine the appropriateness of electrolyzers for offering regulation and load following services, Eichman et al. [12] carried out ramping tests. The tests were carried out on a 40-kW alkaline and a 40-kW PEM electrolyzer. The results show 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. Eichman et al.'s work also shows 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 within a quick succession. The alkaline electrolyzer lagged the PEM electrolyzer significantly in the study and is thus less suitable for providing demand response services. The provision of high value ancillary services help to make the installation and operation of electrolysis technology more economical.

There are a number of disturbances that can lead to a disjoint between energy supply and demand [13]. To accommodate the disturbances and manage the grid, the Independent Electricity Systems Operator (IESO) purchases ancillary services from generators and consumers [14–18]. Ancillary services can be divided into operating reserves (OR) and demand response (DR), as shown in Table 1.

As can be seen from Table 1, the goal of the demand response program is to procure loads which react to signals to modify their energy use. One way to encourage a modification of energy use is to provide a price-based program [19,20]. This system mimics the nature of the Time of Use energy pricing for residential consumers in Ontario, and of the wholesale Hourly Ontario Energy Price (HOEP) for industrial and commercial consumers [13,21]. The eventual goal in Ontario is to have various demand response contractors bid through an auction to provide demand response services, as laid out by IESO's pre-auction report [22,23].

Although there are costs from offering demand response services, such as lost business and inconvenience, end users offering the service may have reduced total electrical costs from the use of low cost off-peak power [20,24,25]. When a high amount of energy demand is shifted to off-peak periods, it becomes easier to utilize renewable energy and manage the province's baseload nuclear power and makes more efficient use of all generation assets. The benefits are not only limited to the customers, but also extends to the operator of the program. If the IESO purchases demand response services from multiple loads, it will reduce electricity prices and its own capital and operations costs [26]. The IESO hopes to reach a demand response capacity of 80 MW through a number of contracts for loads up to 35 MW [18].

Parra et al. [27] carry out a techno-economic evaluations of power to gas energy hub systems with hydrogen production (electrolyzer system) capacities in the MW scale. One of the conclusions of their study shows the benefit of developing power to gas energy systems that can provide multiple services like: 1) Power to Hydrogen, and 2) Power to Methane. By offering multiple services, Parra et al. show that power to gas energy systems can become more economically viable.

Therefore, this study focuses on modeling a 2 MW power to Gas system, co-located at a natural gas pressure reduction station that offers three services, namely: 1) Offsetting CO_2 emissions at natural gas end users by providing hydrogen enriched natural gas; 2) Providing demand response when directed by the Independent Electricity System Operator of the province, and 3) Providing pure hydrogen to a fuel cell vehicle refueling station. A mixed integer non-linear programming problem has been formulated in the General Algebraic Modeling System (GAMS). The objectives being optimized are the economic performance, and the economic benefits from curbing the emission of greenhouse gases from the hub,

Table 1
Ancillary Services provided for IESO [17].

Type	Service	Procured from	Service Time
1. Operating Reserves	Supplementary energy for unforeseen circumstances	Dispatchable loads and generators	2 h [17]
2. Demand Response			
a. Regulation [18]	Manipulation of consumption profile	End-users	Second-to-second
b. Load following [13,19]	Match fluctuations in demand and supply	Generators and loads can participate directly or as aggregated load [20]	5-min to 1-h

while participating in the future demand response auction program [22]. In the auction program the power to Gas facility receives the maximum demand response auction clearing price value [23].

The study also highlights the potential benefit of integrating the power grid with the natural gas grid and also linking the power grid to the future transportation sector that employs the use of zero-emission vehicles like fuel cell vehicles. Schiebahn et al. [28] carry out a techno-economic analysis of the potential energy recovery pathways of power to gas systems (e.g.: providing hydrogen for fuel cell vehicles) in the context of Germany. Their economic evaluation is based on a static electricity pricing. Zhao et al. [29] develop a small scale refueling station solely dependent on renewable energy generation sources. Their work focuses on a decentralized energy system. In comparison to both Schiebahn et al. and Zhao et al.'s work, the study presented here involves development of a more rigorous optimization model that accounts for the variation in the operating cost (dynamic electricity pricing) of the power to gas system on an hourly time index over the course of a year while satisfying hydrogen demand of a fuel cell vehicle refueling station with a daily hydrogen demand capacity of 670 kg. This work also looks at how a power to gas energy hub gains economic incentives in offsetting CO_2 emissions by injecting hydrogen into the existing natural gas infrastructure within the province of Ontario. There is a realizable benefit in linking the power and natural gas grid in Ontario as the electrolytic hydrogen produced comes from a relatively clean energy supply mix (90% of annual energy generation came from clean energy source in 2015) [30]. This in turn leads to a better utilization of the surplus power produced by the grid, in comparison to exporting electricity at a low price to neighboring jurisdictions. Another novelty of this work is the incorporation of ancillary services and analyzing the economic benefits of participating in the provincial demand response auction market. The high ramp up and ramp down rates of polymer electrolyte membranes has been utilized to provide hourly demand response services to provincial power grid of Ontario.

2. Problem definition

Polymer electrolyte membrane (PEM) electrolyzers are known to have a higher durability (i.e. provide better functionality at extreme operating conditions) and are quicker to complete to changes in operating level in comparison to alkaline electrolyzers over their lifecycle [12,31–33]. Therefore, the authors analyze the potential benefits that the electrolyzers can provide through demand response (DR) based on the load following requirements set by the IESO. Natural gas pressure reduction stations serve as an interconnection between the high-pressure transmission-lines which operate at 42–84 bar and low pressure distribution pipelines at 1.03–5.15 bar [34]. As PEM electrolyzers have the ability to produce hydrogen at high pressures in the range of 10–30 bar, it is safe to assume that injecting high pressure hydrogen in to the distribution lines originating from the pressure reduction station will only require pressure regulation through the infrastructure for which is already available at the pressure reduction site. In this study, it is assumed that the two PEM electrolyzer modules produce hydrogen at 30 bar [35] and 21 °C. The safe injection limit of hydrogen into natural gas systems is approximately 5 mol% [34]. In addition to providing demand response services to the power grid, and Hydrogen Enriched Natural Gas (HENG) to natural gas end users, the potential economic and environmental benefits of providing hydrogen for a refueling station has also been considered in this energy hub simulation. The motivation behind this comes from the shift towards a greener transportation sector [36], especially a transition towards a hydrogen economy. As of March 2016, there are 644 fuel cell refueling stations worldwide [37], and a number of different hydrogen fuel cell vehicles are now available commercially. The provision of hydrogen for vehicles is the third high value service (the other two services are: Offsetting CO_2 emissions at natural gas end user and providing demand response to power grid) that the electrolysis technology provides in this study. Although this work is customized to the Ontario electrical generation system, the model can be used use for various electrical generation systems with various generation profiles.

2.1. Hydrogen demand

Pratt et al. [38] highlight three near-term hydrogen filling station capacities: 100 kg per day, 200 kg per day, and 300 kg per day. The filling stations having a capacity of 100 and 200 kg are suitable for large city centers where the demand fits the 'low use commuter or intermittent station classifications' [37]. The 300 kg per filling station is better suited for an urban market with high demand, and can be categorized as a 'High Use Commuter' fueling station. However, the 2 MW PEM electrolyzer systems can meet a daily hydrogen demand of 300 kg with sufficient capacity to spare.

The hydrogen vehicle demand curve in this paper is the 'default Chevron Demand Profile' from the Hydrogen Refueling Station Analysis Model (HRSAM) developed by the National Renewable Energy Laboratory (NREL) [39]. In order to account for variations in the total daily demand placed on the station over a period of one week, variability data from a feasibility analysis of a hydrogen fueling station in Honolulu is considered [40].

The hydrogen demand profile available in the Hydrogen Refueling Station Analysis Model has been used for a refueling station capable of handling 100 kg per day of hydrogen demand. Mukherjee et al. develop a linear programming optimization problem of a power to gas energy hub with fixed storage and hydrogen production capacity (2 MW) [41]. The purpose of the work was to assess the maximum daily hydrogen demand that can be supplied by the 2 MW system while providing demand response service to the power grid. The hydrogen demand profile of the 100 kg per day refueling station is scaled up manually until the optimization problem gives an infeasible solution. In other words this implies that the hydrogen demand placed on the energy hub goes unsatisfied. The conclusion of their work shows that the 2 MW power to gas energy hub can meet a maximum daily hydrogen demand of 670 kg from a refueling station while also satisfying demand response requirements placed on it by the power grid. To improve on the model proposed by Mukherjee et al., the same system configuration is utilized in the work presented here to provide the additional service of offsetting CO_2 emissions at the natural gas end users by linking the power and natural gas grids.

2.2. Energy hub components: H_2 filling station infrastructure

The energy hub designed at the pressure reduction station, and illustrated in Fig. 1, is comprised of:

- 2 × 1 MW PEM electrolyzers [35] for producing hydrogen;
- 1 storage tank with a maximum capacity of 89 kg at 172 bar [42];
- A three stage booster reciprocating compressor capable of handling inlet pressures as low as 20 bar (compression ratio ~ 21) and has a capacity of 87 kg per h; and,
- A pre-storage reciprocating compressor developed by RIX Industries [39] that has a maximum flow handling capacity of 42 kg per h and can compress hydrogen gas from 3 bar to 310 bar.

As shown in Fig. 1, a fraction of the hydrogen produced by the electrolyzer is sent directly to the pressure reduction station where the gas is mixed with natural gas to form HENG and injected in to low pressure distribution lines. The compressors and storage tank unit are a part of an integrated system that provides pure hydrogen to a hydrogen refueling station. Hydrogen produced for satisfying fuel cell vehicle (FCV) fuel demand passes through a pre-storage reciprocating compressor that compresses gas coming in at 30 bar and 21 °C to the storage tank pressure of 172 bar. The lower limit of hydrogen inventory (I_{Min}) within the tank is calculated at 30 bar using the ideal gas equation that has been modified to account for the compressibility factor of hydrogen at 30 bar and 21 °C. The parameters V, R and T are used as denotations for the volume of tank (m^3), the ideal gas constant (m^3 bar per K mol) and the temperature (K) inside the tank (Appendix: A).

$$I_{Min} = \frac{P_{tank,min} \times V \times z}{R \times T} \tag{1}$$

The booster compressor placed outside the tank is used to compress hydrogen gas coming out of the tank to 350 bar, which is considered to be the storage pressure of hydrogen gas on board fuel cell vehicles [39]. The temperature assumed for calculating the properties of hydrogen is taken to be 21 °C which is temperature at which hydrogen is stored on board fuel cell vehicles [39].

