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Development of a process simulation model for energy analysis of hydrogen production from underground coal gasification (UCG)

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ABSTRACT

This paper presents a model to perform energy balances and estimate hydrogen conversion efficiency from UCG-based syngas. The model was developed for H₂ production from UCG-based syngas with and without CCS, along with the co-production of electricity and steam in a conventional combined cycle plant. In this paper, at base case conditions (H₂O-to-O₂ injection ratio of 2 and a steam-to-carbon ratio of 3), the coal-to-H₂ conversion efficiency is estimated to be 58.1% for UCG with and without CCS. For the plant configuration involving no CCS, in addition to H₂ production, approximately 4.7% of coal energy is converted to electricity that is exported to the grid. In the case of UCG–CCS, a minor energy penalty is incurred, wherein the electrical energy exported per unit coal energy is around 2.4%, with a CO₂ capture efficiency of 91.6% being achieved. The H₂ conversion efficiency decreases with rise in H₂O-to-O₂ injection ratio, but increases with fall in steam-to-carbon ratio. Effect of ground water influx in UCG on the H₂ conversion efficiency is minor, whereas H₂ separation efficiency in the pressure swing adsorption (PSA) unit has a major effect.

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Introduction

Canadian crude oil production from the oil sands is projected to rise from 1.8 million barrels per day (bpd) in 2012 to 3.2 and 5.2 million bpd in 2020 and 2030, respectively [1]. The production of hydrogen (H₂), required to upgrade bitumen to synthetic crude oil (SCO), will increase in a similar fashion. Around 2.52 GJ of H₂ energy is required to upgrade one cubic meter of bitumen to SCO [2]. Steam methane reforming (SMR) is the dominant H₂ production pathway in Alberta and leads to

a significant amount of greenhouse house (GHG) emissions, from 8.9 to 14.21 kg of CO₂e per kg of H₂ produced [2–8]. To put things into perspective, H₂ production from SMR accounts for around 43% of the total well-to-upgrading¹ GHG emissions in the Canadian oils sands industry [2]. In 2010, the Alberta oil sands industry contributed around 23% to Alberta's total GHG emissions [9]. With a focus on reduction of GHG emissions, the Government of Alberta has set a target of a 50% reduction in projected business-as-usual GHG emissions in 2050, which is around 200 million tonnes in GHG emissions reduction [9]. Therefore, there is justification to explore and study an

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¹ Well-to-upgrading emissions are those associated with bitumen extraction and upgrading to SCO. In absolute numbers, 0.25 tonnes of CO₂ will be emitted if SMR is used to produce the required amount of H₂ to upgrade one cubic meter of bitumen [2–6].

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Nomenclature

ASU	air separation unit
bpd	barrels per day
CC	combined cycle
CCS	carbon capture and sequestration
CO ₂ e	carbon dioxide equivalent
CRIP	controlled retractable ignition point
ECBM	enhanced coal-bed methane
EOR	enhanced oil recovery
FUNNEL-EGY-H2-UCG	FUNDamental eNGineering principleS-based model for estimation of Energy consumption and production in hydrogen (H ₂) production from Underground Coal Gasification
GHG	greenhouse gas
GJ	gigajoule
GT	gas turbine
HP	high pressure
HRSG	heat recovery steam generator
HT	high temperature
HX	heat exchanger
IGCC	integrated gasification combined cycle
kWh	kilowatt hour
LHV	lower heating value
LP	low pressure
LT	low temperature
MDEA	methyl diethanolamine
MEA	monoethanolamine
MPa	megapascal
MW	megawatt
PSA	pressure swing adsorption
SCG	surface coal gasification
SCO	synthetic crude oil
SMR	steam methane reforming
SRR	syngas reforming reactor
SOFC	solid oxide fuel cell
ST	steam turbine
Tt	trillion tons
UCG	underground coal gasification
WGSR	water gas shift reactor
η_e	electrical energy exported per unit coal energy
η_h	coal to hydrogen conversion efficiency

alternate, less GHG-intensive, hydrogen production pathway for the bitumen upgrading industry.

Coal reserves in Alberta are estimated to be in the range of 2–3 trillion tons (Tt) [10–13]. Of the total reserves, there is the potential to recover around 0.62 Tt (or 25% of total reserves) by surface and underground mining [13]. There is an opportunity to retrieve the remaining 75% of the un-minable coal reserves²

² Initial studies have suggested that three coal zones in Alberta – Ardley, Horseshoe Canyon, and upper Mannville – are suitable for UCG. These three zones constitute around 54% of the total coal reserves. Owing to greater depth, upper Mannville (which has around 16% of the total coal reserves) is the most favorable coal zone for UCG in terms of ground water protection and unwanted overburden subsidence [12].

through technology like underground coal gasification (UCG) [12,14]. In UCG, gasifying agents (a combination of either water and oxygen, steam and air, steam and oxygen, or water and air) are injected into a coal seam, and syngas is produced through chemical reactions that normally occur in surface coal gasifiers [15,16]. This produced syngas can be used to produce electricity, hydrogen, liquid fuels, etc. [15,16]. In a world of anthropogenic induced climate change, UCG has been deliberated as a clean coal conversion technology and a carbon neutral energy pathway [7]. This is due to the fact that while in operation, UCG does not compromise the economic viability and maintains a negligible GHG footprint, especially when combined with CCS [7,17]. UCG is not only a pragmatic technology for clean coal conversion but also has several economic advantages over surface coal gasification (SCG) [14,15,18,19]. UCG significantly reduces the cost of upstream operations such as coal mining, coal handling, coal transport, and coal gasifiers, and leads to low fugitive emissions, low dust, no ash residues, and reduced noise pollution [14,15,18,19]. However, implementation of UCG–CCS technology on an industrial scale remains a challenge in order to gain the merits over other fossil fuel based pathways, especially SMR, for H₂ production. Some of the challenges to adopt UCG technology as an energy production pathway comprise limited process control, inconsistent syngas quality and composition, and environmental risks like ground water contamination and land subsidence [7]. In addition, low natural gas prices diminish the economic competitiveness of UCG-based H₂ against SMR-based H₂, especially in western Canada [7].

