Life Cycle Assessment of Hydrogen Production from Underground Coal Gasification

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Abstract

Western Canada is endowed with considerable reserves of deep un-mineable coal, which can be converted to syngas by means of a gasification process called underground coal gasification (UCG). The syngas can be transformed into hydrogen (H_2) through commercially available technologies employed in conventional fossil-fuel based H_2 production pathways. This paper presents a data-intensive model to evaluate life cycle GHG emissions in H_2 production from UCG with and without CCS. Enhanced oil recovery (EOR) was considered as a sequestration method and included in the LCA. The life cycle GHG emissions are calculated to be 0.91 and 18.00 kg-CO_2-eq/kg-H_2in H_2 production from UCG with and without CCS, respectively. In addition, a detailed analysis of the influence of key UCG parameters, i.e., H_2O-to-O_2 injection ratio, ground water influx, and steam-to-carbon ratio in syngas conversion, is completed on the results. The advantage of adopting UCG-CCS technology for H_2 production is realized over the predominant steam methane reforming (SMR) process; around 15.3 million tonnes of GHG emissions can be mitigated to achieve the projected SCO production rate from the bitumen

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upgrading in 2022. Furthermore, the sensitivity analysis showed that the life cycle GHG emissions is sensitive to the heat exchanger efficiency and the separation efficiency of the pressure swing adsorption (PSA) unit, with increasing values of these parameters causing an increase and a decrease in the magnitude of life cycle GHG emissions, respectively.

Keywords

Underground coal gasification (UCG); life cycle assessment (LCA); hydrogen production; carbon capture and sequestration (CCS); GHG emissions

1. Introduction

Crude oil production from the Canadian oil sands contributed around 51 Mega tonnes (Mt) to Alberta's total greenhouse gas (GHG) emissions of 244 Mt in 2010 [1]. Synthetic crude oil (SCO) production from the Canadian oil sands is anticipated to rise to 1.26 million bpd in 2022 [2], and hydrogen (H_2) demand to upgrade bitumen to SCO, will rise in a corresponding manner. Around 21 kg-H_2 is required to upgrade one cubic meter of bitumen to SCO, which translates to a hydrogen demand of 4.2 Mt/day to produce 1.26 million bpd of SCO in 2022[3, 4]. Currently, H_2 is produced from the steam methane reforming (SMR) process, using natural gas (NG) as a feedstock [5, 6]. Since SMR-based H_2 production has high GHG footprint – 9.1-14.49 kg-CO_2-eq/kg-H_2 [3, 7-11] – there is reason to study alternative ways to produce H_2 for sustainable development of the bitumen upgrading industry.

Underground coal gasification (UCG) involves injecting gasifying agents in an underground coal seam to produce syngas, which can be used to produce electricity, hydrogen, liquid fuels, etc. [12, 13]. UCG not only reduces fugitive emissions, ash residues, etc., but reduces costs of coal mining, coal handling, coal transport, and coal gasifiers [12, 14-16]. Furthermore, CO_2 sequestration can be combined with UCG, mainly because of the close proximity of CO_2 sequestration sites with the un-mineable coal reserves [17-19]. Therefore, keeping in mind the abundant coal reserves in Alberta, which are estimated to be in the range of 2-3 trillion tons[2], UCG along with carbon capture and sequestration (CCS) can potentially be an environmentally benign H_2 production pathway [20-23]. More recently, the feasibility and the operation of UCG for syngas production in Alberta was successfully demonstrated by Swan Hills Synfuels LP [24].

A life cycle assessment (LCA) is a potent tool that uses a cradle-to-grave approach to evaluate the environmental impact of a system [8]. An LCA deals mostly with product systems and focuses on environmental assessment and corresponding consequences. An LCA allows for characterization of the consequences of possible public policy options or scientific alterations and development of novel sustainable energy resources and technologies [8, 10, 25, 26]. There are a large number of studies in the literature that evaluate environmental competitiveness of various H_2 production pathways (both renewable and non-renewable) by implementing LCA. Lee et al. [27] conducted an LCA of H_2 production from naphtha steam reforming, natural gas steam reforming (NGSR), liquefied petroleum gas steam reforming, and water electrolysis with wind power. They concluded that the H_2 production from water electrolysis with wind power has the least global warming potential (GWP). Ozbilen et al. [28] concluded that H_2 production from thermochemical water decomposition cycles is less GHG intensive as compared to NGSR. In

[2] It is reported that around 16% of Alberta's total coal reserves, located in the upper Mannville coal zone in Alberta, can be recovered through UCG [20].

another study by Ruether et al. [29], an LCA for H_2 fuel production in the United States from liquefied natural gas (LNG) and coal was applied. The results of the analysis showed that although H_2 production from coal gasification is more GHG intensive than from LNG gasification, implementation of CCS has a larger environmentally favorable effect with coal than with LNG [29].

Pereira et al. [30] integrated the Greenhouse gases, Regulated Emissions and Energy use in Transportation (GREET) model and the Global Emissions Model for Integrated Systems(GEMIS) to conduct a well-to-wheel analysis of H_2 production from wind and solar energy for Portugal. Moreover, Dufour et al.[31]implemented the LCA of various NG-based H_2 production pathways (i.e., SMR, SMR-CCS, thermal and autocatalytic decomposition of NG) by using SimaPro software. They concluded that H_2 production from SMR-CCS led to 67% lower GHG emissions than conventional SMR. Aspen Plus software was used to conduct a simulation of large-scale H_2 production from water splitting thermo-chemical cycle and the obtained results were then used to implement the LCA in [32]. Furthermore, an exergetic LCA of H_2 production from wind and solar energy showed that although the use of wind and energy has lower fossil and mineral consumption, the cost of H_2 production is 2.25-5.25 times higher than SMR-based H_2 production [9]. Cetinkaya et al. [7] reported that for large-scale operation of H_2 production, NGSR, coal gasification, and thermochemical water splitting with copper-chlorine cycles are more beneficial than wind and solar energy-based pathways.

However, while extensive work has been carried out regarding the LCA of conventional and unconventional H_2 pathways, the evaluation of UCG from an LCA perspective and its comparison with other H_2 production pathways in the literature is very limited. With this in mind, the LCA conducted in this paper will provide a reliable and comprehensive estimate of the GHG mitigation potential of UCG-based H_2 production. The estimates developed in this research can contribute to the sustainable development of GHG intensive sectors, where a considerable hydrogen demand exists (e.g. Western Canada's bitumen upgrading industry). In addition, the insight gained from the LCA has the potential to help the governmental in development and formulation of appropriate policy, and industry in making investment decisions on large-scale implementation of UCG, especially in a carbon constrained energy economy such as Alberta's. Furthermore, the LCA will facilitate the identification of vital areas for minimizing the GHG footprint of a fossil fuel based energy system like UCG.

In this paper, two scenarios – H_2 from UCG with CCS[3] and without CCS – were considered to quantify the environmental competitiveness over conventional methods such as SMR, SMR-CCS, SCG and SCG-CCS. An LCA model – FUNNEL-GHG-H2-UCG (**FUN**damental **En**gineering Principl**E**s-based Mode**L** for Estimation of **G**reenHouse **G**ases in hydrogen (**H2**) production from **U**nderground **C**oal **G**asification) – is developed to estimate the GHG emissions in H_2 production from UCG with and without CCS. In addition, FUNNEL-GHG-H2-UCG takes into account the life cycle GHG emissions associated with CO_2 transportation and sequestration, which none of the aforementioned studies [3, 8, 31] have considered. Following [33], a process modelling approach is applied to estimate the operation emissions in the two scenarios. In this paper, the GHG emissions are estimated based on pertinent data inputs to represent western Canadian conditions as closely as possible.

The paper is structured in the following manner: Section 2 outlines the methodology adopted for the LCA. The results and discussion, and comparative analysis are provided in section 3 and 4, respectively. Finally, the conclusions are presented in section 5.

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[3] This scenario follows the Government of Alberta's target of reducing GHG emissions by 139 Mt through CCS projects in 2050 [1].

2. Methodology

An LCA is a technique used to evaluate the energy and material use associated with an energy production pathway or a product [34]. Moreover, the results of the LCA can help to identify key processes that can be improved to reduce the overall environmental impact [10]. Overall, the LCA methodology can be implemented to evaluate the life cycle GHG emissions associated with an energy production pathway. As per ISO 14040 and ISO 14044 [35], there are four steps for conducting an LCA– goal and scope definition, life cycle inventory analysis, life cycle impact assessment and life cycle interpretation. The first step aims to distinctly define the goal and scope of the study. The purposes for carrying out the LCA and the intended audience are described in the goal of the study. The description of the functional unit used in the current analysis, the unit operations to be studied, and the system boundary are emphasized in the scope of the LCA. The second step – life cycle inventory analysis – involves estimation, calculation or measurement of the energy and material flows within the systems boundary. The third step – life cycle impact assessment – refers to the identification of the impact categories e.g., GWP, human impact, land use, etc., and to allocating the data collected to the appropriate impact categories. Lastly, in the life cycle interpretation step, the results from steps 2 and 3 are combined to evaluate the environmental impact as per the goal of the study. Additionally, appropriate conclusions and recommendations are prepared.

2.1. Goal and Scope

The purpose of this analysis is to evaluate life cycle GHG emissions from H_2 production from UCG. This paper evaluates two scenarios, H_2 production from UCG with CCS (scenario 1) and

H_2 production from UCG without CCS (scenario 2) in Alberta. A geological sequestration method – enhanced oil recovery (EOR) – is used for carbon storage in scenario 1[4].

2.1.1. Functional unit

The functional unit chosen in this paper is 1 kg of H_2. This analysis reports GHG emissions and energy use associated with different unit operations involved in the H_2 production pathway. GHG emissions are reported as kg-CO_2eq/kg-H_2.The net energy ratio (NER), which is a measure of “useful energy” (i.e., H_2 and electricity) production by the system per unit energy consumption of the fossil fuel (i.e., coal), is defined in Eq. (1).

$$\square\square\square = \frac{\square 2\ \square\square\square\square\square\square\ \square\square\square\square\square\square\square\ (\square\square) + \square\square\square\square\square\square\square\square\square\square\square\ \square\square\square\square\square\square\square\ (\square\square)}{\square\square\square\square\square\square\ \square\square\square\square\square\square\square\ \square\square\square\square\square\ (\square\square)} \quad (1)$$

2.1.2. System boundaries

Figure 3 depicts system boundaries for scenario 1 and scenario 2. The starting point of both scenarios is the injection of gasifying agents (H_2O and O_2) through an injection well in an underground coal reactor, which upon gasification produces syngas. The syngas is collected by

[4] EOR was purposefully selected to put into perspective the Government of Alberta’s decision to fund a large-scale CCS project, the Alberta Carbon Trunk Line (ACTL) [5].The ACTL will include a 16 inch, 240 km CO_2 pipeline, which will transport CO_2 from Fort Saskatchewan, Alberta to an EOR site in Clive, Alberta [5].

a production well and is converted to H_2 using conventional technologies employed in SMR- and SCG-based H_2 production pathways. It is important to mention that both scenarios are characterized with capture of CO_2 using a physical solvent – Selexol[5]. Pure H_2 reaches a bitumen upgrading facility by a pipeline after its separation in a PSA unit, and compression. Downstream of the PSA unit, the remaining un-separated gas, called purge gas, is combusted in a combined cycle plant to produce electricity and steam. A portion of the purge gas is burned separately to satisfy the heat duty of a syngas reforming reactor (SRR) in the syngas-to-H_2 conversion section. In scenarios 1 and 2, GHG emissions are mainly associated with combustion of the purge gas in the gas turbine (GT) and the burner in the syngas-to-H_2 conversion section. However, scenario 2 has additional GHG emissions from CO_2venting of the CO_2captured by the Selexol system. The underlying difference between the two scenarios is the absence of CO_2 compression, transportation, and sequestration in scenario 2. In scenario 1, the captured CO_2 is compressed till it reaches a supercritical state and then transported through a pipeline to the sequestration site.