2.3. Demand response

The energy hub provides hourly load following demand response services through load reductions, as directed by the IESO. The hourly load-following requirement of the grid is calculated via the schematic shown in Fig. 2. Through the calculation of the hourly load following requirement, the hours in which the grid has a positive hourly load following most of which needs to be provided from the generator side, demand response service provided by the power to gas energy hub can offset a part of the concerned hour's positive load following requirement.

The first step in developing the demand response data used in this study involves normalizing the twelve 5-min provincial market energy demands in an hour. The historical 5 min market demand data has been provided by the IESO. The normalization is done by calculating the 25 min rolling averages of each of the twelve 5-min market demands. Subsequently, the maximum and minimum rolling averages occurring in an hour are estimated. Following this the difference between the maximum and minimum rolling average is also determined ($Differential_h$).

Since the market demand data includes energy exchanges between the neighboring jurisdictions, the provincial imports and exports of energy occurring in an hour need to be accounted for. The hourly net interchange schedule is estimated by calculating the difference between the hourly imports and exports of energy to and from the province [43]. Upon the determination of the hourly net interchange schedule the hourly load following is calculated by calculating the difference between the terms $Differential_h$ and $Net\ Interchange\ Schedule_h$ [44]. The binary parameter 'DR' is '1' when the electrolyzers need to provide demand response and it is set as '0' when there is no demand response action required.

3. Optimization model

Previous work by Mukherjee et al. [5] has focused on sizing the components of the power to gas energy hub, specifically the hydrogen production and storage systems. The optimization logic to size the energy hub components have been based on the trade-

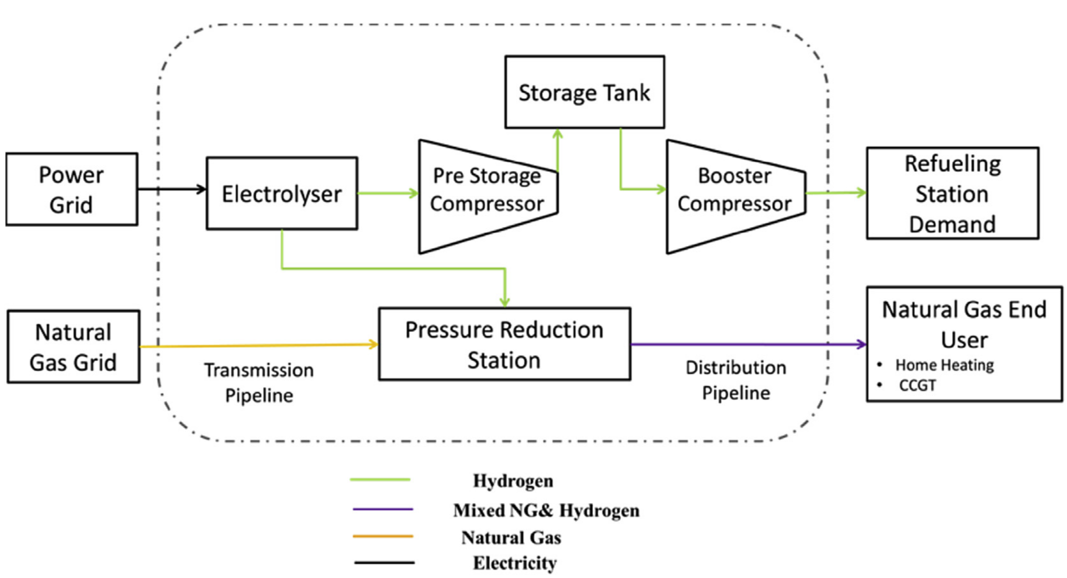

Fig. 1. Conceptual Overview of the Energy Hub.

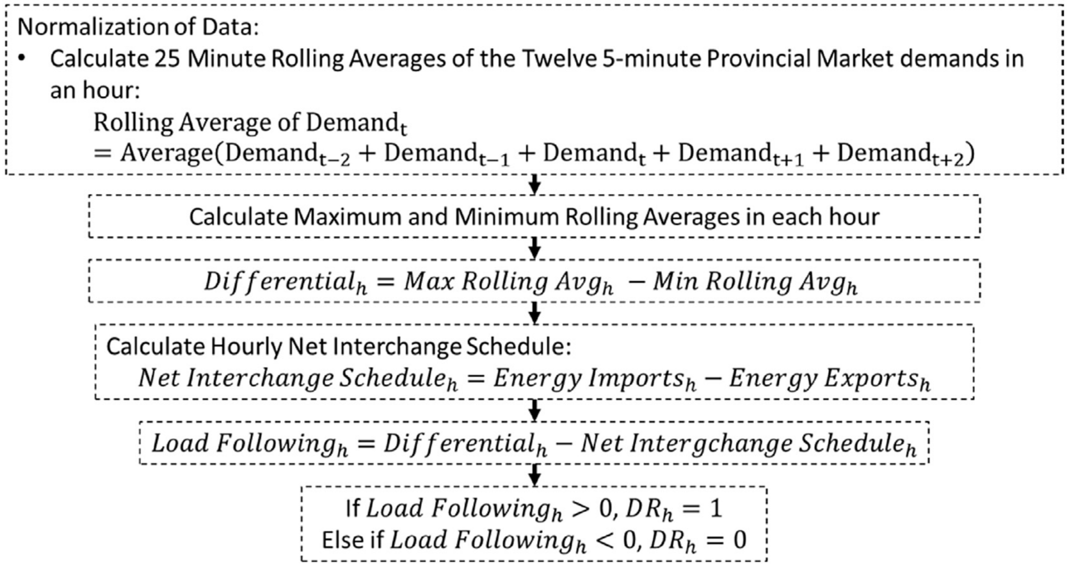

Fig. 2. Schematic showing the development of the demand response data.

off based ε-constraint method [45], where the net cost of the overall system has been minimized subject to emission offset constraints applicable to CO_2 emissions offset from supplying HENG to natural gas end users. While meeting the emission offset targets, the installed system minimizes net cost by achieving energy arbitrage across the two energy systems. The system decides to produce surplus hydrogen and inject some of it in storage tanks when it is inexpensive to buy electricity for producing hydrogen through the electrolyzers. By doing so, when the electricity price peaks, the storage systems can be used to withdraw hydrogen to inject it into the natural gas system providing a uniform service and concentration. In this way cost is reduced during peak electricity price by operating electrolyzers at a lower level. The results from Ref. [5] shows that selling hydrogen to natural gas end users at the energy value of natural gas (Henry hub natural gas spot price) is not economical. However they propose that the energy hub may be more economically feasible while providing ancillary services like grid regulation (demand response), and H_2 fuel supply for fuel cell vehicle refueling stations.

Mukherjee et al. assess the ability of a power to gas system with fixed hydrogen production capacity (2 MW nameplate capacity PEM electrolyzers) to provide demand response and offset CO_2 emissions at natural gas end users by providing hydrogen enriched natural gas [46]. They adopt a multi-objective (Economic and Emissions) optimization approach using the ε-constraint method to model the power to gas energy hub and size a storage and compressor module around the electrolyzer system. The conclusion of their work shows that when 29 storage modules of 21.3 kg capacity each are co-located at the site of electrolyzer system installation, a total of 1905 tonnes of $CO_{2,e}$ emissions can be offset. However, the payback period is more than the project lifetime of 20 years. When the minimum $CO_{2,e}$ emissions to be offset is lowered to 70% of the maximum value, the energy hub can achieve this without any required storage and has a favorable payback period of 11.7 years. Another work carried out by Mukherjee et al. [47] looks at the ability of a 2 MW electrolyzer system to provide hydrogen demand for a fuel cell vehicle refueling station having a 428.6 kg daily demand while also offering hydrogen to natural gas end users. The electroylzer system is also setup to provide frequency regulation services to the power grid. The hydrogen produced for the fuel cell vehicles is sent to the refueling station via the natural gas pipeline network. The hydrogen is separated from the natural gas via pressure swing adsorption units sized at a downstream point in the gas distribution network and then sent to the refueling station. The conclusion of their work shows that the energy hub is economically attractive when on top of receiving incentive for providing frequency regulation service, the hydrogen is sold at a premium price ($ 8 per kg) to both the natural gas end user and the refueling station. They draw this conclusion in comparison to a system where hydrogen to the natural gas system is sold at the natural gas spot price. In this case far less hydrogen is sold to the natural gas end user and the total revenues earned are much lower.

The work presented by Mukherjee et al. in Ref. [46], and [47] show the potential benefits of developing an energy hub with a fixed electrolyzer capacity to provide ancillary services as well as provide hydrogen to both the natural gas and the future transportation sector in Ontario. Although, both articles show that power to gas energy hubs can be competitive in economic terms, the articles base the valuation of the services provided by the energy hub based on what is set either in neighboring jurisdictions (examples of values used: $CO_{2,e}$ tax of Alberta, Canada, hydrogen fuel price from developing US fuel cell vehicle markets, and regulation service pricing from PJM, USA) or what has been set within the province of Ontario without the consideration of power to gas as a potential service provider (e.g. Demand response auction market clearing price in Ontario). Therefore, in this study, the authors utilize the existing pricing structures for each of the individual services, namely: 1) $CO_{2,e}$ emissions offset benefit; 2) Demand response incentive, and 3) Hydrogen fuel price for transportation sector (set as production cost of hydrogen for the energy hub modeled, see section 3.1), as a baseline value and then develop a premium pricing mechanism that give a clear idea on the valuation of the services provided above. This in turn will help the policy makers in the province of Ontario to develop programs for power to gas energy hubs to be able to participate and compete in the energy storage and service provider market. The optimization logic adopted in this work and presented in section 3.1 moves away from the previously adopted multi-objective optimization approach by the authors in their work described above [46], [47]. In the multi-objective approach, the potential monetary incentive of offsetting emissions were calculated post-optimization. In this study the optimization problem is centered around a single objective which incorporates the incentive received from $CO_{2,e}$ emissions offset as a revenue stream contributing to the cash flow objective (see section 3.1). In doing so, one can actually make a decision if the $CO_{2,e}$ emission offset credit adopted is high enough to warrant injection of hydrogen in to the natural gas grid and offset emissions at the end users of natural gas.