Since coal has the highest CO₂ emissions of all fossil fuels per unit of energy produced, the conversion of syngas to electricity or H₂ produces significant amounts of CO₂ emissions [18,20,21]. Carbon capture and sequestration (CCS) technology captures CO₂ using a physical solvent within a pre-combustion arrangement and then stores the CO₂ in an underground geological formation for enhanced oil recovery (EOR) or enhanced coal bed methane (ECBM) recovery [15,20–22]. Moreover, geological sequestration sites (such as saline aquifers) have been found to co-exist with potential UCG sites [17,20,21]. The Western Canadian Sedimentary Basin, in which most of the Alberta's coal reserves are found, has many favorable CO₂ sequestration sites³ [7]. Interestingly, UCG and CCS can be coupled in a process wherein the captured CO₂ is sequestered into a coal seam cavity created upon gasification by using the same injection and production wells [18,21]. A similar integrated UCG–CCS process was discussed for a study area in Bulgaria by Nakaten et al. [23]. Admittedly, with huge un-mineable coal reserves in Alberta and with UCG and CCS potential, a low-carbon H₂ production pathway should be analyzed in terms of sustainable development of the bitumen upgrading industry.

There are a few studies in the literature that discuss H₂ production from UCG. Yang et al. [24] discussed the fundamentals of H₂ production by analyzing the experimental

³ Alberta Carbon Trunk Line, a 40.6 cm, 240 km CO₂ pipeline expected to be operational in 2015, will transport CO₂ collected from current and proposed bitumen upgraders to enhanced oil recovery (EOR) fields in central and southern Alberta [8].

conditions and the UCG process in China. Rogut et al. [25] discussed the potential of UCG for large-scale integration of H₂ production with on-site geological storage of CO₂ in the European Union. Some studies have discussed a techno-economic model for electricity and H₂ production from an integrated UCG–CCS process [7,23]. Nakaten et al. [23] concluded that the UCG–CCS process, integrated with a combined cycle (CC) gas turbine (GT) is an economical, low-carbon option for electricity production in Bulgaria. Prabu et al. [26] developed a model to estimate electrical plant efficiency for an integrated UCG–solid oxide fuel cell system (SOFC) system. Nourozieh et al. [27] conducted a feasibility study for Alberta reservoirs by developing a simulation model for process optimization and prediction of syngas production. Moreover, Swan Hills Synfuels LP has successfully constructed and operated the world's deepest in-situ coal gasification pilot facility in Alberta [28].

With that said, none of the aforementioned authors developed models that provide a holistic evaluation of the energy balances involved in UCG for H₂ production, along with the integration of CCS technology. This holistic approach is especially important to characterize the energy conversion efficiency of UCG as a H₂ production pathway, which provides insight into its competitiveness with other conventional options. In addition, the resolution of the energy flows in the H₂ production from UCG leads to the identification of energy-intensive centers along with improvements in the overall system management. Furthermore, the results can be applied to evaluate the life cycle GHG emissions, and GHG mitigation potential and costs associated with H₂ production from UCG along with consideration of CCS [29,30].

The system design of converting H₂ from syngas produced from UCG is identical to that of H₂ produced from SCG [15,16], and the latter is well understood in various studies [31–42]. Following Refs. [31–42], a model to estimate and analyze key performance estimates (coal-to-H₂ conversion efficiency (η_h) and electrical energy exported to grid per unit coal energy (η_e) of UCG-based H₂ production can readily be developed. The model is called FUNNEL-EGY-H2-UCG (FUNdamental eNGineering princIplEs-based model for estimation of EnerGY consumption and production in hydrogen (H₂) production from Underground Coal Gasification) in this paper. While these studies [31–42] focused more specifically on mineable coal and natural gas as a feedstock, this paper addresses the gap in knowledge in the area of energy balances and the evaluation of plant efficiency in the production of H₂ from unmineable coal resources through UCG. Furthermore, this paper provides a framework through which benchmarking of H₂ conversion efficiency from UCG can be carried out with SCG- and SMR-based H₂ production pathways. FUNNEL-EGY-H2-UCG allows the user to estimate the H₂ conversion efficiency for any type of coal and UCG reservoir conditions. That said, in the current analysis, assumptions pertaining to western Canadian conditions are taken into consideration as closely as possible. This paper also establishes the qualitative and quantitative relationships between key UCG process parameters (H₂O-to-O₂ injection ratio, ground water influx and steam-to-carbon ratio) and plant efficiency. This is completed by analyzing the results for a range of 2–3 for H₂O-to-O₂

injection ratio, 0–0.4 m³/tonne-coal for ground water influx and 2–4 for steam-to-carbon ratio.

The paper is organized in the following fashion. **Methodology section** outlines the unit operations of H₂ production from UCG with and without CCS and the methodology adopted in the development of the data-intensive Aspen Plus model. The results and discussions of the work carried out are presented in **Results and discussion section**. The conclusions are provided in **Conclusion section**.

Methodology

Plant layout overview and system boundary: H₂ production from UCG with and without CCS

The H₂ production pathway from UCG is developed for two different plant configurations: with CCS and without CCS. Fig. 1 shows all the unit operations involved in the hydrogen production pathway for the two plant configurations. The underground coal seam is gasified by injecting H₂O and O₂ via an injection well. Upon gasification, coal produces syngas, which travels through a production well. This syngas is mainly composed of CO, H₂, CH₄, CO₂, and H₂O. Apart from this, the syngas also contains traces of H₂S, C₂H₆, NH₃, and higher hydrocarbons. Based on the composition of the syngas, the H₂ production plant scheme can be derived from existing SCG- and SMR-based H₂ production plant schemes. An extensive review of hydrogen production pathways from surface coal gasification and steam methane reforming, provided in Refs. [4,7,32,33,36,43] was done to determine assumptions for different post-UCG unit operations (see Fig. 1).

The overall system energy flow of the H₂ production pathway is represented by streams shown outside the system boundary (see Fig. 1). The boundary start point is the injection of the gasifying agents for UCG, while the termination point is the H₂ export to a demand site via a pipeline. The difference in the two plant schemes is that CCS uses CO₂ compression, transportation, and sequestration and the configuration without CCS does not. It is important to note that both plant configurations are characterized with CO₂ capture using a physical solvent – Selexol. The H₂ production pathway also consists of a co-generation section, which produces electricity and steam to satisfy the requirements of the different unit operations. Additional electricity produced is exported to the grid outside the system boundary.