Electricity requirement in different unit operations (see Fig. 1) is offset by electricity production in an on-site co-generation plant, and a syngas expander placed after UCG. Additional electricity produced is exported to the grid outside the system boundary, and appropriate emissions credit is awarded. Moreover, diesel use in well drilling, and H_2 and CO_2pipeline construction (see Fig. 1) is placed inside the system boundary; emissions associated with diesel production and distribution are also considered. Similarly, steel use in pipeline construction is placed inside the system boundary. The system boundary termination point is the bitumen upgrading facility for

[5] A higher calorific value of purge gas – 55.15 KJ/kg – is achieved in scenario 2 upon CO_2 removal against a calorific value of 3.15 MJ/kg when no CO_2removal takes place in scenario 2[33, 36].In addition, the purge gas compression power requirement ahead of the GT is also reduced [33].

both scenarios. It is worth mentioning that the emissions associated with CO_2 capture, compression, and transportation is allocated to H_2 production.

Fig. 1

2.2. Life cycle inventory (LCI)

This step includes identification of all unit operations within the system boundary and the quantification of corresponding inputs and outputs [34]. Of the several methodologies for data collection e.g. direct measurement, literature review and process modelling [34], the life cycle inventory (LCI) is conducted by incorporating the results of the FUNNEL-EGY-H2-UCG (**FUN**damental E**n**gineering Princip**lE**s-based Mode**L** for Estimation of **E**ner**GY** consumption and production in hydrogen (**H2**) production from **U**nderground **C**oal **G**asification) developed and presented in [33]. However, in some unit operations of the presented work, the data is collected from the literature and developed as required.

2.2.1. H_2 production from UCG

The plant size for H_2 production is based on gasification of a deep highly volatile B bituminous Manville coal seam. The total gasified coal amount is 118 tonnes per day. The H_2 output is estimated to be 16.28 tonnes per day for a H_2O-to-O_2 injection ratio of 2, and a ground water influx of 0.4 m^3/tonne of coal [33]. Tables 1 and 2 show the composition of coal chosen in the study and the key assumptions associated with different unit operations of the H_2 production pathway from UCG for both scenarios. The H_2 production plant lifetime is assumed to be 40 years and is applicable for both scenarios [6]. The details on the process modeling of the unit operations are given in [33]. It is worth noting that owing to the complexity of the unit operations in the PSA, H_2 separation was modelled as a simple separation process[6] by assuming a separation efficiency of 85% [33, 36, 37]. Furthermore, the heat exchanger network for steam generation was modelled in a similar fashion[7] as employed by authors in [33, 37].

Table 1

Table 2

Table 3 shows the key energy inputs and outputs associated with various unit operations in scenarios 1 and 2. In scenario 1, nearly 91.6% CO_2 is captured [33]; the total flow of captured CO_2 is evaluated to be 247.8 tonne/day [33]. It is important to mention that, of the total gas captured, around 97.4% is CO_2, 0.8% is CH_4, while the remaining gases are non-GHGs.

Table 3

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[6] Post CO_2 capture, the constituents of the H_2-rich and CO_2-free gas (input gas stream to PSA unit) (see Fig. 1) were split into two gas streams – H_2-rich gas, containing 85% of the H_2 in the input gas stream, and purge gas, containing the remaining constituents of the input gas stream [37].

[7] The heat recovered from different unit operations was aggregated and then used for steam production in the co-generation section. A heat exchanger efficiency of 60% was assumed for the base case conditions.

2.2.2. Drilling

UCG involves drilling for the formation of an injection well and a production well. A horizontal drilling technique is used to connect both wells. Injection and production well depth are both assumed to be 1400 m, whereas the length of the horizontal section is 1400 m [24]. Diesel is used for drilling the wells. Total energy consumption in well drilling is calculated based on a correlation developed by Brandt [42] for drilling operations in Canada. Brandt [42] discussed two correlations for diesel use to represent low intensity (Eq. (2)), and high intensity (Eq. (3))drilling operations; *d* is the depth of well, meters; *E* is the diesel energy consumed in drilling a well of depth *d*, in MJ. An average of the results obtained from the two correlations was used to account for diesel use in drilling in this paper.

$$E = 128.765 * d * \exp(0.469 * \frac{d}{1000}) \tag{2}$$

$$E = 366.707 * d * \exp(0.399 * \frac{d}{1000}) \tag{3}$$

2.2.3. CO_2 pipeline specification and EOR well characteristics for sequestration

It is important to reiterate that the operating and infrastructure emissions associated with CO_2 capture, compression, transport, and sequestration are allocated to H_2 production. This is mainly because the primary objective of CO_2 sequestration through EOR is to store the un-wanted CO_2 and not to produce more oil from depleted oil reservoirs[8].

Pipeline is assumed to be the mode of transportation of CO_2 to the geological sequestration site. This is applicable for scenario 1 only. CO_2 is transported as a fluid in its supercritical state; a distance of 100 km from the H_2 production plant to an EOR site is taken as the base case. Based on a pipeline operating pressure of 10.3 MPa [43], the pipeline diameter is calculated by a model developed by Ogden [44]. An iterative methodology is adopted to match an assumed diameter value with the calculated value obtained from the model [44]. CO_2 pipeline is manufactured from carbon steel, with a wall thickness of 15 mm [45-47]. Pipeline construction is also associated with use of a trencher. A trencher model Vermeer T555, suitable for CO_2 pipeline construction is chosen and a trench depth of 3 feet is assumed [48]. Diesel fuel consumption for the given trencher model is 0.88 m^3/day [48]. GHG emissions associated with pipeline construction are amortized over a lifetime of 30 years [46].

After reaching the EOR site, CO_2 is then injected in an EOR well reservoir (only applicable for scenario 1). Table 4 shows EOR well reservoir characteristics considered in the present analysis. Given that reservoir characteristics are site-specific [49], it is worth mentioning that an average of a range of values is used. With the assumed reservoir characteristics and the CO_2flow rate, the total number of wells required is calculated by using a method developed by McCollum et al. [39]. The GHG emissions associated with drilling EOR wellswere calculated using the methodology discussed in section 2.2.2.

Table 4

[8] See note 3

2.2.4. H_2 pipeline specification

Highly pure (99.99%) H_2 is delivered at a pressure of 0.2 MPa bar after its separation in PSA [33, 36]. Pipeline is assumed to be the mode of transportation of H_2 to a bitumen upgrading site. A pipeline length of 100 km is considered as the base case for H_2 pipeline transportation. Typical hydrogen pipeline operating pressure and diameter range from 0.1 to 0.3MPa and 0.25 to 0.30 m, respectively [53]. Considering small-scale H_2 production from UCG and its transportation, a lower value of diameter – 0.25 m is used for pipeline diameter. The compressor power requirement is calculated using Panhandle equation adopted in a similar model developed by Ogden [44]; compressor efficiency is assumed to be 55% [44]. Pipeline construction material and wall thickness are assumed to be carbon steel and 0.75 mm, respectively [54]. Diesel consumption for trenching up to a depth of 1.22 m is calculated using the same assumptions discussed in section 2.2.3 [54]. The GHG emissions associated with H_2 pipeline construction were amortized over a lifetime of 22 years [53].

Based on the discussion above, Table 5 summarizes the LCI data associated with different unit operations of H_2 production with and without CCS. Appropriate emissions factors are allocated to the material and energy use (listed in Table 5) to evaluate the life cycle GHG emissions in scenarios 1 and 2.

Table 5

2.3. Global warming potential (GWP) and main sources of GHG emissions

The environmental impact of a product or energy production pathway over its life cycle can be studied using different environmental indicators. In the present study, GWP– represented by kg-

CO_2-eq/ kg-H_2–is the only impact category of interest. The GWP of other greenhouse gases than CO_2 i.e., CH_4 and nitrous oxide have been accounted for and converted to the CO_2-eq. This paper utilizes a 100-year time horizon for the GWP that is consistent with reporting under the Intergovernmental Panel on Climate Change (IPCC) 2007 report [55].

Operation emissions are associated with combustion of the purge gas (applicable for scenarios 1 and 2) and CO_2 venting from the CO_2 removal section (applicable for scenario 2). The steam requirement in the various unit operations is fulfilled by an in-house co-generation facility. It is important to mention that average emission factors of 0.048 and 0.040 kg-CO_2-eq/kg-H_2 were used to account for construction and manufacturing of the H_2 production plant in scenarios 1 and 2, respectively [29]. The GHG emissions associated with infrastructure are aggregated to evaluate non-operation GHG emissions. The gross life cycle GHG emissions are the sum of operation and non-operation GHG emissions (see Eq. (4); the units are in kg-CO_2-eq/kg-H_2). A credit is given for the export of electricity (in the case of a net positive electricity production) to the grid. Net life cycle GHG emissions are then calculated using Eq. (5). Again the units used in Eq. (5) are kg-CO_2-eq/kg-H_2. Table 6 summarizes emission factor values associated with fuel and material use (listed in Table 5) and the GWP of various GHGs.

[illegible] = [illegible] + [illegible] − [illegible] (4)

[illegible] = ([illegible]) − ([illegible]) (5)

Table 6

2.4. Parametric analysis

This paper discusses the effect of key UCG process parameters (H_2O-to-O_2 injection ratio, ground water influx and steam-to-carbon ratio) on life cycle GHG emissions, both quantitatively and qualitatively. The steam-to-carbon ratio is an important process parameter for syngas-to-H_2 conversion in a conventional SCG-based H_2 production plant [36]. Chiesa et al. [36] examined the effect of steam-to-carbon ratio at the inlet of a high temperature WGSR in H_2 production from SCG; reducing the value of the steam-to-carbon ratio from 1.48 to 0.55 increases the emissions by 45%. The steam-to-carbon ratio is fixed based on the quality of the syngas produced after UCG and the desired percentage of carbon conversion into CO_2 in the WGSRs and SRR. Furthermore, the syngas composition varies with in-situ coal composition and depth. Therefore, the degree of freedom to vary the steam-to-carbon ratio is project specific and is appropriately chosen based on the plant design specification i.e., H_2 production, electricity production in the co-generation plant and GHG emissions.

The H_2O-to-O_2 ratio plays a significant role in the composition of syngas and stability of the UCG operation [24, 57]. The process control of the UCG operation is challenging and involves dynamic control of the H_2O-to-O_2 ratio to achieve a stable quantity and quality of syngas [24]. The degree of freedom to vary the H_2O-to-O_2 ratio was 2 to 3, consistent with the range used in a recent UCG pilot scale project in Alberta [24]; 3 being the maximum value of the ratio [24]. Therefore, it is important to understand the effect of this ratio on H_2 production output and life cycle GHG emissions. Moreover, this allows for choosing an injection strategy to facilitate higher syngas quality [57]. Ground water influx in the UCG affects the quality and the quantity of the produced syngas, which ultimately affects the H_2 output [12, 13]. Since the ground water influx is difficult to estimate, a range of values – 0-0.4 m^3/tonne-coal is considered for analysis [12, 13, 33].

3. Results and discussion

3.1. Life cycle GHG emissions

Table 6 shows a detailed breakdown of operation and non-operation emissions in scenario 1 and 2 estimated by FUNNEL-GHG-H2-UCG. Since the H_2 production pathway in both scenarios is self-sufficient in terms of electricity consumption (see Table 3), there are no GHG emissions for electricity use. The operation emissions in scenario 1 comprise purge gas combustion emissions, whereas in scenario 2, in addition to purge gas combustion emissions, there are emissions associated with venting of gases in the CO_2 removal section. The advantage of the co-generation is realized in both scenarios; the H_2 production pathway is self-sufficient in terms of steam and heat production[9]. This ultimately negates the GHG emissions associated with steam and heat use in different process units – SRR, WGSRs and H_2S stripper.