3.1. Mixed integer non-linear programming formulation

In this section, the calculations of the CO_2 credits and fuel subsidization carried about by the optimization model are discussed. A mixed integer non-linear optimization problem is formulated in the General Algebraic Modeling System. The optimization problem is run for two scenarios, namely: 1) Scenario 1: Baseline price mechanism, and 2) Scenario 2: Adjusted H_2 price mechanism. The two scenarios are developed based on the premise that hydrogen sold to the natural gas end user at the natural gas spot price is not economical [5]. In scenarios 1 and 2, selling price of hydrogen to natural gas end user is set at the natural gas spot price. However, in scenario 2, to account for the losses incurred in selling hydrogen to the natural gas end user, the selling price of the hydrogen to fuel cell vehicle end users is adjusted (or marked up). Scenario 1, does not mark up the price of hydrogen sold to fuel cell vehicles. Equations ((5) and (8) and (12) and (14)–(16) show the process of calculating this adjustment in selling price of hydrogen.

It should be noted that the only difference between scenario 1 and 2 is that scenario 1 doesn't include equations (4), (12) and (15) when modeled in the GAMS software. Every other equation is included in both of the models prepared for scenario 1 and 2.

The symbols used in the equations described in this section are defined in Appendix A and B. Equation (2), below, shows the cash flow objective function formulated for the optimization problem. The main goal is to maximize the cash flow function.

$$\begin{aligned} \mathit{Maximize} : CF &= -O\&M_{Electrolyzer} - C_{Electrolyzer} - (C_{Booster\ Compressor} \\ &\quad \times N_{Booster\ Compressor}) - (C_{Compressor,Pre-Storage} \\ &\quad \times N_{Compressor,\ Pre-Storage}) - \left(C_{Tank\ Storage} \times N_{Tank}\right) \\ &\quad + NR \end{aligned} \tag{2}$$

The cash flow function is comprised of terms that make up the amortized investment including the capital ($C_{Electrolyzer}$) and operating and maintenance ($O\&M_{Electrolyzer}$) costs of the PEM electrolyzers [37]. The objective function also includes the amortized capital and installation costs of the compressor and hydrogen storage system located at the energy hub. The capital cost data for the hydrogen compression and storage system is retrieved from literature examining the future hydrogen economy [39,42]. $N_{Booster\ Compressor}$, $N_{Compressor,\ Pre-Storage}$, and N_{Tank} are parameters that denote the number of booster compressors, pre-storage compressors and tanks used in the energy hub. The coefficients of the parameters: $C_{Booster\ Compressor}$, $C_{Compressor,Pre-Storage}$, and $C_{Tank\ Storage}$ are the amortized capital costs for the booster compressor, pre-storage compressor, and tank. The total capital costs of the components of the energy hub were amortized over a period of (n) 20 years at an interest rate of 8%, which is considered to be the lifetime of the project. The term NR in Equation (2) for scenario 1 is expanded on in Equation (3).

$$\begin{aligned} NR = \sum_{h=1}^{H} \Big[&- \left(F_{H_2,h} \times CR_{Water} \times UC_{Water}\right) - \Big[\Big\{E_h \\ &+ E_{Booster\ compressor,h} + \big(F_{H_2,In,Tank,h} \\ &\times ECF_{Compressor,\ Pre-Storage}\big)\Big\} \times \left(C_{Electricity,h} + TC_h\right)\Big] \\ &+ \left(F_{H_2,Pipe,h} \times HHV_{H_2} \times \left(R_{NG,h} - [\gamma \times \delta]\right)\right) + \big(F_{H_2,Out,Tank,h} \\ &\times LPC_{H_2}\big) - C_{DR,h} + \left(LR_h \times R_{Load\ Reduction} \times DR_h\right)\Big] + \big(EO_{NG} \\ &\times R_{CO_2}\big) \end{aligned} \tag{3}$$

The variable NR is a net monetary stream that is the difference between the earnings and the operating cost of the power to gas energy hub. In addition to the operating and maintenance costs of the PEM electrolyzers, the system also incurs the following operating costs:

- $CR_{Water} \times UC_{Water}$, accounts for the cost ($) of water per kmol of hydrogen produced;
- $C_{Electricity}$, helps in estimating the cost incurred to run the two compressors and the PEM electrolyzers installed in the energy hub;
- E is denoted as the energy consumed by the PEM electrolyzers and it is calculated using Equation (17);
- The term $E_{Booster\ compressor}$ is the kWh of energy consumed by the booster compressor and is calculated using Equation (28);
- $ECF_{Compressor,\ Pre-Storage}$ ($kWh\ per\ kmol\ H_2$) is the energy consumed by the pre-storage compressor per kmol of hydrogen fed to it [39]. The term is pre-calculated because the pre-storage compressor compresses gas coming in from the PEM electrolyzers at 30 bar and 21 °C to the tank storage pressure of 172 bar and 21 °C;
- TC, is a fixed charge added to the total operating cost for using the power transmission lines. It is calculated by multiplying a charge factor by the energy consumed by the electrolyzers, and the two compressors;
- γ (\$ *per MMBtu*) is the rate charged by natural gas distribution utility to supply fuel for compressors located along their pipelines that help in maintaining the pressure of the flow within the pipelines [48];
- δ (%) is the amount of natural gas fuel required by natural gas distribution utility to run their pipeline compressors, on top of the gas is being transported. The requirement is expressed as a percentage of gas to be transported [48], and
- C_{DR} is a term defined to calculate the money owed by the energy hub to the grid at times when the system is actually scheduled to provide its entire contracted capacity for demand response but chooses to offer a demand response curtailment lower than the contracted amount. This term is calculated using Equation (19).

The terms that comprise the earnings of the energy hub include:

- R_{NG}(\$ *per MMBtu*) is the Henry Hub Natural Gas Spot Price that is used as the selling price of hydrogen supplied to the natural gas end users;
- HHV_{H_2} (*MMBtu per kmol*) is the higher heating value of hydrogen used in the study;
- LPC_{H_2} denotes the levelized production cost of hydrogen in scenario 1. The hydrogen is sold to the fuel cell vehicles at the levelized production cost incurred by the energy hub to produce the gas (see equation (5)).

- $R_{Load\ Reduction}$ (\$ per kWh) is the incentive that the power to gas energy hub receives for reducing its load and provide the demand response services to the grid [23];
- DR is a binary parameter which takes a value of '1' when the power to gas system is contracted to provide the demand response service to the grid, and '0' when it does not have to provide the demand response service;
- LR (kWh) is the actual amount of curtailment provided by the PEM electrolyzers at a particular hour;
- EO_{NG} is the amount of CO_2 emissions offset (kg) by sending HENG in place of pure natural gas to the end users. Equation (15) shows how the term is calculated;
- R_{CO_2} is the existing emission credit incentive given to services that reduce their CO_2 emissions. For this study this value has been set at the \$ 15 per tonne of CO_2 emissions carbon tax value used in Alberta, Canada [49]. Once again future analysis will consider the potential for an increase carbon pricing structure, which is likely.

Hourly energy demand data for the pressure reduction station has been made available for the period of November 2012 to October 2013 by Enbridge Inc. Therefore, the natural gas spot price R_{NG} data (Henry Hub Natural Gas Spot Price) and the hourly Ontario energy price ($C_{Electricity}$) [50] for the corresponding timeline has been used in the study.

Equation (4) shows the expression for the net revenue term (NR) for scenario 2. The only difference between equations (3) and (4) is the selling price of hydrogen to the fuel cell vehicles. In this case, LPC_{H_2} is replaced by ASP_{H_2}.

$$NR = \sum_{h=1}^{H}\Big[-\left(F_{H_2,h} \times CR_{Water} \times UC_{Water}\right) - \Big[\Big\{E_h + E_{Booster\ compressor,h} + \left(F_{H_2,In,Tank,h} \times ECF_{Compressor,Pre-Storage}\right)\Big\} \times \left(C_{Electricity,h} + TC_h\right)\Big] + \left(F_{H_2,Pipe,h} \times HHV_{H_2} \times \left(R_{NG,h} - [\gamma \times \delta]\right)\right) + \left(F_{H_2,Out,\ Tank,h} \times ASP_{H_2}\right) - C_{DR,h} + \left(LR_h \times R_{Load\ Reduction} \times DR_h\right)\Big] + \left(EO_{NG} \times R_{CO_2}\right) \tag{4}$$

ASP_{H_2} (\$ per kmol) is the marked up or adjusted selling price at which the hydrogen produced by the electrolyzers is sold to the fuel cell vehicle end users and it is a variable that is calculated using Equation (15).