FUNNEL-EGY-H2-UCG calculates coal-to-H₂ conversion efficiency (η_h) and electrical energy exported to the grid per unit coal energy (η_e) as per Eq. (1) and Eq. (2), respectively. η_e is indicative of electricity production in addition to H₂ production, and is expressed as a percentage of input coal energy after taking into account the electricity consumption in different unit operations.

$$\eta_h = \frac{\text{Hydrogen energy output (LHV basis)}}{\text{Coal energy input (LHV basis)}} \quad (1)$$

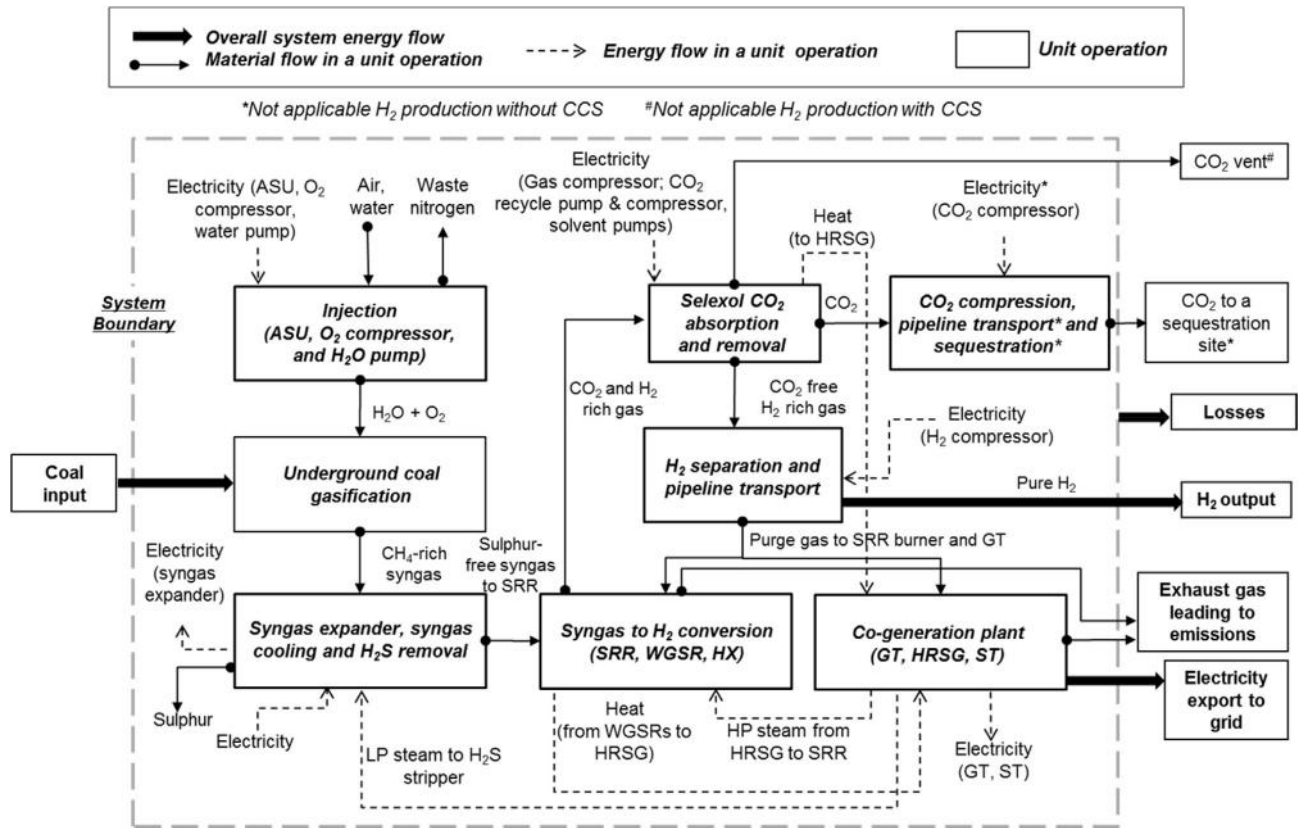


Fig. 1 – Unit operations and system boundary of H₂ production pathways from UCG with CCS and without CCS. All unit operations, except O₂ production in ASU, H₂ separation in PSA and sulphur recovery in Claus unit are modeled in Aspen Plus. Notes: ASU-air separation unit; SRR-syngas reforming reactor; WGSR-water gas shift reactor; HX-heat exchanger; GT-gas turbine; HRSG-heat recovery steam generator; ST-steam turbine.

$$\eta_e = \frac{(\text{Electricity produced} - \text{electricity consumed}) * (1 - \text{transmission losses})}{\text{Coal energy input (LHV basis)}}$$

, or

$$\eta_e = \frac{\text{Net electricity exported to the grid}}{\text{Coal energy input (LHV basis)}}$$

(2)

The underlying assumptions and system components of each unit operation are discussed in the following section of the paper. The Aspen Plus simulation tool is used to model and perform the energy and mass balance of the different unit operations. The inputs and outputs of the Aspen Plus simulation sheet are integrated with a data-intensive Excel-based spreadsheet and the Aspen Simulation Workbook.

H₂ production from UCG – an overview of unit operations

Injection

This unit operation involves the injection of gasifying agents, mainly oxygen and water, at a pressure of 20 MPa and 14 MPa, respectively [28]. Oxygen with 95% purity is produced by an air separation unit (ASU) at a pressure of 0.1 MPa, which consumes 0.26 kWh of electricity per kg of pure O₂ production

[32,33]. It is assumed that the in situ coal gasification reactor is connected by a pair of wells; an injection well is a 1400 m deep and is around 1400 m from a 1400 m high production well [28]. The well diameter is 11.4 cm [28].

Underground coal gasification

The specification of coal used for in situ gasification is shown in Table 1. Due to a lack of production data for hydrogen production from UCG on a large commercial scale for deep coal seams, in situ coal gasification at a small-scale hydrogen production plant was analyzed. In this paper, operational data, mainly type, amount of coal gasified, and injection flow rates of gasifying agents, are taken from a small-scale UCG pilot plant for syngas production operated by Swan Hills Synfuels in Alberta [28]. This pilot project is carried out at a depth of 1400 m, which is one of the deepest of the pilot or

Table 1 – Key assumptions in UCG.