In scenario 1, approximately 91.6% of CO_2 is captured; around 204 kWh of electricity is required to capture and compress one tonne of CO_2. Non-operation emissions are mainly associated with steel and diesel use in H_2 and CO_2 pipeline construction and with diesel use in drilling.

[9]FUNNEL-GHG-H2-UCG is developed in such a way that the heat and steam demand always matches with the heat and steam supply. The model calculates the steam requirement in the SRR, WGSRs and H_2S stripper, and appropriate amount of steam is bled from the co-generation section. An increase in steam demand leads to a decrease in electricity output by the ST or vice versa. Similarly, the model calculates the heat requirement in the SRR unit and allocates appropriate amount of purge gas (main source of heat) to the burner of the SRR and the co-generation plant. An increase in heat requirement also leads to lower GT power output or vice versa.

Gross life cycle GHG emissions are estimated to be 1.8 and 19.8 kg-CO_2-eq/kg-H_2 in scenarios 1 and 2, respectively. Contrastingly, net life cycle GHG emissions, which are calculated using Eq. (5), are lower than the gross life cycle GHG emissions because of a credit for net positive electricity production in scenarios 1 and 2. It is worth mentioning that the credit awarded in scenario 1 is less than in scenario 2 because of higher net electricity production in scenario 2 than in scenario 1 (see Table 3). The net life cycle emissions are evaluated to be 0.9 and 18.0 kg-CO_2-eq/ kg-H_2 in scenarios 1 and 2, respectively.

Table 7

Figures 2 and 3 show a detailed distribution of operation and non-operation GHG emissions in scenarios 1 and 2, respectively. The operation emissions in scenario 1 are mainly associated with combustion of the purge gas, which contribute around 84.4% to gross life cycle GHG emissions. On the other hand, non-operation emissions are around 15.6% of gross GHG emissions. Of the total non-operation emissions, 68.8% are associated with H_2 pipeline construction, while the remaining 31.2% are attributed to CO_2 pipeline construction, drilling of wells in the UCG plant and the EOR site, EOR well leakage, and H_2 production plant construction. Since the diameter of the H_2 pipeline is greater than the diameter of the CO_2 pipeline, the GHG emissions associated with steel use is greater in the former case than the latter case.

Apart from emissions associated with purge gas combustion in scenario 2 (which contribute only 7.4% to gross life cycle GHG emissions), the operation emissions also include emissions from venting of gases in the CO_2 removal section (contributing around 91.1% to gross life cycle GHG emissions). Non-operation emissions contribute only 1.18%. Of the total non-operation emissions in scenario 2, 83% are associated with H_2 pipeline construction, while the remaining 17% are from drilling the UCG wells and H_2 plant construction. Cleary, there are no GHG emissions associated with drilling, leakage in the EOR well, and CO_2 pipeline construction in scenario 2. Overall, the significance of non-operation emissions with respect to gross life cycle GHG emissions can be appreciated in scenario 1 more than in scenario 2. This is because adoption of CCS technology in the former scenario results in lower operation emissions than in the latter scenario. It is worth noting that emissions associated with coal surface mining, coal mine development, and coal transport are negated in H_2 production from UCG, unlike in H_2 production from surface coal gasification (SCG) [7, 14]. The notion of similarity of processes of syngas to H_2 conversion in UCG and SCG is complimented by the fact that the contribution of the operation emissions in the gross life cycle emissions (around 97.8%) in UCG is almost equivalent to reported values of 97% in SCG [7]. A higher percentage in UCG may be attributed to zero emissions associated with coal transport and coal mining.

Fig. 2

Fig. 3

3.2. Sensitivity analysis

A sensitivity analysis was conducted to understand the influence of various input parameters on net life cycle GHG emissions. A variation of ±20% in the input parameters was done to appreciate their effects on the results. Figure 4 shows the sensitivity analysis completed for scenario 1 using base case assumptions. CO_2 and H_2 pipeline transportation distance are found to have weak sensitivities towards net life cycle GHG emissions owing to their low contribution towards the total values. Nevertheless, the net life cycle GHG emissions increase slightly with an increase in transportation distance owing to an increase in diesel and steel use in pipeline construction. The isentropic efficiency of the CO_2 compressor and the pressure ratio in GT are found to have a moderate effect on the net life cycle GHG emissions. The net life cycle GHG emissions moderately increase in a non-linear fashion with increase in pressure ratio in GT owing to the decreased power output of the GT. Due to reasonable contribution of the CO_2 compressors in the total power consumption (around 30%) in scenario 1, the net life cycle GHG emissions decrease with an increase in the CO_2 compressor efficiency; with an increase in the efficiency, the power consumption decreases, ultimately increasing the net power output and emissions credit for export of electricity to the grid.

The significance of H_2 separation efficiency in the sensitivity analysis is realized on observing a sharp increasing trend in the net life cycle GHG emissions. The observed trend is counterintuitive as an increase in the H_2 separation efficiency will not only increase the H_2 output but cause a significant decrease in the power output of the GT and the ST. With an increase in the H_2 separation efficiency by 10%, the power output of the GT and ST decreases by 44% and 27%, respectively, and ultimately the emissions credit is reduced by 85%. Overall, the net life cycle GHG emissions increase from 0.91 to 1.50 kg-CO_2-eq/kg-$H_2$with an increase in the H_2 separation efficiency in the PSA by 10%. The heat exchanger efficiency also has a major effect on the net cycle GHG emissions, with values increasing by 62.3% upon a drop in the efficiency by 10%. This is mainly due to reduced ST power output in the co-generation plant, eventually resulting in a lower emissions credit. Lastly, GT inlet temperature has a high sensitivity towards the net life cycle GHG emissions. A non-linear decreasing trend is observed due to low GT power output upon decreasing the GT inlet temperature.

Fig. 4

3.3. Net energy ratio (NER)

NER is calculated using Eq. (1). Figure 5 shows the energy balance for scenarios 1 and 2. This energy balance allows for identification of key energy consumption within and outside the system boundary for scenarios 1 and 2. NER is calculated as 0.59 and 0.61 for scenarios 1 and 2, respectively. The aforementioned NER values indicate that, the aggregate amount of energy extracted from coal is less than the energy content of the coal. This NER also accounts for the energy used in the production of electricity and steam required for operating the H_2 plant in scenarios 1 and 2. Furthermore, the NER in scenario 2 is greater than in scenario 1; this is mainly due to zero energy consumption in CO_2 compression in scenario 2, which ultimately leads to higher electricity export to grid.

Fig. 5

3.4. The effect of steam-to-carbon ratio on life cycle GHG emissions

Figure 6 shows the effect of the steam-to-carbon ratio on the H_2 production and the amount of CO_2 captured in scenario 1. It is important to note that a similar trend is obtained for H_2 production in scenario 2 because the unit operations up to H_2 production are the same in both scenarios. For a fixed steam-to-carbon ratio, H_2 production falls slightly with increase in ground water influx (see Fig. 6). The reason is two-fold. First, H_2 content in the syngas from UCG falls, while CH_4 content rises [33].Second, steam consumption in the SRR unit increases to maintain a fixed steam-to-carbon ratio; this makes up for the deficit in H_2 content in the syngas by converting CH_4 into H_2in the SRR unit[33]. In addition, the amount of CO_2 captured also falls with an increase in ground water influx. Ultimately, an increasing trend of the gross and net life cycle GHG emissions in both scenarios is seen with increase in ground water influx (see Fig. 7).

The effect of the steam-to-carbon ratio can be appreciated over gross and net life cycle GHG emissions in both scenarios (see Fig. 7). With a rise in the steam-to-carbon ratio, H_2 production increases; this stems from the fact that an augmented flow of steam will favor CH_4 conversion into H_2 in the SRR unit. At the same time, increased CH_4 conversion also escalates the amount of CO_2 in the reformed syngas post SRR and WGSR units, the effect of which is eventually realized in improved CO_2 capture. However, the percentage increase in H_2 production (13%) is greater than the percentage increase in CO_2 captured or vented (5%) in both scenarios. As a result, gross life cycle GHG emissions drop with a rise in steam-to-carbon ratio in both scenarios.

Contrastingly, the effect of the steam-to-carbon ratio on the net life cycle GHG emissions is not straight forward in either scenario. With an increase in the steam-to-carbon ratio, an increasing trend is observed in the net life cycle GHG emissions in scenario 1, as compared to a decreasing trend in scenario 2. With a rise in the steam-to-carbon ratio from 2 to 4, net life cycle GHG emissions reduce from 20.38 to 16.57 kg-CO_2-eq/kg-H_2 in scenario 2, while it increases from 0.56 to 1.10 kg-CO_2-eq/kg-H_2 in scenario 1. The reason for the observed trends is multifold. First, with an increase in the steam-to-carbon ratio, the GT power output decreases; due to decreased CH_4 flow in the purge gas, the calorific value of the purge gas falls, which results in lower GT power output for a higher steam-to-carbon ratio. Second, a penalty is enforced on the output of the ST because of rise in steam consumption in the SRR unit. Third, there is an increased energy penalty in capture and compression of CO_2 in scenario 1; the CO_2 content of the syngas after its processing in SRR and WGSRs increases with increase in steam-to-carbon ratio (see Fig. 6).

These three factors (drop in power output of ST and GT, and energy penalty for CCS) result in lower net power output for a higher steam-to-carbon ratio. Eventually, the emissions credit for the export of electricity to the grid declines with a rise in the steam-to-carbon ratio. Since the values of gross life cycle GHG emissions in scenario 1 are much lower than in scenario 2 (see Fig. 7), the effect of the emissions credit on net life cycle GHG emissions is greater in scenario 1 relative to scenario 2. A marginal increasing trend in net life cycle GHG emissions is therefore, achieved in scenario 1 compared to a significant decreasing trend in scenario 2 with increase in steam-to-carbon ratio.

Fig. 6

Fig. 7

3.5. The effect of the H_2O-to-O_2 injection ratio on life cycle GHG emissions

Figure 8 shows the effect of the H_2O-to-O_2 injection ratio on the H_2 production output and the total CO_2 captured for a fixed steam-to-carbon ratio of 3. Clearly, both output variables have great sensitivity towards the H_2O-to-O_2 injection ratio; with an increase in H_2O-to-O_2 injection ratio from 2 to 3, the H_2 output and the flow rate of captured CO_2 decrease by around 3.4% and 6.3%, respectively. This trend is mainly attributable to an increase in CH_4 content, while a decrease in H_2 flow in the syngas after UCG is observed [33].

The effect of the H_2O-to-O_2 injection ratio is clearly transferred to the gross life cycle GHG emissions in scenarios 1 and 2 (see Fig. 9). The decrease in flow of "captured CO_2" results in an increase in CO_2 content of the purge gas. This combined effect of a rise in CO_2 content of purge gas and fall in H_2 output, H_2 production output, eventually increases the gross life cycle GHG emissions from 1.8 to 2.3 kg-CO_2-eq/kg-H_2in scenario 1 and 19.75 to 21.65 kg-CO_2-eq/kg-H_2 in scenario 2, with rise in the H_2O-to-O_2 injection ratio from 2 to 3. Contrastingly, the increase in net life cycle GHG emissions is marginal in scenario 1. This is mainly because the GHG emissions credit award for increased power output compensates for decreased flow of "captured CO_2" in scenario 1.

Fig. 8

Fig. 9

4. Comparative assessment with other studies and GHG mitigation potential

This section compares life cycle GHG emissions in H_2 production from UCG with other H_2 production pathways. H_2 production from UCG-CCS is found to be more environmentally competitive than H_2 production without CCS. The competiveness of H_2 production from UCG in terms of GHG emissions can be appreciated when the life cycle GHG emissions are compared with other H_2 production pathways. For the comparative assessment, a number of fossil fuel and renewable energy based H_2 production pathways are considered; they are listed in Table 8. Clearly, a wide range of scenarios is present in SCG and SMR, with regards to different plant configurations and schemes (with or without co-generation, only electricity co-production and only steam co-production).