The levelized production cost of hydrogen(LPC_{H_2}) is calculated by taking the ratio of total cost incurred in producing the gas (denoted by C_{H_2}) over the total amount of hydrogen produced (T_{H_2}) over the course of the entire modeling timeframe (Nov 2012–Oct 2013).

$$\frac{C_{H_2}}{T_{H_2}} = LPC_{H_2} \tag{5}$$

The variable C_{H_2} accounts for both the amortized capital costs of the energy hub infrastructure as well as the operating and maintenance cost incurred while operating the components of the hub. The terms used to calculate C_{H_2} is determined by using Equation (5). The terms included in Equation (6) are a part of equations (2) and (3) and have already been explained in detail.

$$C_{H_2} = O\&M_{Electrolyzer} + C_{Electrolyzer} + \left(C_{Booster\ Compressor} \times N_{Booster\ Compressor}\right) + \left(C_{Compressor,Pre-Storage} \times N_{Compressor,\ Pre-Storage}\right) + \left(C_{Tank\ Storage} \times N_{Tank}\right) + \sum_{h=1}^{H}\Big[\left(F_{H_2,h} \times CR_{Water} \times UC_{Water}\right) + \Big[\Big\{E_h + E_{Booster\ compressor,h} + \left(F_{H_2,In,Tank,h} \times ECF_{Compressor,\ Pre-Storage}\right)\Big\} \times \left(C_{Electricity,h} + TC_h\right)\Big] + \left(F_{H_2,Pipe,h} \times HHV_{H_2} \times \gamma \times \delta\right)\Big] \tag{6}$$

The hydrogen produced every hour is related to the energy bought from the grid at the hourly energy price (HOEP) via Equation (7). The $EF_{Electrolyzer}$ coefficient on the right hand side in Equation (7) is determined based on the ratio of the PEM electrolyzer efficiency and the higher heating value of hydrogen [35].

$$F_{H_2,h} = EF_{Electrolyzer} \times E_h \tag{7}$$

The annual hydrogen production of the energy hub can be calculated by summing the $F_{H_2,h}$ over the entire year (Nov 2012–Oct 2013) or 8760 h (H), as seen in Equation (8) below.

$$T_{H_2} = \sum_{h=1}^{H} F_{H_2,h} \tag{8}$$

Since the energy hub provides hydrogen to both the natural gas end users as well as the fuel cell vehicles at refueling station, the hydrogen coming out of the electrolyzer (F_{H_2}) is split in to two streams, as in Equation (9), $F_{H_2,In,Tank}$ and $F_{H_2,Pipe}$.

$F_{H_2,In,Tank}$ is the flow of hydrogen directed through the pre-storage compressor and then sent to the tank storage unit. $F_{H_2,Pipe}$ on the other hand is the hydrogen flow sent to the pressure reduction station where it mixes with natural gas and is then injected into the distribution pipelines which takes the HENG to the natural gas end users.

$$F_{H_2,h} = F_{H_2,In,Tank,h} + F_{H_2,Pipe,h} \tag{9}$$

At any given hour (h), the amount of hydrogen stored within the tank is determined by doing a simple inventory balance as shown in Equation (10).

$$I_{H_2,h} = I_{H_2,h-1} + F_{H_2,In,Tank,h} - F_{H_2,Out,Tank,h} \tag{10}$$

The index $h-1$ indicates the previous time point. I_{H_2} denotes the hydrogen inventory within the tank at the end of hour h. $F_{H_2,Out,\ Tank}$ is the amount of hydrogen taken out of the tank and sent to the booster compressor before being sent to the refueling station. The maximum and minimum amount of hydrogen that can be stored in the tank at any instant is set by the upper (I_{Max}) and lower (I_{Min}) bounds shown in Equation (11) below.

$$I_{Min} \le I_{H_2,h} \le I_{Max} \tag{11}$$

As the higher heating value of hydrogen is lower than the higher heating value of natural gas, it is intuitive that selling hydrogen to natural gas end user at a price set at the natural gas energy value is going to be less economical. Also, since the levelized hydrogen production cost calculated in Equation (5) accounts for both the hydrogen produced for the natural gas end user and the refueling station, hydrogen sold to the pipeline is undervalued. Therefore, the monetary loss in selling hydrogen at a lower price to the natural gas end user is used to adjust the selling price of hydrogen to fuel cell vehicles.

The monetary loss while selling hydrogen to the natural gas end user on an energy basis (HHV_{H2}) by using the Henry Hub Natural Gas Spot Price ($ per MMBtu) is calculated from the difference between the levelized production cost and the hourly spot price as seen in equation (12) below.

$$L = \left\{ LPC_{H_2} - \sum_{h=1}^{H} (HHV_{H_2} \times R_{NG,h}) \right\} \times F_{H_2,Pipe,h} \tag{12}$$

The summation of all of the hydrogen sold to the fuel cell vehicle over the course of a year is estimated by summing hydrogen withdrawn from the tank storage as seen in Equation (13).

$$T_{H_2,FCV} = \sum_{h=1}^{H} F_{H_2,Out,\ Tank,h} \tag{13}$$

The variable $R_{H_2,FCV}$ in Equation (14), is used to estimate the revenue earned if the hydrogen sent to the refueling station is sold at levelized production cost determined from Equation (5).

$$R_{H_2,FCV} = T_{H_2,FCV} \times LPC_{H_2} \tag{14}$$

Using the values of $T_{H_2,FCV}$ (kmol) and $R_{H_2,FCV}$ ($) from Equations (13) and (14), the adjusted selling price of hydrogen sent to refueling station has been estimated in equation (15), below.

$$ASP_{H_2} = \frac{(L + R_{H_2,FCV})}{T_{H_2,FCV}} \tag{15}$$

The total CO_2 emissions offset is calculated by adding the emissions reduced at natural gas end users (EO_{NG}).

$$EO_{NG} = \sum_{h=1}^{H} \left[O_h \times \left(EMF_{NG} + EMF_{NG,production} \right) - \left(F_{H_2,Pipe,h} \times EMF_{H_2} \right) \right] \tag{16}$$

Equation (16) outlines the process for calculating potential CO_2 emissions offset by selling HENG to natural gas end user. The term 'O' in the above equation denotes the amount of natural gas displaced with hydrogen and is calculated by taking the difference of natural gas flow when energy demand placed at the pressure reduction is satisfied solely with natural gas (X_{NG}) and natural gas flow ($F_{NG,Pipe}$) when HENG is used to satisfy the energy demand as shown in Equation (17).

$$O_h = X_{NG,h} - F_{NG,Pipe,h} \tag{17}$$

The calculated offset is then multiplied by the sum of the emission factors of natural gas combustion and natural gas production to get the actual emissions offset with the use of HENG as an energy vector. Emission factor of natural gas (EMF_{NG}, *kg of* $CO_{2,e}$ *per kmol of NG burnt*) is the amount of CO_2 emitted when natural gas is burnt by its end user. The emissions associated with the production of natural gas are given by $EMF_{NG,production}$ (*kg* $CO_{2,e}$ *per kmol of NG produced*) [51].

The emission factor associated with using electricity in the electrolyzers to produce hydrogen is that of the power grid (kg of CO_2 per kWh of electricity produced). Using this value and multiplying it with the efficiency factor (kWh of electricity consumed per kmol of hydrogen produced) of the PEM electrolyzers gives the value for EMF_{H_2}.

The amount of energy consumed by the electrolyzers is governed by Equation (18). The parameter E_{max} denotes the maximum energy consumption possible by the electrolyzers at a given hour (2000 kWh). In order to give the electrolyzers the flexibility to vary their consumption from one hour to another, a variable named $Ereduce_h$ is defined.

$$E_h \le E_{max} - LR_h \tag{18}$$

The variable LR in Equation (18) denotes the amount of load reduction offered in hours when the electrolyzers are required to reduce their energy consumption based on the load following demand response logic described in Subsection 2.3. The contracted curtailment amount (CCA) of the electrolyzers to offer demand response is set at 2000 kW in an hour. The Independent Electricity System Operator (IESO) sets the minimum amount of demand response offered by a contracted facility to be 1000 kW in an hour [52]. Equation (19) is used to limit the amount of load reduction offered by the electrolyzers in a given hour to 1000–2000 kW (CCA).

$$1000 \times DR_h \times \alpha_h \le LR_h \le CCA \times DR_h \times \alpha_h \tag{19}$$

The term α is used as a binary variable that gives the optimization problem the flexibility to choose between either offering or not offering the demand response service in a particular hour.

The IESO administers a clawback (C_{DR}) charge in hours where a facility cannot provide the entire contracted curtailment amount. Equation (20) is used to take into account this clawback charge when the electrolyzers are not able to offer a demand response of 2000 kWh (CCA).

$$C_{DR,h} = (UF_h \times R_{Load\ Reduction} \times CCA) \tag{20}$$

The clawback charge is calculated by initially multiplying the unavailability factor (UF) with the contracted curtailment amount. This product can also be defined as the difference between the contracted curtailment amount and the actual load reduction provided by the electrolyzers. The original incentive offered by the IESO for providing the demand response service is then multiplied to this difference to calculate the clawback charge. The unavailability factor is an estimate of the fractional decrease in demand response offered and is calculated by Equation (21).

$$UF_h = \frac{CCA - LR_h}{CCA} \times DR_h \tag{21}$$

The pure hydrogen demand from the refueling station that is placed on the energy hub is determined using Equation (22), where the flow of hydrogen coming out the tank storage unit ($F_{H_2,Out,\ Tank}$) should be equal to the pure hydrogen demand (D_{H_2}).

$$D_{H_2,h} = F_{H_2,Out,\ Tank,h} \tag{22}$$

The energy demand placed at the pressure reduction station is denoted by $D_{NG}(MMBtu)$. Since the natural gas end users are supplied with HENG, a heat content energy balance is used to make sure that the total energy demanded by the natural gas end users is satisfied. Therefore, the sum of energy content of hydrogen and natural gas injected into the distribution lines should be equal to D_{NG}, as illustrated in Equation (23).

$$\left(F_{H_2,Pipe,h} \times HHV_{H_2}\right) + \left(F_{NG,Pipe,h} \times HHV_{NG}\right) = D_{NG,h} \tag{23}$$

Since natural gas pipelines can be subjected to hydrogen embrittlement at high concentrations of hydrogen, a safe upper limit on the hydrogen injectability has been set with the help of Equation (24).

$$F_{H_2,Pipe,h} \le \theta \times F_{NG,Pipe,h} \tag{24}$$

The mole fraction factor in the above equation is set such that hydrogen content in the HENG blend does not exceed 5 mol%. This upper bound is set based on the analysis published in a report by Melaina et al. on blending hydrogen in natural gas pipelines [34].