Parameter/values		Sources/comments	
Coal type		High volatile B bituminous manville coal	[28]
UCG reservoir temperature		60 °C	[27]
UCG reservoir pressure		11.5 MPa	[27]
Coal composition			[28]
Ultimate analysis		Proximate analysis	
Parameter	%	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	Average of the range 26.8–30.2 MJ/kg [7,47]
Coal gasified (tonnes/day)		118	[28]
Oxygen injection (tonnes/day)		45	[28]
Water/Oxygen injection mass ratio		2	[28]

commercial UCG projects around the world [19,28]. Owing to greater coal seam depth, the operating pressure of the UCG reactor in Alberta, Canada ranges from 10 to 12.5 MPa [28,44]. High operating pressures result in low water influx in the gasification zone of the UCG reactor and high gas losses from the rock formation [15,16].

The authors in Ref. [28] describe a controlled retractable ignition point (CRIP)⁴ technique that was used to gasify coal underground. The CRIP technique and high operating pressure result in the production of high quality syngas, low heat losses, and improvement of the overall gasification efficiency [19,45]. The initial UCG reservoir temperature and pressure are assumed to be 60 °C and 11.5 MPa, respectively [27]. Heat loss to the surrounding strata in UCG is difficult to estimate and depends on the properties of the dry rock above the coal seam [15,19]. Also, the UCG process reaches a heat balance on its own [19]. With that said, a nominal temperature decrease of 100 °C in the syngas is assumed in this paper to address the heat losses in the UCG reactor. Another factor that is difficult to estimate in UCG is the rate of ground water influx in gasification, which not only affects the composition of the syngas but also the quality and quantity of the syngas [15,16]. It is also reported in the literature that the influx water will either be part of the gasification reactions or cool the gases in the reactor [16]. It is assumed in the present analysis that ground water (amounting to 0.4 m³/tonne of coal)⁵ takes part in the gasification reaction, and its effect on η_h , and η_e is addressed.

One of the most important considerations in estimating H₂ production from UCG is the composition of the syngas collected from the production well. The process of UCG is similar to surface coal gasification, from a chemical and a

thermodynamic perspective [48]. The in situ coal will undergo a series of chemical reactions, namely coal drying, pyrolysis, char gasification, boudouard, steam gasification, hydrogen gasification, CO combustion, gas-steam shift, and methane-steam shift⁶ [44,49]. Coal is characterized in Aspen Plus in the form of products obtained after pyrolysis, that is, char, tar, H₂S, C₂H₆, CO, CH₄, NH₃, CO₂, H₂, ash, and H₂O. The mass flow rates of each of these constituents are estimated in a similar fashion as done by the authors of [44], using a mathematical model provided by Ref. [50]. The syngas composition is estimated based on the minimization of the Gibbs free energy of the UCG reactor using the Peng–Robinson equation of state in Aspen Plus. The model developed is predicated upon the assumption that the UCG reactor reaches equilibrium with the following: surrounding strata, ground water influx, heat losses and gasifying agents (H₂O and O₂) at a given point of time. The UCG process is represented by two RGibbs reactors in Aspen Plus. The second RGibbs reactor accounts for heat losses in the UCG reactor by specifying the assumed temperature decrease of 100 °C. However, there are limitations with this methodology. The resolution of syngas losses to the surrounding rocks and dynamic temperature-pressure profile in the in situ coal seam and its effect on the syngas composition are beyond the capacity of the model presented.

The composition of the syngas on a dry molar basis based on 118 tonnes per day of coal extracted by UCG for an H₂O-to-O₂ injection ratio of 2 and a ground water influx of 0.4 m³/tonne of coal is given in Table 2. The composition of the produced gas obtained from the model is consistent with reported values in the literature for a variety of coal, i.e., H₂:

⁴ The CRIP technique uses coiled tubing for injection through an injection well that is drilled horizontally until it reaches the foot of a production well. Fresh coal is reached by retracting the coil when the cavity has matured (because of which the syngas quality becomes poor) [19].

⁵ A ground water influx rate of 0.4 m³/tonne of coal is assumed for stable and continuous gas production [46].

⁶ Coal drying: Wetcoal → Drycoal + H₂O, $\Delta H^0 = 40$ kJ/mol; Pyrolysis: Drycoal → Char + Volatiles, $\Delta H^0 \sim 0$ kJ/mol; Char gasification: C + O₂ → CO₂, $\Delta H^0 = -393$ kJ/mol; Steam gasification: C + H₂O → H₂ + CO, $\Delta H^0 = +131$ kJ/mol; Boudouard: C + CO₂ → 2CO, $\Delta H^0 = +172$ kJ/mol; Hydrogen gasification: C + 2H₂ → CH₄, $\Delta H^0 = -75$ kJ/mol; CO combustion: CO + 1/2O₂ → CO₂, $\Delta H^0 = -283$ kJ/mol; Gas-steam shift: CO + H₂O ↔ CO₂ + H₂, $\Delta H^0 = -41$ kJ/mol; Methane-steam shift: CH₄ + H₂O ↔ CO + 3H₂, $\Delta H^0 = +206$ kJ/mol.

Table 2 – Composition of the syngas produced from UCG.

Dry gas mol%					Total volume of dry gas	Calorific value of syngas
CH ₄	CO ₂	CO	H ₂	H ₂ S	Nm ³ /h	MJ/Nm ³
10.77%	20.73%	33.69%	34.63%	0.19%	11168.26	10.55

11–35%; CO: 2–16%; CH₄: 1–8%; CO₂: 12–28%; H₂S: 0.03–3.5% [19]. Considering the high operating pressures in UCG, there is likely to be considerable CH₄ in the produced gas, unlike in low operating pressures, where the CH₄ percentage is lower than that of gas [28,44]. This is mainly due to the fact that the hydrogenating gasification reaction ($C + 2H_2 \rightarrow CH_4$) is favorable at a high underground reactor pressure [28,44]. The product gas is treated with steam to convert CH₄ into water gas (H₂ + CO) in a reforming reactor to improve η_h . This reactor is called a syngas reforming reactor (SRR) in this paper.