Figure 10 shows a comparison of life cycle GHG emissions between UCG, SCG, SMR, wind, hydro, and solar energy based H_2 production pathways. It is evident from Fig. 10 that there exists a wide range of values for life cycle GHG emission in the literature for SCG and SMR. This might be due to the consideration of a different system boundary, coal composition, set of assumptions, jurisdiction, etc.[10]. For example, in pathway 7.1 [8],amine absorption technology is utilized for CO_2capture (with 85% efficiency); additional steam and electricity use (other than in H_2production) for CCS system is derived from electricity producing NGCC-CCS plant. Moreover, the authors assume CO_2 compression pressure of 13.5 MPa for its transport to a storage site via a 300 km pipeline. Equipment emissions associated with CCS system are considered and no credits are awarded for steam additional steam produced by the system. In comparison, the LCA model discussed in [3] uses default values for estimating the energy consumption in CCS (pathways 7.2-7.4 and 5.1-5.3) without explicitly stating the CO_2 capture technology, underlying process assumptions and associated equipment emissions. The pathways with electricity co-production (4.3, 5.2, 6.3 and 7.3) have greater GHG footprint than with steam co-production counterpart (4.4, 5.3, 6.4.2 and 7.4, respectively). This is mainly because the emissions credit awarded for electricity export in the former cases is higher than for steam export in the latter cases.

The UCG-CCS pathway has a significantly lower GHG footprint than other fossil fuel based H_2 production pathways for all plant configurations, except SCG-CCS with steam co-production. The advantage of integrating CCS technology with UCG can be realized as this pathway becomes competitive with even renewable energy-based H_2 production pathways – wind, solar and hydro. To put this into perspective, if H_2 were produced from UCG-CCS instead of the predominant SMR process, nearly 15.3 Mt of GHG emissions would be mitigated per year in the bitumen upgrading industry of Alberta in 2022. This GHG abatement potential is calculated

[10] These reasons can also be used to explain higher value of net life cycle GHG emissions in H_2 production from UCG without CCS than some reported values in the literature for SCG-based H_2 production pathway without CCS (see Fig. 10).To put this into perspective, the emissions associated with electricity production from UCG are evaluated to be 0.843 tonnes-CO_2-eq/MWh as compared to 0.88 tonnes-CO_2-eq/MWh from SCG in Alberta (see Table 6).

based on SCO production of 0.20 million m^3/day in 2022 [4], H_2 requirement of 2.52 GJ-H_2/m^3-SCO [3] and an average value of life cycle GHG emissions (around 10.8 kg-CO_2e/kg-H_2) for SMR-based pathway without CCS reported by authors in [7-11]. With that said, large-scale implementation of UCG-CCS technology still remains a challenge in order to gain the environmental advantages over other pathways, especially SMR, for H_2 production. Some of the challenges to implement UCG technology include low process control, lack of consistency of syngas quality and composition, and other associated environmental risks e.g., ground water contamination and land subsidence [6]. Furthermore, low natural gas prices decrease the economic competitiveness of producing $H_2$from UCG technology as compared to SMR technology, especially in western Canada [6].

Table 8

Fig. 10

4. Conclusion

This paper examined life cycle GHG emissions of H_2 production from UCG for two scenarios with and without CCS by developing the FUNNEL-GHG-H2-UCG. The net life cycle GHG emissions are estimated to be 0.91 and 18.00 kg-CO_2-eq/kg-H_2in H_2 production from UCG with and without CCS, respectively. Adoption of CCS technology leads to a substantial reduction in total life cycle emissions in H_2 production from UCG. Purge gas combustion and venting of gases in the CO_2 removal section are the major contributing factors in the net life cycle GHG emissions. On the other hand, energy and material use in drilling, H_2 and CO_2 pipeline transportation, and other construction contributed around15.6% and 1.2% towards life cycle GHG emissions in H_2 production with and without CCS, respectively.

Furthermore, the net life cycle GHG emissions increase marginally with a rise in the H_2O-to-O_2 injection ratio and the steam-to-carbon ratio in H_2 production from UCG with CCS. In addition, the sensitivity analysis showed that the net life cycle GHG emissions are most sensitive to the separation efficiency of the PSA and the efficiency of the heat exchanger. The net energy ratios were estimated to be 0.59 and 0.61 in H_2 production with and without CCS, respectively.

UCG-CCS is found to have a lower life cycle GHG emissions footprint in comparison to other conventional H_2 production pathways (SCG, SCG-CCS, SMR and SMR-CCS); only exception being SCG-CCS with steam co-production. UCG-CCS based H_2 is also comparable with wind, hydro, and solar based H_2 in terms of GHG emissions. If the traditional SMR process is replaced by UCG-CCS process for H_2 production in the bitumen upgrading industry, a reduction of around 15.3 Mt in GHG emissions can be achieved in 2022.

Acknowledgments

The authors thank the NSERC/Cenovus/Alberta Innovates Associate Industrial Research Chair Program in Energy and Environmental Systems Engineering and the Cenovus Energy Endowed Chair Program in Environmental Engineering for funding the research project. The authors are thankful to Astrid Blodgett for editorial assistance in this paper.

References

[1] Alberta Government. Alberta's Clean Energy Future. Climate Change. Available at: http://www.oilsands.alberta.ca/FactSheets/CChange_FSht_Sep_2013_Online.pdf. 2013.

[2] Energy Resources Conservation Board. ST98-2013. Alberta’s Energy Reserves 2012 and Supply/Demand Outlook 2013–2022. May 2013. Available at: http://www.aer.ca/documents/sts/ST98/ST98-2013.pdf.

[3] Wang M. GREET, Model 4.02a; Argonne National Laboratory,U.S. Department of Energy. 2012.

[4] Canadian Association of Petroleum Producers (CAPP). Crude oil: forecasts, markets and transportation. Available at: http://www.capp.ca/getdoc.aspx?DocId=247759&DT=NTV. June 2014.

[5] Cole S, Itani S. The Alberta Carbon Trunk Line and the Benefits of CO2. Energy Procedia. 2013;37:6133-9.

[6] Olateju B, Kumar A. Techno-economic assessment of hydrogen production from underground coal gasification (UCG) in Western Canada with carbon capture and sequestration (CCS) for upgrading bitumen from oil sands. Applied Energy. 2013;111:428-40.

[7] Cetinkaya E, Dincer I, Naterer GF. Life cycle assessment of various hydrogen production methods. International Journal of Hydrogen Energy. 2012;37:2071-80.

[8] Dufour J, Serrano DP, Gálvez JL, González A, Soria E, Fierro JLG. Life cycle assessment of alternatives for hydrogen production from renewable and fossil sources. International Journal of Hydrogen Energy. 2012;37:1173-83.

[9] Granovskii M, Dincer I, Rosen MA. Exergetic life cycle assessment of hydrogen production from renewables. Journal of Power Sources. 2007;167:461-71.

[10] Koroneos C, Dompros A, Roumbas G, Moussiopoulos N. Life cycle assessment of hydrogen fuel production processes. International Journal of Hydrogen Energy. 2004;29:1443-50.

[11] Spath P, Mann M. Life Cycle Assessment of Hydrogen Production via Natural Gas Steam Reforming. NREL/TP-570-27637; 2005.

[12] Burton E, Friedmann J, Upadhye R. Best practices in underground coal gasification. Contract W-7405-Eng-48. Livermore, CA: Lawrence Livermore National Laboratory.2006.

[13] Gregg DW, Edgar TF. Underground coal gasification. AIChE Journal. 1978;24:753-81.

[14] Bhutto AW, Bazmi AA, Zahedi G. Underground coal gasification: From fundamentals to applications. Progress in Energy and Combustion Science. 2013;39:189-214.

[15] Khadse A, Qayyumi M, Mahajani S, Aghalayam P. Underground coal gasification: A new clean coal utilization technique for India. Energy. 2007;32:2061-71.

[16] Pana C. Review of Underground Coal Gasification with Reference to Alberta's Potential. Energy Resources Conservation Board. Alberta Geological Survey. 2009.

[17] Friedmann SJ, Upadhye R, Kong F-M. Prospects for underground coal gasification in carbon-constrained world. Energy Procedia. 2009;1:4551-7.

[18] Roddy DJ, Younger PL. Underground coal gasification with CCS: a pathway to decarbonising industry. Energy & Environmental Science. 2010;3:400-7.

[19] Self S, Reddy B, Rosen M. Review of underground coal gasification technologies and carbon capture. International Journal of Energy and Environmental Engineering. 2012;3:1-8.

[20] Richardson RJ. Alberta’s 2 Trillion Tonnes Of ‘Unrecognized’ Coal. Available at: eipa.alberta.ca/media/43006/alberta_2_trillion_tonnes_coal.pdf. 2010.

[21] Beaton A, Langenberg W, Pană C. Coalbed methane resources and reservoir characteristics from the Alberta Plains, Canada. International Journal of Coal Geology. 2006;65:93-113.

[22] Beaton A, Pana C, Chen D, Wynne D, Langenberg CW. Coalbed methane potential of Upper Cretaceous- Tertiary strata, Alberta Plains. Alberta Energy and Utilities Board, EUB/AGS Earth Sciences Report 2002-06. 2002.

[23] Energy Resources Conservation Board. Alberta's energy reserves 2008 and supply/demand outlook 2009–2017. Available at: http://www.aer.ca/documents/sts/ST98/st98-2009.pdf. 2009.

[24] Swan Hills SynFuels. Swan Hills In-Situ Coal Gasification Technology Development. Final Outcomes Report. Prepared for: Alberta Innovates – Energy and Environment Solutions. Available at: http://www.ai-ees.ca/media/6876/swan_hills.pdf 2012.

[25] Udo de Haes HA, Heijungs R. Life-cycle assessment for energy analysis and management. Applied Energy. 2007;84:817-27.

[26] Wagner U, Geiger B, Schaefer H. Energy life cycle analysis of hydrogen systems. International Journal of Hydrogen Energy. 1998;23:1-6.

[27] Lee J-Y, Yu M-S, Cha K-H, Lee S-Y, Lim TW, Hur T. A study on the environmental aspects of hydrogen pathways in Korea. International Journal of Hydrogen Energy. 2009;34:8455-67.

[28] Ozbilen A, Dincer I, Rosen MA. Comparative environmental impact and efficiency assessment of selected hydrogen production methods. Environmental Impact Assessment Review. 2013;42:1-9.

[29] Ruether. J, Ramezan. M, Grol. E. Life-Cycle Analysis of Greenhouse Gas Emissions for Hydrogen Fuel Production in The United States from LNG and Coal. National Energy Technology Laboratory. DOE/NETL-2006/1227. 2005.

[30] Pereira SR, Coelho MC. Life cycle analysis of hydrogen – A well-to-wheels analysis for Portugal. International Journal of Hydrogen Energy. 2013;38:2029-38.

[31] Dufour J, Serrano DP, Gálvez JL, Moreno J, García C. Life cycle assessment of processes for hydrogen production. Environmental feasibility and reduction of greenhouse gases emissions. International Journal of Hydrogen Energy. 2009;34:1370-6.