$$F_{H_2,In,Tank,h} \le N_{Compressor,\ Pre-Storage} \times F_{Max,Compressor,\ Pre-Storage} \tag{25}$$

Hydrogen sent to the tank needs is compressed to 172 bar. In order to constrain the electrolyzer system from producing more than the compressor can handle in a particular hour, as shown in Equation (25), the hydrogen sent to the pre-storage compressor ($F_{H_2,In,Tank}$) should be less than or equal to the maximum flow that the compressor can handle ($F_{Max,Compressor,\ Pre-Storage}$). Similarly, the hydrogen coming out of the tank that is sent to the refueling station needs to be compressed to a pressure of 350 bar, which is the vehicle tank storage pressure. Therefore the flow of hydrogen sent to the booster compressor ($F_{H_2,Out,Tank}$) cannot exceed the maximum flow capacity of the compressor ($F_{Max,\ Booster\ compressor}$) itself, as illustrated in Equation (26).

$$F_{H_2,Out,Tank,h} \le N_{Booster\ Compressor} \times F_{Max,\ Booster\ compressor} \tag{26}$$

The energy consumed by the pre-storage compressor is fixed per kmol of hydrogen passed through the compressor because the compression ratio always remains the same (172:30). However, the energy consumed by the booster compressor is subject to variation because of the variation in the pressure of the incoming gas from the tank. The hydrogen coming out of the tank is assumed to have the same pressure as the gas pressure inside the tank.

The change in gas inventory also changes the pressure inside the tank. This is monitored using modified gas law (Equation (27)) where the compressibility factor (z) of hydrogen is used to take in to account its effect on pressure. The z for hydrogen in Equation (27) is estimated at different pressure and temperature conditions using a lookup table developed in Matlab Simulink model by Peng [33]. V, R *and* T are set as parameters and denote the volume of tank (m^3), the ideal gas constant (m^3 bar per K mol) and the temperature (K) inside the tank.

$$P_{tank,h} = \frac{I_{H_2,h} \times R \times z_h \times T \times 1000}{V} \tag{27}$$

The pressure inside the tank derived from equation (26) is then assumed to be the pressure of the hydrogen flow going into the booster compressor. Based on the formula given in a report prepared by NREL [39], the theoretical work done by the booster compressor ($W_{Booster\ compressor,theoretical}$, *kJ per kmol*) is calculated using Equation (28) below.

$$W_{Booster\ compressor,theoretical,h} = \frac{\bar{z}R_{comp}Tk}{k-1}\left[\left(\frac{P_{out}}{P_{tank,h}}\right)^{\frac{k-1}{k}} - 1\right] \tag{28}$$

The parameters used in Equation (27) include: R_{comp} (*kJ per kmol* – *K*), universal gas constant used for booster compressor; k, heat capacity ratio of hydrogen; P_{out} (*bar*), outlet pressure of compressor; $\bar{z}$, the variable compressibility factor of hydrogen going in to the booster compressor, as a function of $Pressure = \frac{P_{tank}+P_{out}}{2}$; and, Temperature, which is assumed to be a constant set at tank storage temperature.

In Equation (29) the ratio of theoretical work and the efficiency of the booster compressor, η, is multiplied with the incoming hydrogen from the tank to estimate energy consumed in kJ per hour units. Therefore in order to have units of kWh, the kJ per hour term is divided by 3600, the number of seconds in an hour.

$$E_{Booster\ compressor,h} = \frac{W_{Booster\ compressor,theoretical,h} \times F_{H_2,Out,Tank,h}}{\eta \times 3600} \times 1\ hour \tag{29}$$

It should be noted that in work done by Mukherjee et al. [41], the model was similar to what scenario 1 in this study looks like. However, it did not include hydrogen injection into the natural gas grid. Therefore, it did not have equations ((3), (9), (23) and (24), that are the new additions in scenario 1. Scenario 2 presented in this study is a new addition as well and was not included in Ref. [41]. Equations ((4) and (9) and (12)–(17) and (23) and (24) are the new additions to the model developed for scenario 2.

4. Results and discussion

The results from the mixed integer non-linear optimization model formulated in the previous section are presented here. The model is run for the electricity pricing in the time period November 2012–October 2013. Solutions to the problem have been obtained by using the mixed integer non-linear programming (MINLP) solver DICOPT available in Version 22.6 of the General Algebraic Modeling System (GAMS) software.

The results and discussion section here in are split into 3 sections. Section 4.1 discusses the pricing mechanisms at which scenario 1 (Baseline price mechanism) and scenario 2 (Adjusted H_2 price mechanism) are run at. Section 4.2 talks about the observed operating characteristics of the energy hub, and section 4.3 presents the premium pricing mechanisms for the three services offered by the energy hub.

4.1. Pricing mechanisms: scenario 1 and scenario 2

Scenario 1 sells hydrogen to the refueling station at the levelized production cost (equation (5)). Hydrogen is sold to the natural gas end user on an energy value basis (using the Henry Hub Natural Gas Spot Price, $ per MMBtu) in scenario 1.

In scenario 2, the revenue lost in selling hydrogen to the natural gas end user is recovered by adjusting the selling price of hydrogen to the refueling station. The adjustment is estimated using equations ((5) and (8) and (12) and (14)–(16).

The values of the demand response incentive and the $CO_{2,e}$ emission offset benefit were kept the same for both scenarios 1 and 2. The only difference is in the selling price of hydrogen to the refueling station. Table 2 shows the unit values of each of the potential revenues of the energy hub for both scenarios.

As seen in Table 2, the levelized hydrogen production cost (LPC) of hydrogen is estimated to be $3.006 per kg of hydrogen produced for scenario 1. The annual monteary loss of selling hydrogen at the natural gas energy value has been calculated to be $210,269 for scenario 2 using equation (12). This value is used in adjusting the selling price of hydrogen to fuel cell vehicles for scenario 2. The consequent result shows a $0.66 per kg (of hydrogen) increase from the value in scenario 1.

4.2. Operating regime of energy hub

Analyzing the variation in hourly energy consumption by the electrolyzer system and the hourly hydrogen concentration levels maintained within the natural distribution pipeline system are of interest. However, the sheer size of the data makes it difficult to capture the variations of these primary decision variables.

Table 2
Pricing Mechanism for Scenario 1 and Scenario 2.

Scenario #	H_2 Selling Price to Refueling Station ($ per kg)	H_2 Selling Price to Natural Gas End User ($ per MMBtu)	Demand Response Incentive ($ per kWh)	$CO_{2,e}$ Emissions Offset Benefit ($ per kg)
1	3.006	Hourly Henry Hub Spot Price	0.0215	0.015
2	3.665	Hourly Henry Hub Spot Price	0.0215	0.015

Therefore, to better analyze this data, their weekly averages have been calculated and shown in Figs. 3 and 4.

The weekly average of hourly energy consumption profiles of the electrolyzer module while operating under scenario 1 (Baseline Price Mechanism) and scenario 2 (Adjusted H_2 Price Mechanism) have been compared in Fig. 3. It is seen that the weekly average of the Hourly Ontario Electricity Price is the primary parameter that influences the energy consumption profiles for the electrolyzers in the energy hub.

There is no significant variation in the energy consumption profile for scenario 1 with respect to price of electricity. The reason behind this trend can be attributed to the fact that the electrolyzers in scenario 1 only run to meet hydrogen demand from the refueling station. Since the energy consumption profile has been averaged over a period of a week and there are only 801 h spread across the year when the electrolyzer provides demand response, the drop in energy consumption while providing demand response is not seen in Fig. 3.

When the electrolyzer module runs under scenario 2 (Adjusted H2 Price Mechanism), the revenue lost in selling hydrogen to the natural gas pipeline on an energy basis is used to modify the selling overall price of hydrogen sent to the refueling station. An inverse relationship between the electricity price and the energy consumption profile has been observed. This phenomena can be termed as energy arbitrage where the electrolyzers run at maximum capacity and produce excess hydrogen that is stored in the on-site storage tank during low electricity prices. This enables the system to lower its energy consumption during hours of high electricity price and withdraw excess gas stored in the tank to meet refueling station demands. Thereby, helping in lowering operating cost of the energy hub. Another conclusion from Fig. 3 is that the hourly average capacity factor of the electrolyzer system throughout the year is lower in case of scenario 1 (66%) when compared to its capacity factor in case of scenario 2 (94%). Injection of hydrogen in to the natural gas pipeline contributes to scenario 2 having a higher capacity factor.

The variation in weekly average of hourly hydrogen concentration within the natural gas pipeline (for scenario 2) has been plotted and shown in Fig. 4. The hydrogen produced by the electrolyzer module changes with the variation in energy consumed by the system. Hydrogen is sold on an energy value basis (Henry Hub Spot Price, $ per MMBtu) to the natural gas end user. Since hydrogen has a lower energy content in comparison to natural gas, more hydrogen needs to be injected to make up for the energy loss. In order to maximize the primary cash flow objective (equation (2)), the energy hub tries to achieve energy arbitrage in this case by making use of the price differential that exists between the cost of electricity ($ per kWh) and the selling price of natural gas ($ per MMBtu). The system reduces the amount of hydrogen injected in to the pipeline when this price differential is not favorable.