Hydrogen sulphide (H₂S) removal

Sulphur needs to be removed from the product gas obtained from UCG both for economical operation and to avoid poisoning the catalysts in the reforming reaction of the methane present in the product gas [43]. This is unlike in surface coal gasification plant schemes with CCS, where H₂S is co-captured with CO₂ downstream of water-gas shift reactions [32,33,39,40]. Additionally, prior to H₂S removal, the highly pressurized product gas obtained from UCG is expanded in a turbine to around 3 MPa⁷ to generate electricity and then cooled to 25 °C [43]. The heat extracted from the gas is used to raise the temperature of the sulphur-free gas, which is put into the SRR. The polytropic efficiency of the syngas expander is assumed to be 88% [32]. H₂S capture is carried out in an absorption tower with dimethyl ether of polyethylene glycol (Selexol) as a solvent and an operation pressure of 3 MPa [32,33,36,43]. The process flow scheme from H₂S absorption to stripping is derived from Ref. [36].

The solubility of CO₂ in Selexol is about 8.93 times less than that of H₂S [51]. However, the amount of CO₂ absorbed in Selexol is significantly greater than the amount of H₂S absorbed. This is because of higher mole concentration of CO₂ than of H₂S in the product gas [32] (see Table 2). Therefore, after stripping H₂S from Selexol, the solvent is fed to a CO₂ absorption tower downstream of water–gas shift reactors (WGSRs) to capture the CO₂. Close to 99% of H₂S is removed from the product gas, which is consistent with the 99% H₂S removal efficiency reported in the literature [31,32,36]. Steam (6 MJ, 0.6 MPa steam per kg of sulphur [32]) required to strip H₂S from the solvent is produced from a heat recovery steam generator (HRSG) in a co-generation plant. The above assumptions are also valid for plant schemes without CCS. Sulphur is recovered in a Claus plant, which consumes 98 kWh of electricity per tonne of sulphur removed⁸ [52]. Additional electricity is required to treat tail gas coming from

the Claus plant and is assumed to be 463 kWh per tonne of sulphur removed⁸ [52].

Syngas to H₂ conversion

The sulphur-free and CH₄-rich syngas is processed in a series of reactors to produce H₂: a steam reforming reactor (SRR) and high temperature (HT) and low temperature (LT) WGSRs. Table 3 shows all the assumptions pertinent to this unit operation. A steam-to-carbon ratio of 3 is assumed in order to get the maximum H₂ output upon syngas conversion [43]. Carbon flow is calculated based on the molar flow of CH₄ and CO in the UCG produced syngas. The syngas is then converted to H₂ in a series of HT and LT WGSRs. A heat exchanger network is modeled in a simplified fashion to use the heat recovered from the WGSRs to produce HP and LP steam in an HRSG. Purge gas, which is produced after the removal of H₂ downstream of CO₂ removal, is burned to satisfy the heat duty of the SRR.

CO₂ removal and transportation

To integrate hydrogen production from UCG with CCS, CO₂ is absorbed, removed, and compressed before its transportation to a sequestration site [31,33,53]. CO₂ is absorbed using Selexol as a solvent because Selexol consumes less energy than other solvents like methyl diethanolamine (MDEA) [33]. The absorbed CO₂ is then separated in a series of flash chambers and finally compressed to a pressure of 15 MPa in five stages [33,53]. The solvent also absorbs H₂ in the absorption tower. Therefore, the solvent coming from the first flash chamber is compressed and recycled back to the absorption tower to avoid loss of H₂ [31]. The pressure drop between the first flash chamber and the absorption tower is achieved with a hydraulic turbine [31]. The work extracted from the hydraulic turbine is then used to satisfy a portion of solvent recycle pump work [31]. Table 4 shows key assumptions employed for this unit operation. In H₂ production without CCS, the advantage of CO₂ removal (see Fig. 2) is appreciated by

Table 3 – Key assumptions in SRR and WGSR.

Parameter	Value	Sources
SRR		
Steam-to carbon-ratio	3	[43]
Temperature/pressure in SRR, °C/MPa	800/3	[43]
WGSR		
Pressure loss in WGSRs	4%	[32]
Temperature of gas inlet to HT-WGSR, °C	350	[31]
Temperature of gas outlet from HT-WGSR, °C	450	[31]
Temperature of gas inlet to LT-WGSR, °C	250	[31]
Temperature of gas outlet from LT-WGSR, °C	275	[31]
Pressure loss in HXs	2%	[32]
Temperature of gas inlet for CO ₂ absorption, °C	25	[31]

⁷ The pressure value is based on values in the literature of steam methane reforming reaction in H₂ production from natural gas plant schemes [43].

⁸ Owing to complexity of the processes involved in the Claus plant, the sulphur recovery and tail gas treatment are not modeled in Aspen Plus.

Table 4 – Key assumptions for CO₂ capture, removal and compression.

Parameter	Value	Sources/comments
<i>CO₂ absorption and removal</i>		
Solvent pump efficiency	75%	[32]
Recycle compressor isentropic efficiency	85%	[40]
Recycle compressor mechanical efficiency	98%	[40]
Pressure in CO ₂ absorber, MPa	5	[32]
Pressure of flash chambers, MPa	1.7, 0.9, 0.32, 0.11	Values indicate pressure level in chambers 1, 2, 3, and 4, respectively [32]
<i>CO₂ compressor</i>		
Stage 1 discharge pressure, MPa	0.24	[53]
Stage 2 discharge pressure, MPa	0.56	[53]
Stage 3 discharge pressure, MPa	1.32	[53]
Stage 4 discharge pressure, MPa	3.02	[53]
Stage 5 discharge pressure, MPa	7.38	[53]
Booster pump discharge pressure, MPa	15	[53]
Final discharge temperature, °C	25	[53]
Compressor isentropic efficiency	75%	[53]

achieving a higher heating value of purge gas (55.15 MJ/kg) post H₂ separation than a CO₂-rich purge gas of low heating value (3.15 MJ/kg) when no CO₂ removal takes place [32]. Additionally, the purge gas compression power required in the GT section is likely to be reduced, when CO₂ removal takes place ahead of H₂ separation in PSA.

Pipeline is assumed to be the mode of transportation of CO₂ to an enhanced oil recovery site. CO₂ is transported as a liquid, and a distance of 100 km from the CO₂ capture site to an EOR site is taken as the base case. CO₂ has a critical pressure of 7.38 MPa; that is, it behaves as a liquid at pressure values greater than 7.38 MPa [53]. Therefore, CO₂ is compressed to a pressure of 15 MPa by means of a five-stage compressor power train [32,40,53,54]. Table 4 shows the key assumptions pertaining to the CO₂ compressors. With an increase in pressure of the captured CO₂, the temperature also increases in each stage. Since the operating temperature in the compressor power train is assumed to be 31 °C, the temperature of the captured CO₂ is decreased through the heat exchanger after

each stage. The heat recovered from the heat exchangers is used in the HRSG section to produce steam.