[32] Smitkova M, Janíček F, Riccardi J. Life cycle analysis of processes for hydrogen production. International Journal of Hydrogen Energy. 2011;36:7844-51.
[33] Verma A, Olateju B, Kumar A, Gupta R. Development of a Process Simulation Model for Energy Analysis of Hydrogen Production from Underground Coal Gasification (UCG). International Journal of Hydrogen Energy (in review).
[34] Ozbilen A, Dincer I, Rosen MA. Life cycle assessment of hydrogen production via thermochemical water splitting using multi-step Cu–Cl cycles. Journal of Cleaner Production. 2012;33:202-16.
[35] International Organization for Standardization. ISO 14040:2006 and ISO 14044:2006: environmental management – life cycle assessment – principles and framework.
[36] Chiesa P, Consonni S, Kreutz T, Robert W. Co-production of hydrogen, electricity and CO2 from coal with commercially ready technology. Part A: Performance and emissions. International Journal of Hydrogen Energy. 2005;30:747-67.
[37] Molburg JC, Doctor RC. Hydrogen from steam-methane reforming with CO2 capture. Argonne National Laboratory. Available at: http://seca.doe.gov/technologies/ccbtl/refshelf/papers/pgh/hydrogen from steam methane reforming for carbon dioxide cap.pdf; June 2003.
[38] Yang LH. A Review of the Factors Influencing the Physicochemical Characteristics of Underground Coal Gasification. Energy Sources, Part A: Recovery, Utilization, and Environmental Effects. 2008;30:1038-49.
[39] McCollum DL, Ogden JM. Techno-economic models for carbon dioxide compression, transport and storage & correlations for estimating carbon dioxide density and viscosity. Institute of Transportation Studies, University of California, Davis (2006).
[40] Mansouri Majoumerd M, De S, Assadi M, Breuhaus P. An EU initiative for future generation of IGCC power plants using hydrogen-rich syngas: Simulation results for the baseline configuration. Applied Energy. 2012;99:280-90.

[41] Cormos C-C. Integrated assessment of IGCC power generation technology with carbon capture and storage (CCS). Energy. 2012;42:434-45.

[42] Brandt AR. Oil depletion and the energy efficiency of oil production: The case of California. Sustainability. 2011;3: 1833–54.

[43] Heddle G, Herzog H, Klett M. The Economics of CO2 Storage. Massachusetts Institute of Technology, Laboratory for Energy and the Environment; MIT LFEE 2003-003 RP; 2003.

[44] Ogden JM. Conceptual Design of Optimized Fossil Energy Systems with Capture and Sequestration of Carbon Dioxide; DOE Award Number: DE-FC26-02NT41623. 2004.

[45] Hertwich EG, Aaberg M, Singh B, Strømman AH. Life-cycle Assessment of Carbon Dioxide Capture for Enhanced Oil Recovery. Chinese Journal of Chemical Engineering. 2008;16:343-53.

[46] Serpa J, Morbee J, Tzimas E. Technical and Economic Characteristics of a CO2 Transmission Pipeline Infrastructure; European Commission Joint Research Centre Institute for Energy;. 2011.

[47] Demofonti G, Spinelli CM. Technical challenges facing the transport of anthropogenic CO2 by pipeline for carbon capture and storage purposes; PTC 6th Pipeline Technology Conference. 2011.

[48] Vermeer. T555 COMMANDER® 3 Tractor. Available at: http://www2.vermeer.com/vermeer/NA/en/N/equipment/trenchers_pipeline/t555iii. Accessed: December 2013.

[49] Gunter B, Longworth H. Overcoming the Barriers to Commercial CO2-EOR in Alberta, Canada; Prepared for Alberta Innovates Energy and Environment Solutions. 2013.

[50] Hussain D, Dzombak DA, Jaramillo P, Lowry GV. Comparative lifecycle inventory (LCI) of greenhouse gas (GHG) emissions of enhanced oil recovery (EOR) methods using different CO2 sources. International Journal of Greenhouse Gas Control. 2013;16:129-44.

[51] Khoo HH, Tan RBH. Life cycle investigation of CO2 recovery and sequestration. Environmental Science and Technology. 2006;40:4016-24.

[52] Encana. Life of the Well. Available at: http://www.encana.com/pdf/communities/usa/LifeOfTheWell2011.pdf. Accessed: December 2013. 2011.

[53] Amos WA. Costs of Storing and Transporting Hydrogen. National Renewable Energy Laboratory. NREL/TP-570-25106. 1998.

[54] Remp LH. DOE Hydrogen Pipeline Working Group Workshop. Air Products. Available at: https://www1.eere.energy.gov/hydrogenandfuelcells/pdfs/hpwgw_airprod_remp.pdf. 2005.

[55] Intergovernmental Panel on Climate Change (IPCC). Climate Change 2007. Synthesis Report. A report submitted to the Intergovernmental Panel on Climate Change. Available at: http://www.ipcc.ch/pdf/assessment-report/ar4/syr/ar4_syr_full_report.pdf. 2008.

[56] Savage B. Memorandum. Notice of Change for Emission Factor for Increased Grid Electricity Usage. Government of Alberta, Environment and Water Available at: http://environmentgovabca/info/library/8429pdf. 2011.

[57] Nourozieh H, Kariznovi M, Chen Z, Abedi J. Simulation Study of Underground Coal Gasification in Alberta Reservoirs: Geological Structure and Process Modeling. Energy Fuels. 2010;24:3540–50.

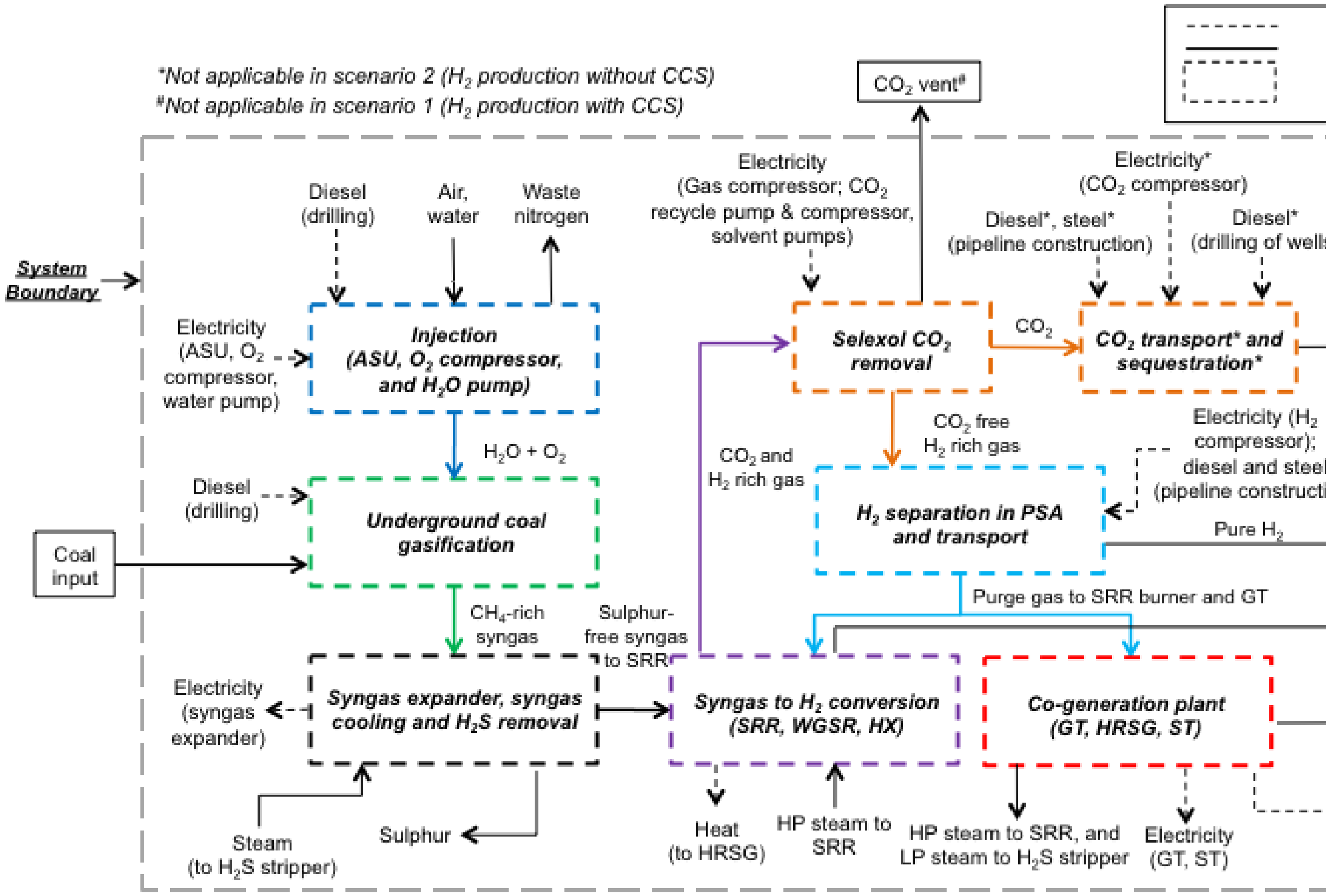

Fig. 1: System boundary of the study. The boundaries are the same for scenarios 1 and 2, except for the absence of CO_2 transport, and sequestration in the latter scenario. Notes: ASU-air separation unit; SRR-syngas reforming reactor; WGSR-water gas shift reactor; HX-heat exchanger; GT-gas turbine; HRSG-heat recovery steam generator; ST-steam turbine.

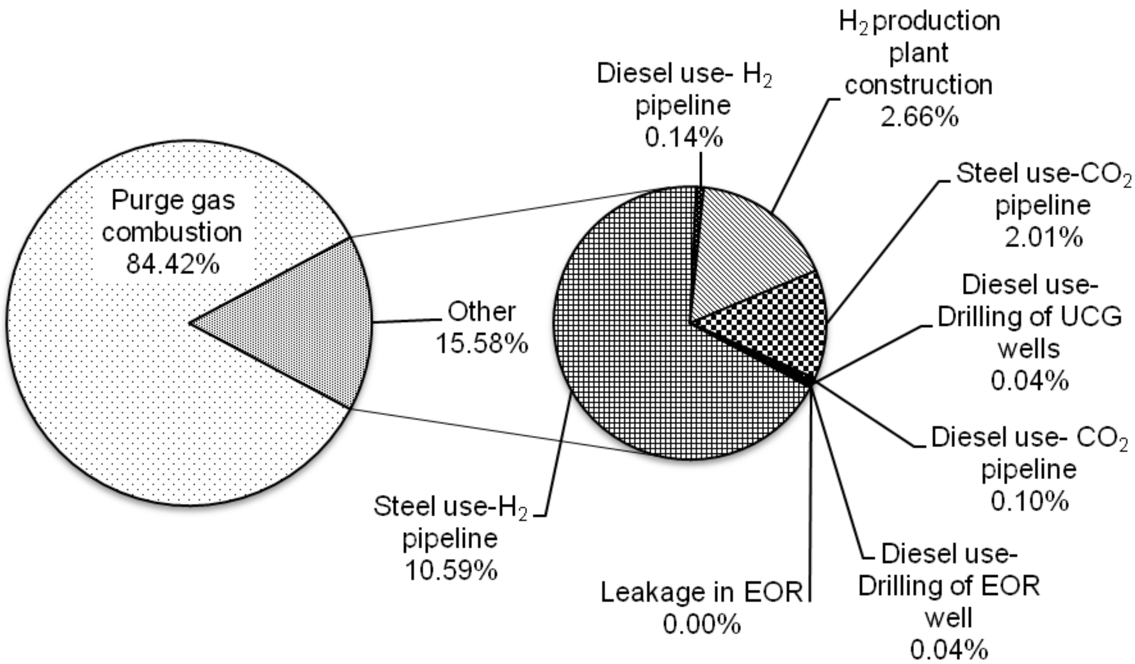

Fig. 2: Life cycle GHG emissions distribution in scenario 1 (H_2 production from UCG with CCS). "Other" indicates non-operation GHG emissions. The distribution is based on gross life cycle GHG emissions.