The maximum amount of hydrogen that can be injected in to the distribution lines in an hour cannot exceed 5 mol%. It is seen in figure that the maximum weekly average of hourly hydrogen concentration is 0.072 mol%. The corresponding maximum for all of the hours in scenario 2 (Adjusted H_2 Price Mechanism) is calculated to be 0.546 mol%. This maximum concentration is well below the 5 mol% safety limit. It should be noted that in scenario 1 (Baseline Price Mechanism), the optimization problem deems hydrogen injection into the natural gas pipeline not economical because the hydrogen is being sold at the natural gas energy price. However, scenario 2 (Adjusted H_2 Price Mechanism) recovers the loss in selling hydrogen injected into pipeline on an energy basis by adjusting the selling price of hydrogen sold to the fuel cell vehicles. So it produces hydrogen for injecting into the natural gas pipeline. This indicates that a regulatory incentive pricing structure for the hydrogen injected into the natural gas system would make the overall system economical. Justification for such incentives could be reduction of overall electrical system emissions, allowing for

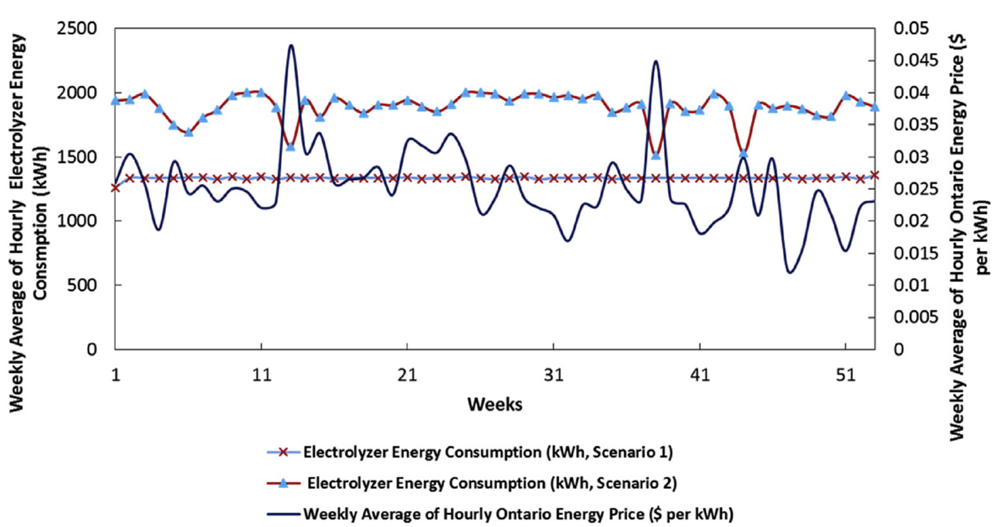

Fig. 3. Comparison of Weekly Average of Hourly Energy Consumption of the Electrolyzer Module for Scenario 1 (Baseline Price Mechanism) and Scenario 2 (Adjusted H_2 Price Mechanism).

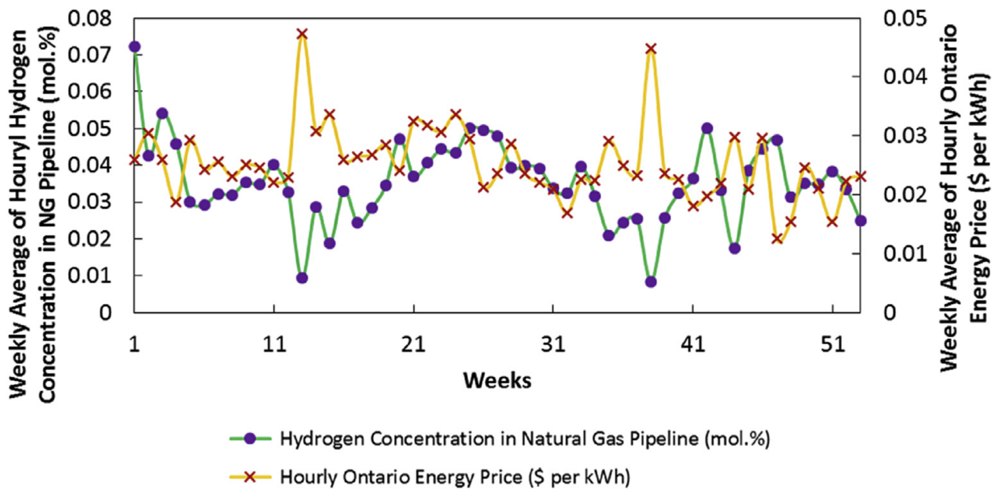

Fig. 4. Weekly Average of Hourly Hydrogen Concentration in Natural Gas Distribution Pipelines for Scenario 2 (Adjusted H_2 Price Mechanism).

increased penetration of wind and solar energy, reduction of the losses associated with selling excess peak baseload power at a loss, and promotion of the market penetration of zero emission vehicles.

Since a blend of HENG is sent to the natural gas end user, there can be potential $CO_{2,e}$ emissions offset at the end user. The system achieves a maximum $CO_{2,e}$ emissions offset of 427 tonnes at the natural gas end user. The zero-emission fuel cell vehicles can offset a total of 953 tonnes of carbon that would come from internal combustion (ICE) vehicles. The value is calculated based the annual driving distance of ICE vehicles in Ontario, and the emission factor of gasoline vehicles as well as the emission factor of the hydrogen fuel produced via electrolysis for the 254 fuel cell vehicles serviced at the refueling station. However, this emission offset associated with the fuel cell vehicles occurs outside the energy hub system boundary and therefore is calculated after the optimization problem was run.

4.3. Development of premium pricing mechanisms

Fig. 5 shows the step by step procedure of determining the new pricing mechanism for each of the three individual services that the energy hub is designed to provide in this study. Note that the equation in Fig. 5 is the same as equation (30). The following paragraphs describe this post-processing calculation in more detail.

The first step (second bubble) in the schematic in Fig. 5 shows the estimation of the net present value and the payback period for the optimization problem results from scenarios 1 and 2.

The net present value of the energy hub at the end of its 20 year lifetime when operating under scenario 1 (Baseline Price Mechanism) and scenario 2 (Adjusted H_2 Price Mechanism) is calculated to be -$263,222 and -$213,883, respectively. Upon projecting the calculation beyond the twenty year time period, it is seen that scenario 1 has a payback period of 26 years, whereas scenario 2 has a payback period of 24 years. This implies that even after accounting for the monetary loss incurred in hydrogen injection to the natural gas pipeline, the pricing mechanism in scenario 2 is not suitable for the project to have a positive net present value at the end of its 20 year lifetime, and a modification of the incentive pricing structure would be required.

The energy hub earns its revenue from providing: 1) Hydrogen to fuel cell vehicles; 2) Demand response; 3) Hydrogen enriched natural gas to natural gas end users, and 4) Offsetting $CO_{2,e}$ emissions at natural gas end users. Out of these four revenue streams, the price at which hydrogen is sold to the natural gas end user cannot be changed. However, the remaining three services provided by the energy hub could have premium prices associated with them.

The payback period for scenario 2 (Adjusted H_2 Selling Price Mechanism) is shorter in comparison with what is observed for scenario 1 (Baseline Price Mechanism). Therefore, in this study, the premium pricing structure is developed with respect to scenario 2. The pricing mechanism in scenario 2 is used as a basis for determining the additional incentive required. Three premium price mechanisms have been proposed for scenario 2, each one used for enabling the energy hub achieve an NPV equal to zero within a shorter project lifetime. The project lifetimes of interest are 8, 9 and 10 years, respectively. The sum of the amortized capital costs of the individual energy hub components shown in equation (2) is $302,024. This value when multiplied by 20, gives the total investment ($6,040,478) over the course of 20 years. The term '*Total Capital Investment*' used in the equation shown in the third bubble in Fig. 5 denotes this value.

The term '$NR_{Required}$' on the right hand side of the equation in the third bubble in Fig. 5 denotes the net annual revenue required for the energy hub to have a NPV equal to zero at the end of shorter project lifetimes of 8, 9 and 10 years, respectively. Current net annual revenue (*NR*) for scenario 2 is $304,401 (determined from equation (4)). r and n' denotes the discount rate (8%) and the project lifetimes (n'), 8, 9 and 10 years, respectively.

The net annual revenue earned by the energy hub needs to be much higher than the values observed from price mechanism used in scenario 2. Required net annual revenue ($NR_{Required}$) values of $1,05,1132, $966,958, and $900,209 for project lifetimes of 8, 9 and 10 years, respectively, have been estimated. The difference between $NR_{Required}$ and *NR* is termed as the additional monetary incentive required (bubble 4 in Fig. 5). Based on this logic, additional monetary incentive requirements of $746,731, $662,557, and $595,808 with respect to a net annual revenue value of $304,401 for scenario 2 have been calculated.

Under scenario 2, 92.4% of the total revenues are earned via selling hydrogen to the fuel cell vehicles, followed by a 1.7% and 0.7% contribution from providing demand response and offsetting $CO_{2,e}$ emissions, respectively. The remaining 5.2% of the revenue share is from selling hydrogen to natural gas end users. The selling price of the hydrogen sold in the natural gas market cannot be changed in the model as proposed. Therefore the percentage contributions of the first three revenue streams are used to proportionately split the additional monetary incentive requirements into

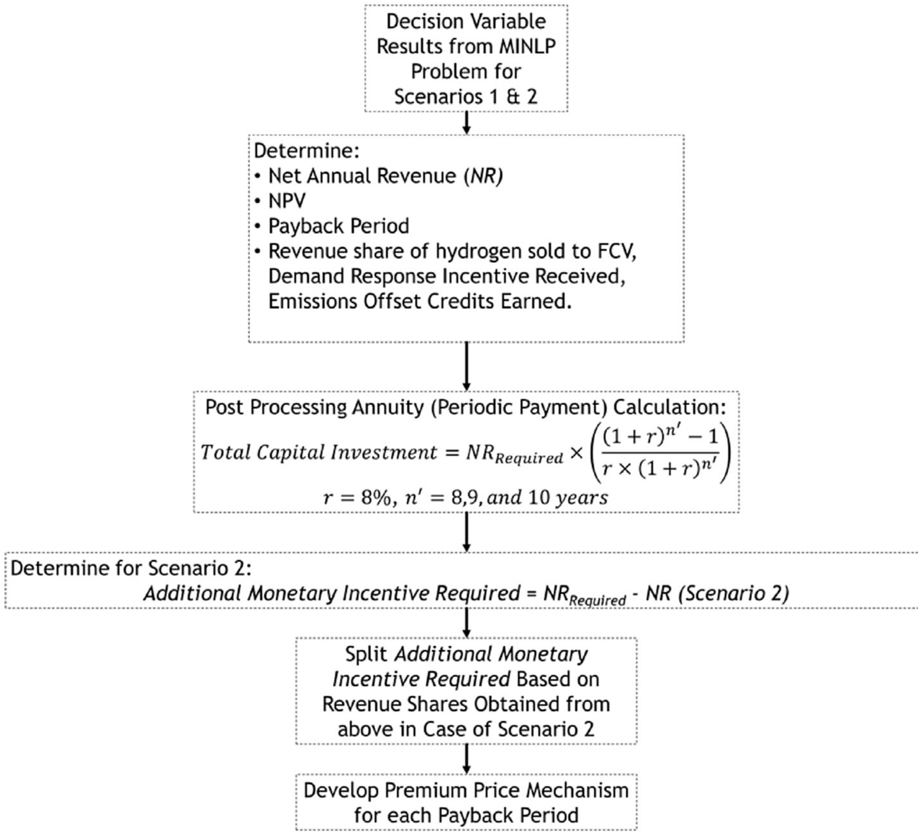

Fig. 5. Process schematic for determining premium pricing mechanism.

the hydrogen selling price, the demand response incentive and the $CO_{2,e}$ emissions offset credit (bubbles 5 and 6 from Fig. 5).