H₂ removal and transportation

For plant schemes with and without CCS, H₂-rich gas after CO₂ removal is processed in a PSA unit to separate H₂ at an efficiency of 85% [32]. Since PSA processes require an elaborate and independent model for their assessment, the H₂ separation is represented as a simple separation process, with an efficiency of 85% [32,43]. The remaining gas, known as purge gas, consists of the inseparable H₂ and some CH₄. A portion of the purge gas is then processed to produce electricity and steam in a co-generation plant, while the other portion is burned to satisfy the heat duty of the SRR. High purity (99.99%) H₂ is delivered at a pressure of 2 MPa from PSA [32]. Pipeline is assumed to be the mode of transportation of H₂ to an oil sands upgrading site. A pipeline length of 100 km is used as the base case for H₂ transportation. Typical hydrogen pipeline operating pressures and diameters range from 1 to 3 MPa and 0.25–0.30 m, respectively [55]. Considering the exit H₂ gas pressure from PSA, the average of the range is used for the operating pressure in the present analysis. The efficiency of the H₂ compressor is assumed to be 55% [56]. Considering the small-scale H₂ production from UCG and the transportation of H₂, a lower value, 0.25 m, is used for pipeline diameter. The compressor power requirement is calculated using the method developed by Ogden [56].

Co-generation plant

This section includes several components, mainly gas turbine (GT), HRSG, and steam turbine. The amount of purge gas fed to the burner is calculated based on the amount of heat duty required in the SRR. The remaining purge gas is compressed, combusted, and then expanded in a GT to produce electricity. The amount of air fed to the GT combustor is specified based on a turbine inlet temperature of 1300 °C. The HRSG produces high-pressure (HP) and low-pressure (LP) steam from heat recovered from the SRR and the WGRs as well as exhaust gas from the GT. The HP steam, at 3 MPa, is fed to the SRR, and the LP steam, at 0.6 MPa, is fed to the H₂S stripper. Table 5 shows key assumptions employed for this unit operation. The

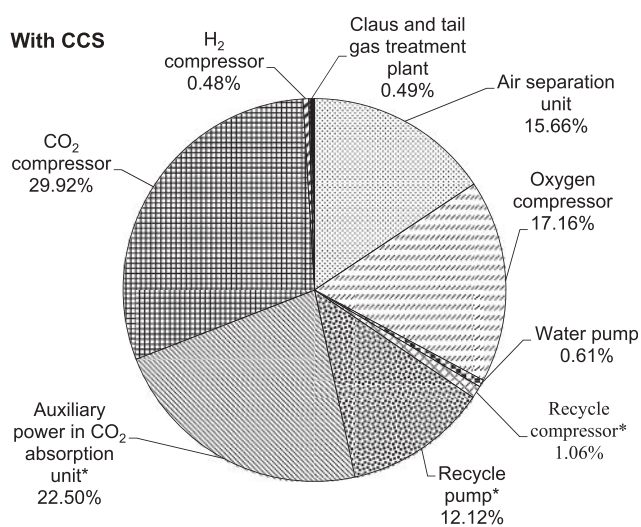


Fig. 2 – Power distribution for H₂ production from UCG with CCS. *Applies to the CO₂ removal section.

Table 5 – Key assumptions for a co-generation plant.

Parameter	Values	Sources/comments
<i>Gas turbine</i>		
Mechanical efficiency	99.5%	[40]
Polytropic efficiency of turbine	88%	[32]
Polytropic efficiency of compressor	85%	[32]
Ambient air temperature/pressure, °C/MPa	15/0.1	[40]
Turbine inlet temperature, °C	1300	[32]
Pressure ratio	14.8	[32]
Turbine outlet pressure, MPa	0.11	[40]
Efficiency of electric generator	98.7%	[32]
<i>Steam turbine</i>		
Steam pressure (HP/LP), MPa	3/0.6	Based on steam pressure requirement in SRR, and H ₂ S stripper
Isentropic efficiency of turbine	85%	[33]
Mechanical efficiency of turbine	99.5%	[40]
Pump efficiency	75%	[32]
Efficiency of electric generator	98.7%	[32]

temperature of the exhaust gas is assumed to be 100 °C [33]. Based on an average heat exchanger efficiency of 60%; heat losses in heat recovery are assumed to be 40%. Auxiliary power consumption is assumed to be 2% of the gross power output [31,32]; this makes up for the power consumption in the process and feed-water pumps [32]. Additionally, a transmission loss of 6.5% of net electricity or additional electricity produced is accounted for in estimating η_e (see Eq. (2)) [2].

Scope of assumptions and model results

The input data and assumptions used in FUNNEL-EGY-H2-UCG are both generic and site-specific in nature. All the site-specific assumptions are associated with two unit operations – injection and UCG. These input data include coal type, UCG reservoir depth and pressure, and characteristics of injection gasifying agents. These inputs have direct implications on the quality and quantity of the syngas produced that ultimately affects the H₂ conversion efficiency. On the other hand, all the assumptions considered in the unit operations described in sections Hydrogen sulphide (H₂S) removal to Co-generation plant are generic. In other words, the FUNNEL-EGY-H2-UCG can be used to evaluate H₂ conversion efficiency from any type of UCG coal seam. Based on the above discussion and model assumptions, the energy and material balance was performed in Aspen Plus. The process flow diagrams and input–output flows associated with each unit process are enclosed in Appendix A of the paper in the Supplementary Section.