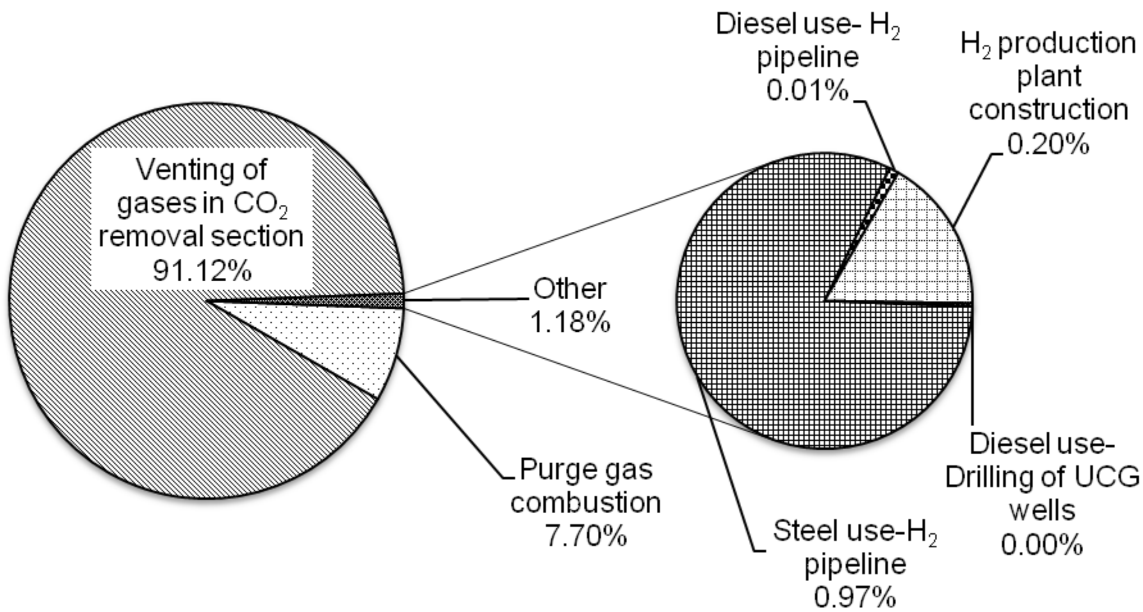

Fig. 3: Life cycle GHG emissions distribution in scenario 2 (H_2 production from UCG without CCS). "Other" indicates non-operation GHG emissions. The distribution is based on gross life cycle GHG emissions.

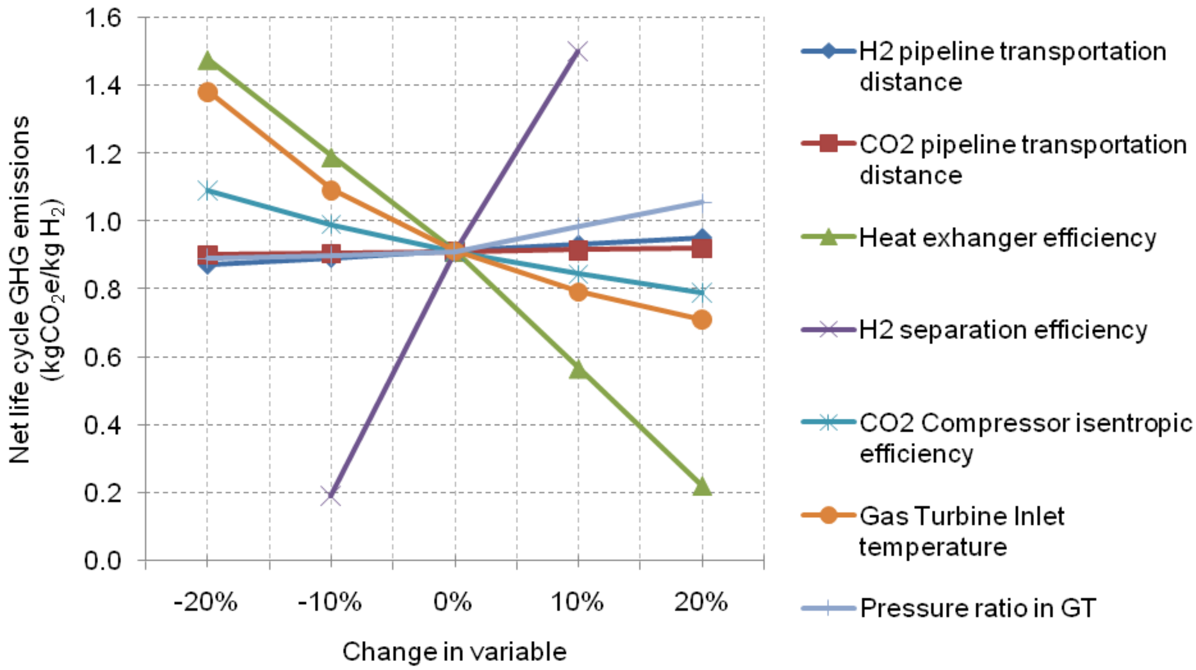

Fig. 4: Sensitivity analysis for scenario 1. The analysis is done for base case assumptions (the H_2O-to-O_2 injection ratio is 2, ground water influx is 0.4 m^3/tonne of coal, and the steam-to-carbon ratio is 3).

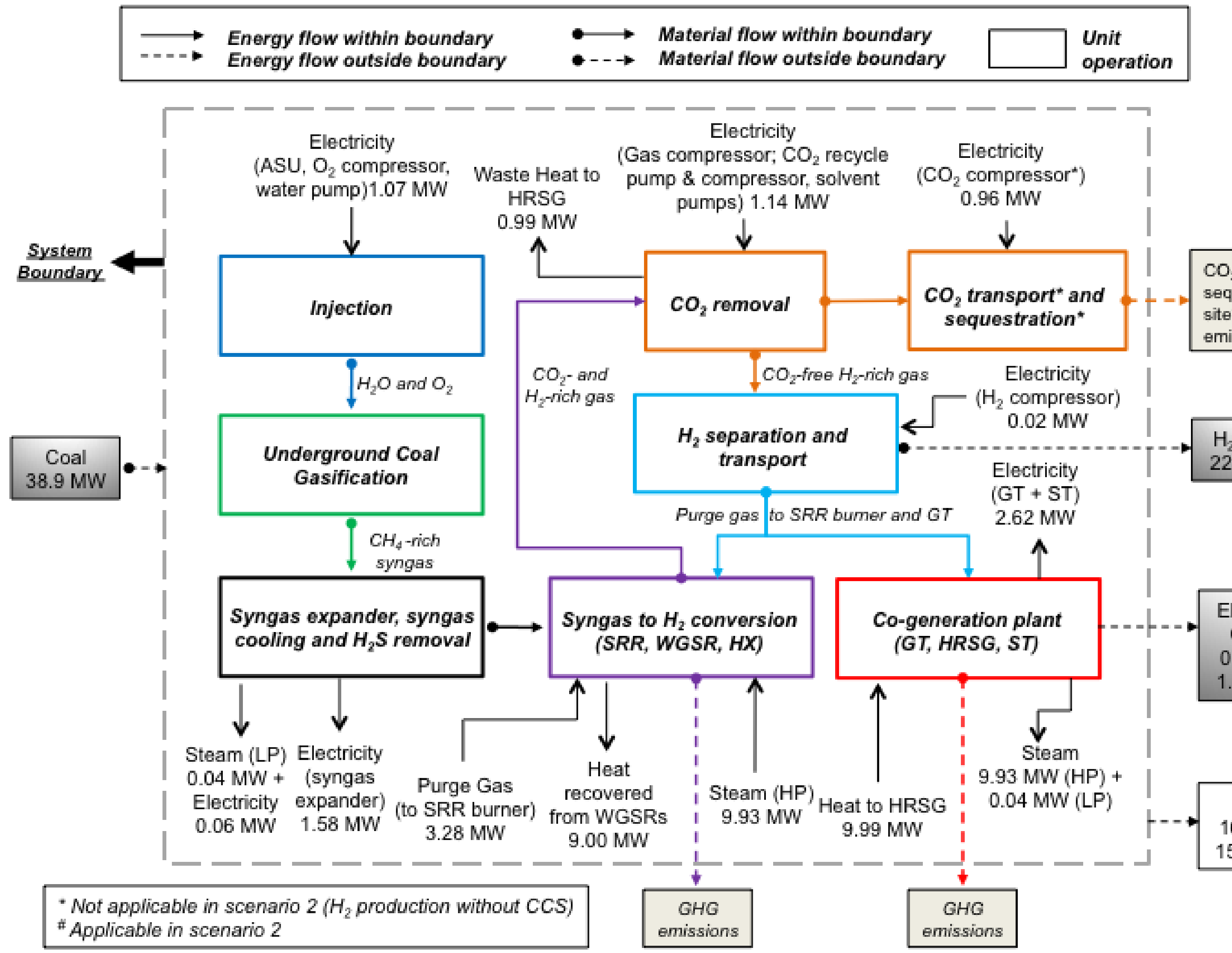

Fig. 5: Energy balance in scenarios 1 and 2 for base case assumptions i.e. total coal input – 118 tonne/day, H_2O-to-O_2 injection ratio – 2 and ground water influx – 0.4 m^3/tonne of coal.

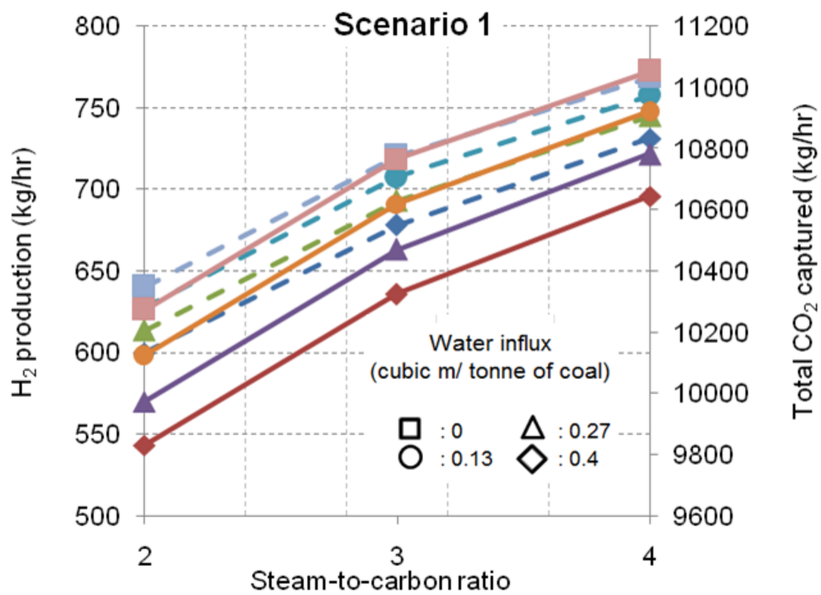

Fig. 6: The effect of the steam-to-carbon ratio on H_2 production and amount of CO_2 captured using Selexol technology in scenario 1 with different ground water influx rates and a fixed H_2O-to-O_2 injection ratio of 2. Dash lines represent H_2 production and solid lines represent total CO_2 captured.