Fig. 6 shows the required selling price of hydrogen to the fuel cell vehicles to achieve the project lifetime of 8, 9 and 10 years, respectively. In each of the three project lifetimes, a base selling price of $3.66 per kg of hydrogen has been used (from the earlier result of scenario 2). Based on this, a simple percentage increase in required selling price of hydrogen shows that a project lifetime of 8 years requires the maximum percentage increase of 83% followed by 74% and 66% increase for project lifetimes of 9 and 10 years, respectively. Currently, the selling price of hydrogen in the US ranges between $5–10 per kg of hydrogen as illustrated by the National Hydrogen Association [53]. The maximum price of hydrogen ($6.71 per kg) from the results presented in Fig. 5 is therefore well within the price range existing in the North American market.

The IESO in its auction report [23] sets a demand response incentive of $0.0215 per kWh or $516 per MW-day. This price is used as a basis upon which the projected increase in the demand response incentive has been estimated for each of the three project lifetimes as seen in Fig. 7. A maximum demand response incentive of $0.039 per kWh ($936 per MW-day) is required for the energy hub to achieve a project lifetime of 8 years. The power to gas energy hub is considered to be a novel concept and in future markets the introduction of innovative technologies to provide grid support will require a higher incentive price for them to be economically

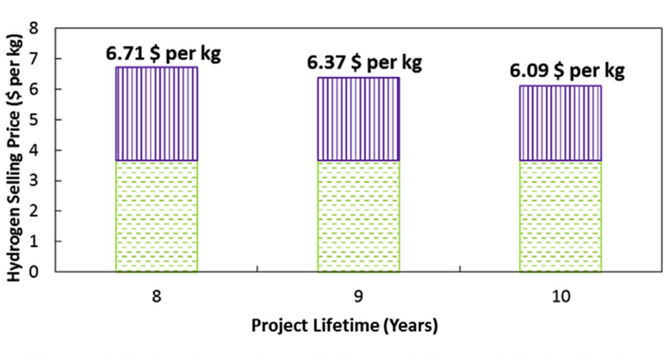

Fig. 6. Premium Pricing for Hydrogen Sold to Fuel Cell Vehicles for Project Lifetimes of 8, 9 and 10 Years for Scenario 2.

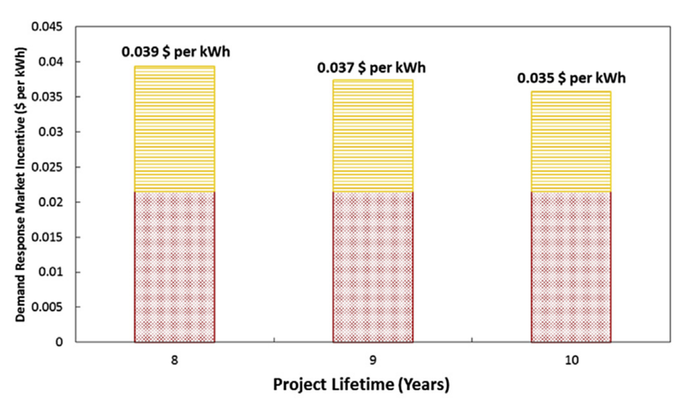

Fig. 7. Demand Response Incentive for Project Lifetimes of 8, 9 and 10 Years in scenario.

feasible.

A $CO_{2,e}$ credit value of $ 15 per tonne of CO_2 emissions currently is used in the province of Alberta in Canada [49]. This serves as a preliminary credit value and used as a basis in Fig. 8. The calculated emission credit values in Fig. 8 range from $27.5 to $24.95 per tonne of $CO2_{,e}$. The monetary value associated with offsetting $CO_{2,e}$ emissions and earning credits supports the industries making a financial case for the use of green technology. The province of Alberta plans to increase the carbon tax it charges to emitters to $ 20 per tonne of $CO_{2,e}$ at the beginning of 2017 and increase it further to $30 per tonne of $CO_{2,e}$ in 2018 [54]. On the other hand, Ontario plans to implement the cap and trade program within the province and the government has been seeking feedback from industry to determine cap levels and permit credit values. The province has set a short term optimistic goal to reduce greenhouse gas emissions by 15% by 2020. California already has a cap and trade program and their program is being used as a reference to set up the system within Ontario [55]. There is no set credit value mentioned in Ministry of the Environment and Climate Change's report. However, comparing current emission credit/tax values from Alberta ($15 per tonne of $CO_{2,e}$) and California ($12.69 per tonne of $CO_{2,e}$) [49,56], the carbon pricing structure required as shown in Fig. 7 bodes well for the use of power to gas to offset $CO_{2,e}$ emissions at the natural gas end users.

The adaptability of power to gas energy systems is more favorable for countries undergoing a transition towards a renewable energy economy and which also have an existing natural gas infrastructure in place. This is validated by work done by de Boer et al. [3].

The economics of the 2 MW plant modeled and optimized in this study looks promising considering the fact that some of the premium pricing mechanisms shown lie well within the ranges of studies carried out internationally (e.g.: Hydrogen fueling price analysis done by National Hydrogen Association, USA [53]). On the other hand premium pricing structures for carbon emissions adopted across the world have been variable. A 2013 report published by 'The Climate Group' shows a wide variety of carbon prices adopted across the world with values ranging from as high as $615 per tonne of $CO_{2,e}$ to as low as $3 per tonne of $CO_{2,e}$ [57]. As more countries adopt either strict carbon taxes or a cap and trade mechanism, the experience of operating such programs might lead to a standardization on the carbon pricing.

The pricing structure for energy storage systems capable of providing ancillary services such as demand response to the power grid in Ontario is relatively new and it will take more time to account for power to gas systems to be able to compete in the provincial demand response market. However, due to the use of PEM electrolyzers that are able to regulate their operating levels in the matter of milliseconds, participating in the higher value frequency regulation market might be an attractive alternative. Mukherjee et al. [47] have reported payback periods as low as 8 years for a 2 MW electrolyzer module providing frequency regulation to the power grid and selling hydrogen to natural gas end user at a premium price. Therefore, it shows that it could be more economical to participate in ancillary services markets that require faster response in comparison to providing hourly demand response.

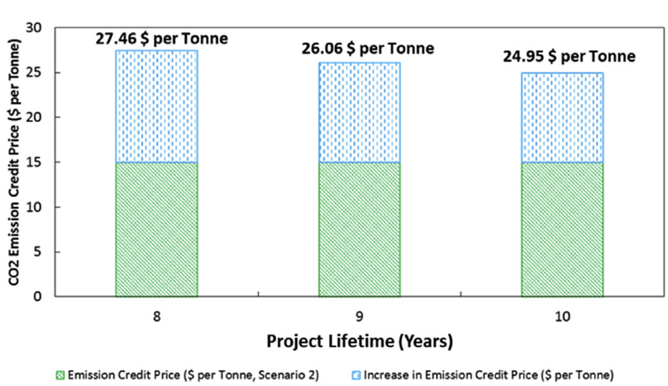

Fig. 8. CO_2 Emission Offset Credit for Project Lifetimes of 8, 9 and 10 Years for Scenario 2.

One of the potential applications of the power to gas energy system could be to use hydrogen in the catalytic methanation process. Götz et al. and Rönsch et al. [58,59] conduct a review of large scale power to gas systems that use electrolytic hydrogen produced from renewable generation sources in methanation plants. The methane produced from the plants can be injected in to the natural gas grid for storage or to be used by the end user. Although this energy recovery pathway has not been analyzed in this work, the potential scalability of power to gas system is very much a realizable goal as seen from literature. The scaling will also enable such energy hubs to help in transitioning towards the adoption of zero emission vehicles.

5. Conclusions

In this study, the potential benefits of the energy recovery pathways of a power to gas energy hub of predetermined size has been demonstrated through the development of a mixed integer nonlinear programming (MINLP) problems. The 2 MW energy hub modeled in this study earns revenue from providing: 1) Hydrogen to 254 fuel cell vehicles on a daily basis; 2) Demand response ancillary service to the power grid; 3) Hydrogen enriched natural gas to the natural gas end user, and 4) Emission reduction service credit at the natural gas end user from burning hydrogen enriched natural gas, which is a cleaner fuel. The first MINLP problem (Scenario 1) run under the baseline price mechanism where hydrogen to natural gas end user and the fuel cell vehicles is sold at an energy e equivalent value of the natural gas spot price ($ per MMBtu) and the levelized hydrogen production cost ($ per kg), respectively. In the second MINLP problem (Scenario 2), the selling price of hydrogen to the fuel cell vehicle is adjusted to account for the loss in selling hydrogen to natural gas end user at the natural gas spot price, which is lower than the cost incurred in producing that hydrogen. It is seen that hydrogen is injected in to the natural gas pipeline only in scenario 2, where the optimization model is allowed to adjust its selling price of hydrogen to fuel cell vehicles. Therefore, the operating regime of the polymer electrolyte membrane (PEM) electrolyzer system for scenario 1 remains less variable, and they operate near 70% of full load, only to satisfy hydrogen demand of the fuel cell vehicles. The energy consumption profile of the electrolyzers in scenario 2 is, however, dependent on the hourly Ontario electricity price. When the price of electricity increases, the electricity consumption of the electrolyzers in scenario 2 decreases, primarily in order to minimize the cost incurred in producing hydrogen for both the fuel cell vehicle end users and the natural gas end user. The selling price of hydrogen to fuel cell vehicles under scenario 1 has been calculated to be $3.006 per kg, whereas the adjusted selling price of hydrogen to the fuel cell vehicles in scenario 2 is estimated to be $3.66 per kg. The adjustment in price is not significant as the electrolyzers only produce hydrogen for direct injection in to the pipelines when the electricity price is low.