Results and discussion

Power requirement in different unit operations: H₂ production from UCG with and without CCS

Table 6 shows key parameters of FUNNEL-EGY-H2-UCG and a detailed breakdown of the total power consumption in producing H₂ from UCG with and without CCS. Based on a coal LHV of 28.5 MJ/kg and input of 118 tonnes/day [28,47] (see Table 1), the total rate of coal input energy is calculated as

38.92 MW. This value is the same in H₂ production both with and without CCS. The gross power output from the syngas expander, ST and GT, estimated to be 4.23 MW for a steam-to-carbon ratio of 3, is also the same for both plant configurations. The total system power requirement in H₂ production without CCS is less than in H₂ production with CCS; there is a net power output (which is exported to the grid) of 0.93 MW and 1.83 MW in addition to H₂ production with CCS and without CCS, respectively. η_h , which represents the fraction of the coal energy converted to H₂ energy (see Eq. (1)), is calculated as 58.08% for both plant configurations. Since the net power output is different in the two plant configurations, η_e is estimated to be 2.39% and 4.69% (see Eq. (2) and Table 6) in H₂ production with CCS and without CCS, respectively. Evidently, the increased η_e in the H₂ production plant configuration with no CCS is due to the “no CO₂ compressor” power requirement. This increase of 2.3% in η_e is consistent and can be compared with reported values in the literature for H₂ production from SCG with CO₂ capture [32]. CO₂ capture efficiency, calculated as 91.6%, is also found to be in close agreement with existing values in various studies and models [2,31–34,38,41].

The benefit of the co-generation is realized in both plant configurations as the H₂ production pathway becomes self-sufficient in terms of steam and heat production (see Table 6). This is attributable to the fact that the FUNNEL-EGY-H2-UCG is developed in such a way that the heat and steam requirement in different unit operations matches with the heat and steam production in the co-generation section. The model calculates the steam requirement in the SRR, WGSRs and H₂S stripper, and appropriate amount of steam is produced in the co-generation section. An increase in steam demand (applicable in a case when a higher steam-to-carbon ratio is assumed) leads to a reduction in electricity output by the ST and vice versa. Moreover, the model calculates the heat requirement in the SRR unit and allocates appropriate amount of purge gas (the main source of heat) to the burner of the SRR, and GT in the co-generation section for electricity production.

Figs. 2 and 3 show the power distribution in different unit operations of H₂ production from UCG with and without CCS. Injection, which comprises an ASU, O₂ compressor, and water pump, consumes around 33.4% and 47.7% of the total power requirement in H₂ production with and without CCS,

Table 6 – Key model parameters, output and heat balance for different unit operations in H₂ production from UCG with and without CCS.

Parameter	Values		Comments
	H ₂ production with CCS	H ₂ production without CCS	
Coal input (LHV basis), MW _{th}	38.92	38.92	
H ₂ O-to-O ₂ injection ratio	2	2	
Ground water influx, m ³ /tonne of coal	0.4	0.4	
Steam-to-carbon ratio	3	3	Represents the amount of steam required for syngas reforming in SRR, calculated based on the molar flow of carbon (CO + CH ₄) in the syngas.
<i>Injection</i>			
ASU, MW	0.50	0.50	
Oxygen compression, MW	0.55	0.55	
Water pumping, MW	0.02	0.02	
<i>Expander and H₂S removal</i>			
Syngas expander, MW	–1.58	–1.58	Negative value indicates power output.
Claus and tail gas treatment plant, MW	0.02	0.02	
<i>CO₂ removal, and transport</i>			
Recycle compressor, MW	0.03	0.03	
Recycle pump, MW	0.39	0.39	
Auxiliary power in CO ₂ absorption unit ³ , MW	0.72	0.72	Power consumption of solvent pump and gas compressors.
CO ₂ compressor, MW	0.96	0	
CO ₂ capture efficiency	91.2%	0	Represents the ratio of the amount of CO ₂ captured to the amount of CO ₂ in the feed gas.
Purity of captured CO ₂ (mol%)	97.4%	0	Remaining gas consists of CH ₄ and other gases.
Total CO ₂ emissions, kg/h	1031.3	12207.4	
<i>H₂ separation and transport</i>			
H ₂ compressor, MW	0.02	0.02	
<i>Co-generation section</i>			
Gas turbine, MW	–1.16	–1.16	Negative value indicates power output.
Steam turbine, MW	–1.46	–1.46	Negative value indicates power output.
Gross power ⁶ , MW	–4.20	–4.20	Sum of electricity output from gas turbine, syngas expander, and steam turbine; this value includes auxiliary power consumption (2% of gross power output) and losses in the electrical generator (1.3% of gross power output).
Net power, MW	–0.93	–1.83	Difference of gross power output and electricity requirement in all other unit operations. Also includes a transmission loss of 6.5%. Negative value indicates power output.
H ₂ output (LHV basis), MW	22.61	22.61	
H ₂ conversion efficiency, η _h	58.08%	58.08%	See Eq. (1); LHV of H ₂ is 120 MJ/kg.
Electrical energy exported per unit coal energy, η _e	2.39%	4.69%	See Eq. (2).
<i>Heat balance</i>			
Heat requirement in SRR, MW	3.28	3.28	This requirement is met by purge gas.
Heat recovered from WGSRs, MW	9.00	9.00	The heat recovered is sent to the co-generation section for steam production. Heat exchanger efficiency is assumed to be 60%.
LP steam to H ₂ S stripper, MW	0.04	0.04	This requirement is met by the co-generation section.
HP steam to SRR, MW	9.93	9.93	This requirement is met by the co-generation section.
Heat recovered from CO ₂ absorption section, MW	0.99	0.99	The heat recovered is sent to the co-generation section for steam production. Heat exchanger efficiency is assumed to be 60%.

respectively. The power requirement in the CO₂ removal is also significant and contributes 35.7% and 50.9% to the total power consumption in H₂ production with CCS and without CCS, respectively. CO₂ compressors contribute around 29.9% and 0% of the total power requirement in H₂ production with and without CCS, respectively. This zero power requirement in the “no CCS” plant configuration is because there is no CO₂ compression. Only a fraction of the total electricity consumption is taken for H₂ compression and sulphur recovery, with values of approximately 1% in H₂ production with CCS

and 1.4% in H₂ production without CCS. Unarguably, with an increase in the scale of operation or pipeline transportation distance, the pipeline configuration may require additional booster stations to overcome the increased friction losses and keep the flow in a liquid state. In that case, the total power requirement is likely to increase. The H₂ compressor requirement in both plant configurations is, however, insignificant compared to other system components' power requirements. This is mainly because the small-scale H₂ pipeline operation requires less pressure increase in the inlet