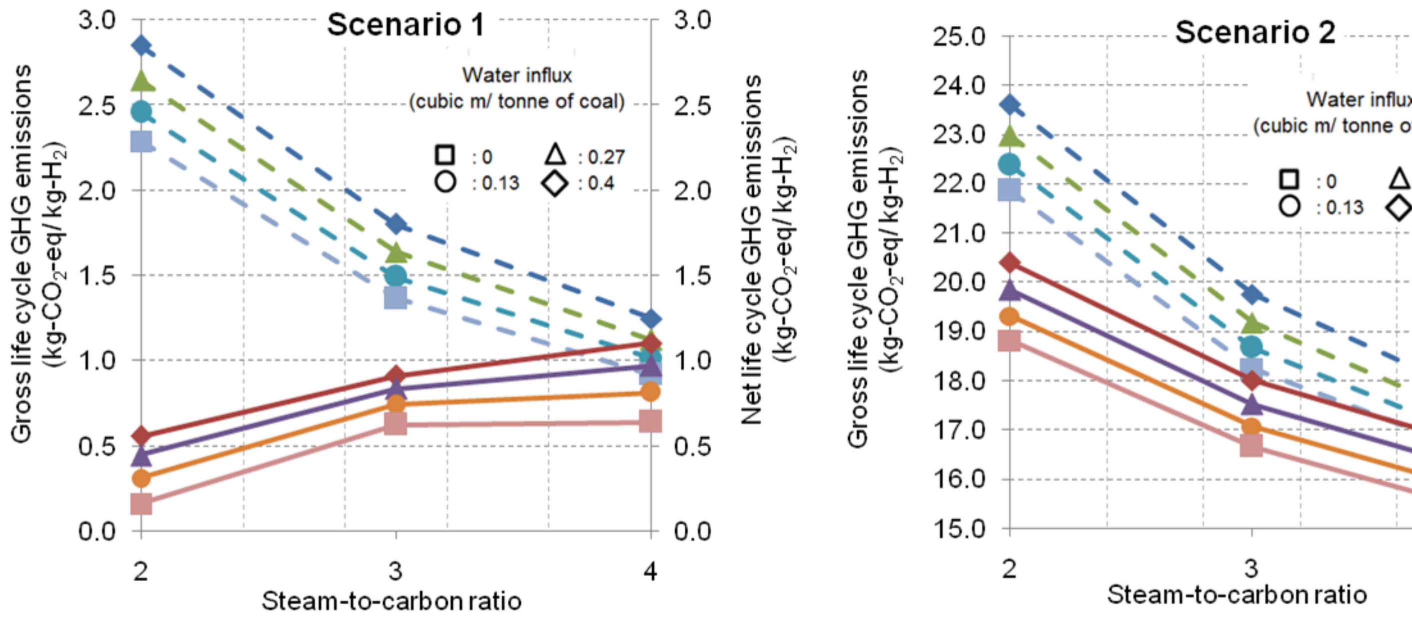

Fig. 7: The effect of the steam-to-carbon ratio on gross and net life cycle GHG emissions in scenarios 1 and 2 with different ground water influx rates, but a fixed H_2O-to-O_2 injection ratio of 2. Dash lines represent gross life cycle GHG emissions and solid lines represent net life cycle GHG emissions.

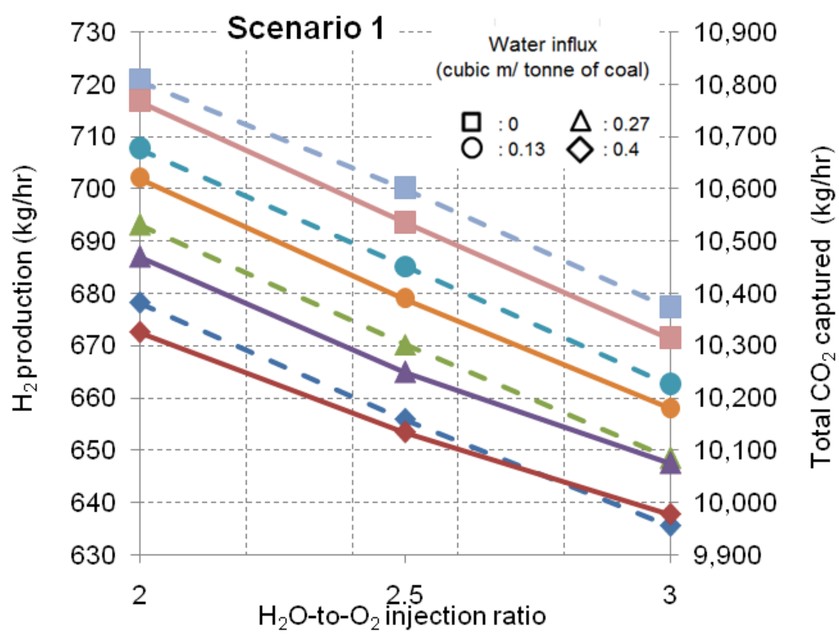

Fig. 8: The effect of the H_2O-to-O_2 injection ratio on H_2 production and amount of CO_2 captured using Selexol technology in scenario 1 with different ground water influx rates, but a fixed steam-to-carbon ratio of 3. Dash lines represent H_2 production and solid lines represent total CO_2 captured.

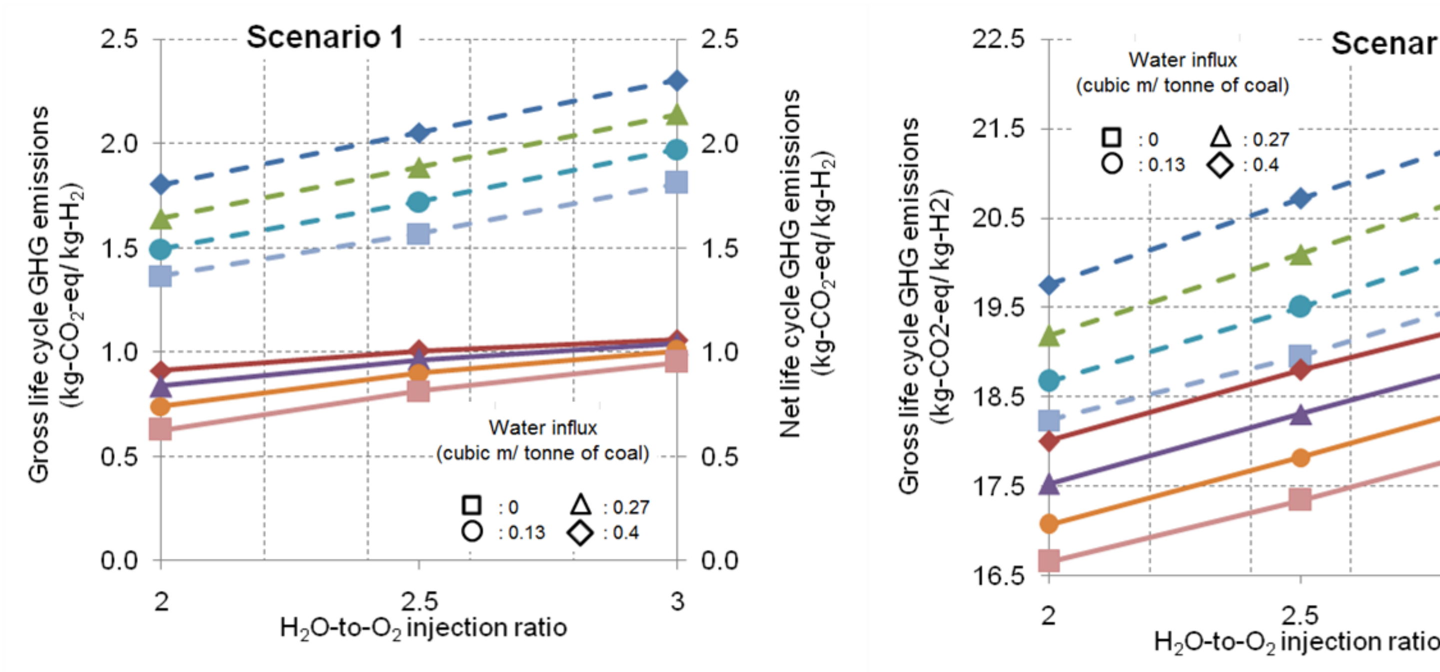

Fig. 9: The effect of the H_2O-to-O_2 injection ratio on gross and net life cycle GHG emissions in scenarios 1 and 2 with different ground water influx rates, but a fixed steam-to-carbon ratio of 3. Dash lines represent gross life cycle GHG emissions and solid lines represent net life cycle GHG emissions.

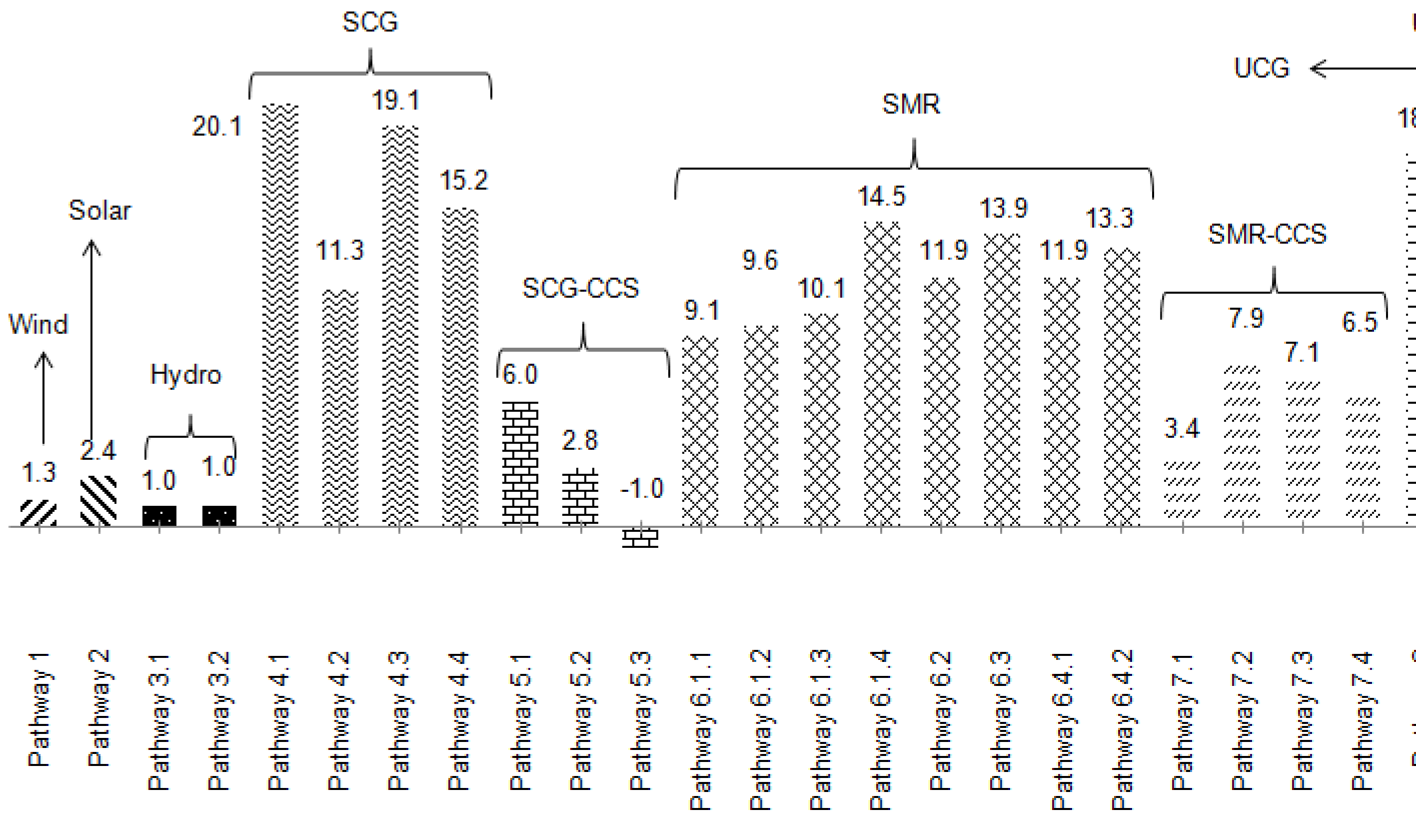

Fig. 10: Comparative analysis of net life cycle GHG emissions in various H_2 production pathways. Pathways 1-3 are renewable energy-based, while pathways 4-9 are fossil-fuel based H_2 production pathways.