In a post processing annuity calculation, the amount of annual net revenues required for energy hub to have an NPV equal to zero for a discount rate of 8% and project lifetimes of 8, 9 and 10 years, have been determined. The net annual revenue of the energy hub for scenario 2 is chosen as a basis to determine the additional revenues required for each of the three project lifetimes. The revenue share from selling hydrogen to the fuel cell vehicles, providing demand response and earning emission offset credits have been estimated to be 92.4%, 1.7%, and 0.7%, respectively. Based on these revenue shares, the additional revenue required for each of the three project lifetimes has been split among these three concerned revenue streams to develop the premium price mechanisms required. The hydrogen selling price to fuel cell vehicles is estimated to be between $6.09–6.71 per kg for the project lifetime range considered in the study. The power to gas energy hub requires a maximum demand response incentive of $0.039 per kWh ($936 per MW-day) for a project lifetime of 8 years. Therefore, in order for the energy hub to be competitive in the demand response auction, the incentive required for demand response can be lowered at the expense of increasing the hydrogen selling price to fuel cell vehicles as the required hydrogen selling prices lie closer to the lower end of the range given by the National Hydrogen Association. A maximum $CO_{2,e}$ emission credit incentive of $27 per tonne of $CO_{2,e}$ emissions is required for the shortest project lifetime of 8 years.

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Appendix A. List of parameters

Parameter	Value
$C_{Booster\ Compressor}(\$)$, Annual investment on total capital cost of booster compressor	37367.92334
$C_{Compressor,Pre-Storage}(\$)$, Annual investment on total capital cost of compressor pre-storage	25441.99036
$C_{Electricity}(\$\ per\ kWh)$, Hourly Ontario energy price	Time series data of electricity price for a year (2012–2013).
$C_{Electrolyzer}(\$)$, Annual investment on total capital cost of electrolyzer	Confidential
$CR_{Water}(l\ of\ Water\ per\ kmol\ of\ H_2\ produced)$, Water consumption rate of electrolyzer	Confidential
$C_{Tank\ Storage}(\$)$, Annual investment on total capital cost of tank storage	30421.51423
$D_{H_2}(kmol)$, Hourly hydrogen demand at a fuel cell vehicle refueling station	Time series data of hydrogen demand over the course of a year.
$D_{NG}(MMBtu)$, Hourly natural gas energy demand at a natural gas pressure reduction station.	Time series data of varying natural gas energy demand for a year (2012–2013).
$ECF_{Compressor,\ Pre-Storage}(kWh\ per\ kmol\ H_2)$, Energy consumed by compressor per kmol of H_2 compressed	2.5042
$EF_{Electrolyzer}$ kmol of H_2 produced per kWh energy consumed by electrolyzer	Confidential
$E_{max}(kWh)$, Maximum energy rating of electrolyzer	2000
$F_{Max,Booster\ compressor}(kmol)$, Maximum inflow to the compressor	43.5
$F_{Max,Compressor,\ Pre-Storage}(kmol)$, Maximum inflow to the compressor	21
$I_{Max}(kmol)$, Upper limit on hydrogen inventory inside tank	45.39133304
$I_{Min}(kmol)$, Lower limit on hydrogen inventory inside tank	8.516043857
$N_{Booster\ Compressor}$, Number of booster compressors	1
$N_{Compressor,\ Pre-Storage}$, Number of compressors Pre-storage	1
N_{Tank}, Number of tanks used for storing hydrogen	1
$P_{out}(bar)$, Output pressure of booster compressor, based on refueling station requirements	350
$P_{tank,min}(bar)$, Minimum pressure level to be maintained in tank	30
$R_{CO_2}(\$\ per\ kg\ of\ CO_2)$, Emission credits for reducing a kilogram of CO_2 emissions	0.015
$R_{Load\ Reduction}(\$\ per\ kWh)$, Monetary incentive provided per kWh of demand response offered	0.0215
$R_{NG}(\$\ per\ MMBtu)$, Hourly Henry hub natural gas spot price.	Time series data of natural gas price for a year (2012–2013).
$R_{comp}(kJ\ per\ K-mol)$, Universal gas constant used for booster compressor	8.314
$UC_{Water}(\$\ per\ liter\ of\ Water)$, Unit cost of water	0.00314
n', Set project lifetime (years)	8, 9 and 10
η, Booster compressor efficiency	0.65
$CCA\ (kWh)$, Contracted curtailment amount	2000
DR, Binary parameter denoting hours in which demand response needs to be provided.	0 or 1
$EMF_{H_2}(kg\ of\ CO_2\ per\ kmol\ of\ H_2)$, Emission factor of hydrogen produced via electrolysis.	Time series data that varies with emission factor of the electricity produced by power grid.
$EMF_{NG,production}\ (kg\ CO_{2,e}\ per\ kmol\ of\ NG\ produced)$, Emissions incurred in producing a kmol of natural gas	12.074
$EMF_{NG}\ (kg\ of\ CO_{2,e}\ per\ kmol\ of\ NG)$, CO_2 equivalent emissions released per kmol of natural gas combusted	42.129
H, Total number of hours in a year	8760
$HHV_{H_2}\ (MMBtu\ per\ kmol)$), High heating value of hydrogen	0.27176
$HHV_{NG}\ (MMBtu\ per\ kmol)$, High heating value of natural gas	0.8053
$O\&M_{Electrolyzer}\ (\$)$, Annual operating and maintenance cost of electrolyzer	Confidential
$R\ (m^3\ bar\ per\ K-mol)$, universal gas constant	8.314×10^{-5}
$T\ (K)$, Temperature inside tank	294.15
$TC\ (\$\ per\ kWh)$, Fee charged for transmission of electricity	0.008652778
$V\ (m^3)$, Maximum volume capacity of tank	7.0523
i (%), Discount rate	8%
k, Heat capacity ratio of hydrogen	1.4091
n, Project lifetime in years	20
$\gamma\ (\$\ per\ MMBtu)$, Rate charged by gas utility to supply fuel for operating pipeline compressors	0.054839982
δ (%), The amount of natural gas fuel supplied to gas utility to run their pipeline compressors, on top of the gas being transported. Denoted as a ratio of fuel to gas being transported through pipelines.	0.00844
θ, Molar hydrogen injectability limit in natural gas (NG) grid	0.052632
$\tau(\$)$, Total investment needed for installing the energy hub	5915379.754

Appendix B. List of variables

ASP_{H_2} ($\$$ *per kmol*), Adjusted selling price of H_2 to fuel cell vehicles
C_{H_2} ($\$$), Annual cost of producing hydrogen
C_{DR} ($\$$ *per h*), Amount of monetary clawback if the contracted curtailment amount (CCA) is not offered as demand response
$E_{Booster\ compressor}$ (*kWh*), Hourly energy consumption of booster compressor
EO_{NG} (*kg*), Emission offset from combustion of hydrogen enriched natural gas compare to combustion of pure natural gas
$F_{H_2,In,Tank}$ (*kmol per h*), Hydrogen injected in the tank
$F_{H_2,Pipe,h}$ (*kmol per h*), Amount of hydrogen injected in to the pipeline every hour
F_{H_2} (*kmol per h*), Amount of H_2 produced every hour
$F_{H_2,Out,\ Tank}$ (*kmol per h*), Hydrogen withdrawn from the tank
$F_{NG,Pipe,h}$ (*kmol per h*), Amount of natural gas flowing through the pipeline every hour
I_{H_2} (*kmol*), Amount of hydrogen in tank at a given time point
LPC_{H_2} ($\$$ *per kmol*), Levelized production cost of H_2
P_{tank} (*bar*), Pressure inside the hydrogen storage tank
$R_{H_2,FCV}$ ($\$$), Annual revenue from selling hydrogen to FCVs
$T_{H_2,FCV}$, Total hydrogen sold to FCVs throughout the year
T_{H_2} (*kmol*), Total annual hydrogen production
$W_{Booster\ compressor,theoretical}$ (*kJ per kmol*), Theoretical work required to operate the booster compressor
X_{NG} (*kmol per h*), Flow of natural gas in pipeline when energy demand is satisfied with pure natural gas
$\bar{z}$, Compressibility factor of hydrogen going in to booster compressor as function of $Pressure = \frac{P_{tank}+P_{out}}{2}$, and Temperature (which is assumed to be constant).
CF, Annual cash flow of the energy hub
E (*kWh*), Hourly energy consumption level of electrolyzer
Ereduce (*kWh*), Hourly reduction in energy consumption of electrolyzer
L, Annual revenue lost in selling hydrogen at natural gas spot price ($)
LR (*kWh*), Hourly load reduction (demand response) offered by electrolyzer
NPV, Net present value
NR ($\$$), Net annual revenue
O (*kmol per h*), Amount of natural gas replaced by hydrogen
UF, Unavailability factor, fraction of CCA not offered
z, Compressibility factor of hydrogen as a function of temperature and pressure inside tank
α, Binary variable to decide if a scheduled demand response signal is satisfied by the electrolyzers or not.
β *($)*, New net annual revenue

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