Nomenclature

ASU	air separation unit
ACTL	Alberta Carbon Trunk Line
CCS	carbon capture and sequestration
CO_2-eq	carbon dioxide equivalent
EOR	enhanced oil recovery
FUNNEL-	FUNdamental Engineering principlEs-based modeL for estimation
EGY-H2-	of EnerGY consumption and production in hydrogen (H2) production from
UCG	Underground Coal Gasification
FUNNEL-	FUNdamental Engineering principlEs-based modeL for estimation of
GHG-H2-	GreenHouse Gases in hydrogen (H2) production from
UCG	Underground Coal Gasification
GEMIS	Global Emissions Model for Integrated Systems
GHG	greenhouse gas
GREET	Greenhouse Gases, Regulated Emissions and Energy Use in Transportation
GT	gas turbine
GWP	global warming potential
HP	high pressure
HRSG	heat recovery steam generator
Kg	kilogram
LCA	life cycle assessment
LCI	life cycle inventory
LHV	lower heating value
LP	low pressure

MJ	megajoule
Mt	million tonne
MW	megawatt
MWh	megawatt hour
NER	net energy ratio
NG	natural gas
NGSR	natural gas steam reforming
PSA	pressure swing adsorption
SCG	surface coal gasification
SCO	synthetic crude oil
SMR	steam methane reforming
SRR	syngas reforming reactor
ST	steam turbine
WGSR	water gas shift reactor
D	depth of well, meter
E	diesel energy consumption in well drilling, megajoule

Table 1: Coal composition assumed in the study. Data adapted from [6, 24]

Ultimate Analysis		Proximate Analysis	
Paramete r	***%***	***Parameter***	***%***
Ash	9.7	Moisture	4.7
Carbon	74.5	Ash	9.3
Hydrogen	3.6	Volatile Matter	30.5
Nitrogen	1.1	Fixed Carbon	55.5
Sulphur	0.4		
Oxygen	10.7		
LHV of coal, MJ/kg		28.5	

Table 2: Key assumptions for calculation of power requirement and production in the different unit operations in scenarios 1 and 2

Parameter	Applicable scenario	Values	Sources/comments
UCG, syngas to H_2 conversion			
H_2O to O_2 injection ratio in UCG	1, 2	2	[24, 33]
Ground water influx, m^3/tonne of coal	1, 2	0.4	[33, 38]
Steam-to-carbon ratio in SRR[1]	1, 2	3	[33, 37]
CO_2 compressor[2]			
Compressor isentropic efficiency	1	0.75	[39]
GT			
Mechanical efficiency	1, 2	99.5 %	[40]
Isentropic efficiency	1,2	88%	[36]
Turbine inlet temperature, ^oC	1,2	1300	[36]
Pressure ratio	1,2	14.8	[36]
HRSG, ST			

HP steam temperature, °C	1,2	510	Based on steam energy requirement in the SRR [33, 37]
HP steam pressure, bar	1,2	30	
LP steam temperature, °C	1,2	302	Based on steam energy requirement in the H_2S stripper [33, 36]
LP steam pressure, bar	1,2	6	
Isentropic efficiency	1,2	85%	[41]
Mechanical efficiency	1,2	99.5 %	[40]
Pump efficiency	1,2	75%	[36]
Heat exchanger efficiency	1,2	60%	[33]

[1] Calculated based on the molar flow of CO and CH_4 in the syngas, which is fed to SRR

[2] Applicable for compression of CO_2 which is captured using Selexol technology, in a five-stage compressor train

Table 3: Input data and assumptions for different unit operations in H_2 production from UCG with and without CCS

Parameter	Values		Source
	Scenario 1	Scenario 2	
Coal input, tonne/day	118	118	[24, 33]
H_2 output, tonne/day	16.28	16.28	[33]
Injection (ASU, O_2 compressor, H_2O pump)[1], MW	1.07	1.07	[33]
Syngas expander power output, MW	1.58	1.58	[33]
H_2S removal (Claus and tail gas treatment plant)[2],			[33]
MW	0.02	0.02	
SelexolCO_2 removal, MW	1.14	1.14	[33]
CO_2 compressor[3], MW	0.96	0	[33]
H_2 compressor, MW	0.02	0.02	[33]
Gas turbine power output, MW	1.16	1.16	[33]
Steam turbine power output, MW	1.46	1.46	[33]
Total power consumption, MW	3.21	2.25	
Total power output, MW	4.20	4.20	[33]
Net electricity export to grid[4], MW	0.93	1.83	[33]

[1]Based on an O_2 input of 45 tonne/day; O_2 and H_2O injection pressure is 20 MPa bar and 14 MPa, respectively

[2]H_2S captured with using Selexol. Sulphur is recovered in a Claus plant after stripping of H_2S from the solvent

[3] The captured CO_2 is compressed above its critical pressure to around 15 MPa using a five-stage compressor train for suitable pipeline transportation

[4]Difference of total power output and total power consumption. A loss of 6.5% is assumed while transmission of electricity from the H_2 production plant to the grid

Table 4: EOR well reservoir characteristics for CO_2 sequestration

Parameter	Value	Sources/comments
Depth of reservoir[1], m	1635.4	[49]
Reservoir thickness[1], m	27.2	[49]
Reservoir pressure[1], MPa	14.7	[49]
Permeability of reservoir, md	5	[39]
CO_2 leakage rate per annum	0.01%	Applicable over 100 years [50, 51]
Life of EOR well, years	25	Average life of an oil well ranges from 20 to 30 years [52]

[1]Average of range of values for different EOR pilot projects in Alberta

Table 5: LCI data associated with H_2 production from UCG with and without CCS

Parameter	Values	
	Scenario 1	Scenario 2
Injection		
Amortized diesel use in drilling of UCG injection and production wells, MJ-diesel/kg-H2	0.016	0.016
H_2 production		
Heat requirement in SRR unit, MJ/kg-H_2	17.41	17.41
Total heat recovered by HRSG, MJ/kg-H_2	53.04	53.04
Total electricity consumed in H_2 production, MJ/kg-H_2	17.03	11.93
Total electricity produced in H_2 production, MJ/kg-H_2	22.30	22.30
Total electricity export in H_2 production, MJ/kg-H_2	4.93	9.69
HP steam use in SRR unit, MJ/kg-H_2	52.71	52.71
HP steam produced in co-generation plant, MJ/kg-H_2	52.71	52.71
LP steam produced in co-generation plant, MJ/kg-H_2	232.20	232.20
LP steam use in sulphur recovery unit, MJ/kg-H_2	232.20	232.20
Total CO_2 captured in H_2 production, tonne-CO_2/day	247.8	247.8
Total GHGs vented (after CO_2 removal), tonne-CO_2-eq/day	0.0	293.0
CO_2 produced from exhaust of GT and purge gas burner, tonne-CO_2-eq/day	24.8	24.8
H_2 pipeline transport		
Amortized diesel use in H_2 pipeline construction, MJ-diesel/kg-H_2	0.033	0.033
Total steel use in H_2 pipeline construction, tonne	6093.2	6093.2
Amortized steel use in H_2 pipeline construction, kg-steel/kg-H_2	0.047	0.047
CO_2 transport and sequestration		

Amortized diesel use in CO_2 pipeline construction, MJ-diesel/kg-H_2	0.030	-
Total steel use in CO_2 pipeline construction, tonne	1578.7	-
Amortized steel use in CO_2 pipeline construction, kg-steel/kg-H_2	0.009	-
Amortized diesel use in drilling of CO_2 sequestration well, MJ-diesel/kg-H_2	0.010	-

Table 6: Emission factors associated with fuel and material use and the GWPs of GHGs relative to CO_2

Parameter	Value	Source
Emission factors		
Grid-electricity use[1], tonnes-CO_2-eq/MWh	0.88	[56]
On-site electricity production[2], tonnes-CO_2-eq/MWh	-0.65[2]	[56]
Diesel use, kg-CO_2-eq/MJ	0.074	[3]
Production of virgin steel, kg-CO_2-eq/kg-steel	4.972	[3]
GWP		
CO_2	1	[3]
CH_4	25	[3]
N_2O	298	[3]

[1] Applicable for Alberta, Canada

[2]Negative value indicates a credit will be given for electricity supply from the site to the grid

Table 7: Life cycle GHG emissions in different unit operations of H_2 production with and without CCS. The results are presented for the base case of an H_2O-to-O_2 injection ratio of 2, steam-to-carbon ratio of 3 and ground water influx of 0.4 m^3/ tonne-coal

Parameter	Values (kg-CO_2-eq/ kg-H_2)	
	Scenario 1	**Scenario 2**
Operation emissions		
Emissions from the CO_2 removal section	0	17.998
Purge gas combustion[1]	1.521	1.521
Electricity use in H_2 production	0	0
Electricity use in H_2 pipeline transport[2]	0	0
Electricity use in CO_2 pipeline transport[3]	0	-
Non-operation emissions		
Drilling of injection and production well in UCG	0.001	0.001
Drilling and leakage in EOR	0.001	-
CO_2 pipeline construction	0.038	-
H_2 pipeline construction	0.193	0.193
H_2 production plant construction[4]	0.048	0.040
Emissions credit for electricity supply to grid	0.890	1.750
Gross life cycle GHG emissions	1.801	19.752
Net life cycle GHG emissions	0.912	18.003

[1] This value represents emissions associated with combustion of purge gas both in the GT and the burner of the SRR unit

[2] Inlet compressor power requirement for H_2 pipeline transport to the bitumen upgrading site is calculated based on the method discussed in section 2.2.4.This takes into account the pressure losses during pipeline operation without any additional compression. Since, the in-house co-generation plant satisfies

the electricity consumed by the inlet compressor, there are no GHG emissions associated with electricity use in both scenarios.

[3]CO_2 is compressed to 15 MPa (above its supercritical pressure). The in-house co-generation plant satisfies the electricity consumed by the compressors. This negates the GHG emissions associated with electricity use. Moreover, there is no additional electricity consumption during the operation ofCO_2 pipeline to the sequestration site. In order to account for the pressure losses during the operation, calculation of appropriate pipeline diameter is done using the method discussed in section 2.2.3.

[4]The GHG emissions associated with H_2 production plant construction in scenario 1 are slightly higher than in scenario 2 because of additional equipment emissions associated with CO_2 compressors required forCO_2pipeline operation in scenario 1.

Table 8: Description of various H_2 production pathways considered in a comparative analysis of life cycle GHG emissions

Pathway Number	Pathway description	Source
Pathway 1	Water electrolysis using electricity generated by wind turbines	[10]
Pathway 2	Integrated photo voltaic system	[7]
Pathway 3.1	Water electrolysis using electricity generated by a hydro plant	[10]
Pathway 3.2		[7]
Pathway 4.1	SCG without co-generation	[3]
Pathway 4.2	SCG with co-generation	[7]
Pathway 4.3	SCG with electricity co-production	[3]
Pathway 4.4	SCG with steam co-production	[3]
Pathway 5.1	SCG-CCS without co-generation	[3]
Pathway 5.2	SCG-CCS with electricity co-production	[3]
Pathway 5.3	SCG-CCS with steam co-production	[3]
Pathway 6.1.1	SMR without co-generation	[9]
Pathway 6.1.2		[10]
Pathway 6.1.3		[8]
Pathway 6.1.4		[3]
Pathway 6.2	SMR with co-generation	[7]
Pathway 6.3	SMR with electricity co-production	[3]
Pathway 6.4.1	SMR with steam co-production	[11]
Pathway 6.4.2		[3]
Pathway 7.1	SMR-CCS	[8]

Pathway 7.2	SMR-CCS without co-generation	[3]
Pathway 7.3	SMR-CCS with electricity co-production	[3]
Pathway 7.4	SMR-CCS with steam co-production	[3]
Pathway 8	UCG with co-generation	Present model
Pathway 9	UCG-CCS with co-generation	Present model