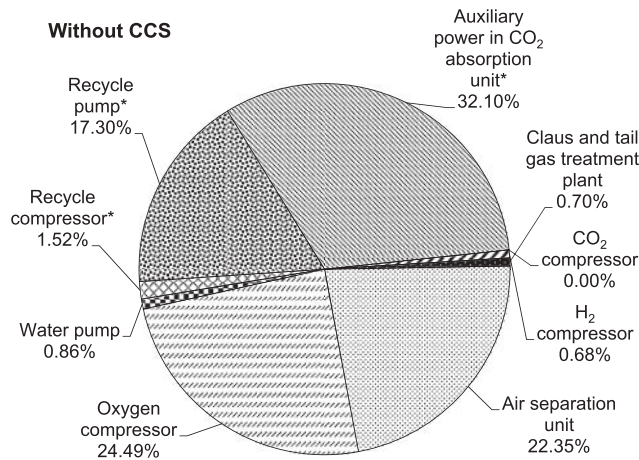


Fig. 3 – Power distribution for H₂ production from UCG without CCS. *Applies to the CO₂ removal section.

pipeline booster station in order to maintain the assumed operating pressure of the pipeline. Conversely, for a large-scale H₂ production plant, the power requirement is likely to increase to overcome the increased friction losses in the pipeline.

Fig. 4 depicts energy input and energy output associated with different operations in the two H₂ production plant

configurations (with and without CCS). The only noticeable difference in the energy balance diagram for the two plant configurations is in the CO₂ compressor requirements, the consequence of which is realized in a higher export of electricity to the grid in H₂ production without CCS than with. The losses, which are the difference of total energy inputs and total energy outputs, are estimated as 15.36 MW and 14.46 MW in H₂ production with and without CCS, respectively.

The effect of the steam-to-carbon ratio on η_h and η_e

The steam-to-carbon ratio plays an important role in the conversion of syngas into H₂ in an SCG-based H₂ production plant [32]. Chiesa et al. [32] demonstrated that by increasing the steam to carbon from 0.55 to 1.48 in the SCG-based H₂ production plant increases the H₂ production by 26%. Therefore, it becomes equally important to investigate the effect of this parameter in UCG-based H₂ production plant efficiencies. The steam-to-carbon ratio is defined as the ratio of steam molar flow in the SRR and molar flow carbon (in the form of CH₄ and CO) in the UCG-based syngas. Fig. 5 shows the effect of the steam-to-carbon ratio on η_h and η_e in H₂ production from UCG with and without CCS. Considering the fact that the ground water influx rate in the UCG reactor is difficult to estimate, the analysis was done for various ground water influx rates ranging from 0 to 0.4 m³ per tonne of coal. Carbon molar flow is calculated based on the product gas available from the

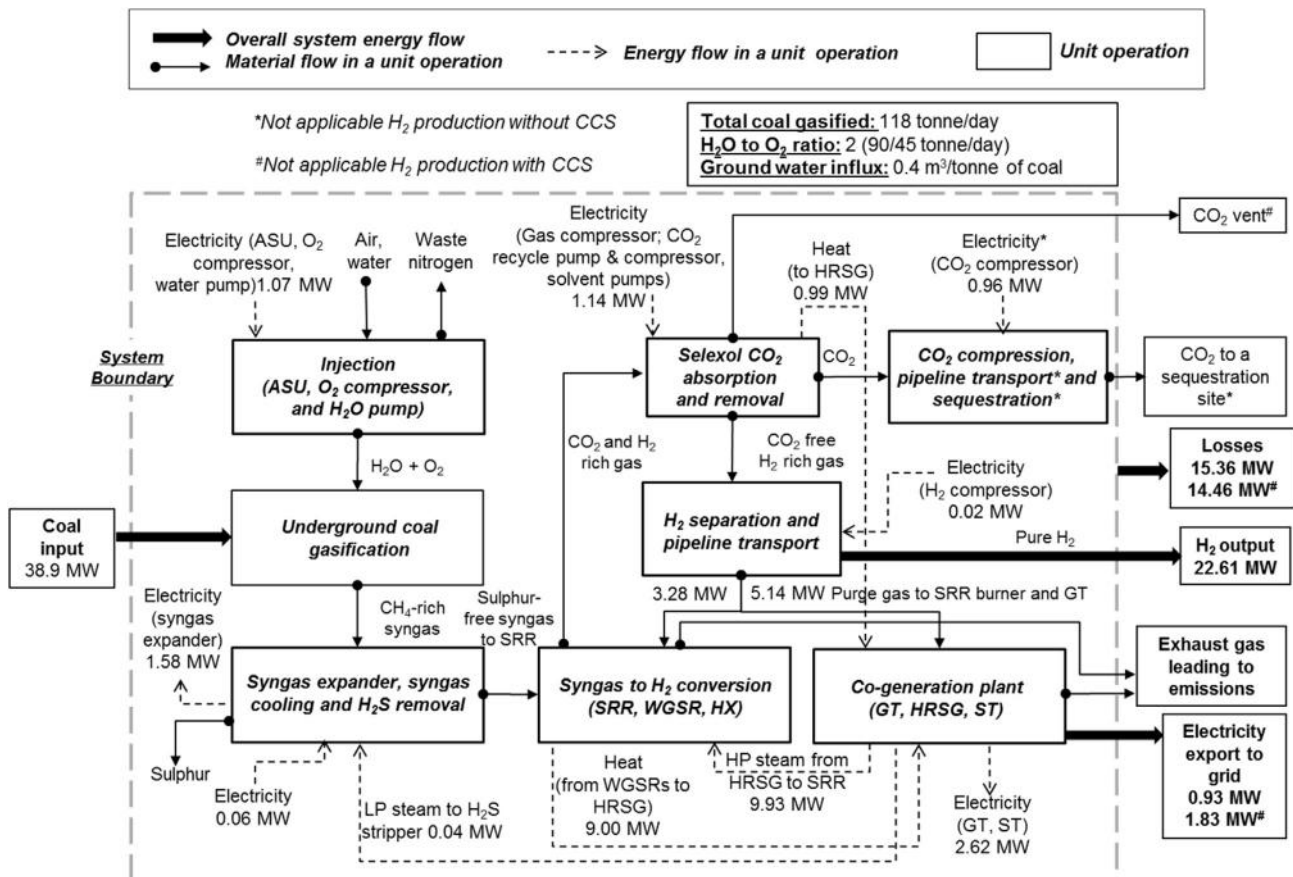


Fig. 4 – Energy balance diagram: H₂ production from UCG with and without CCS.

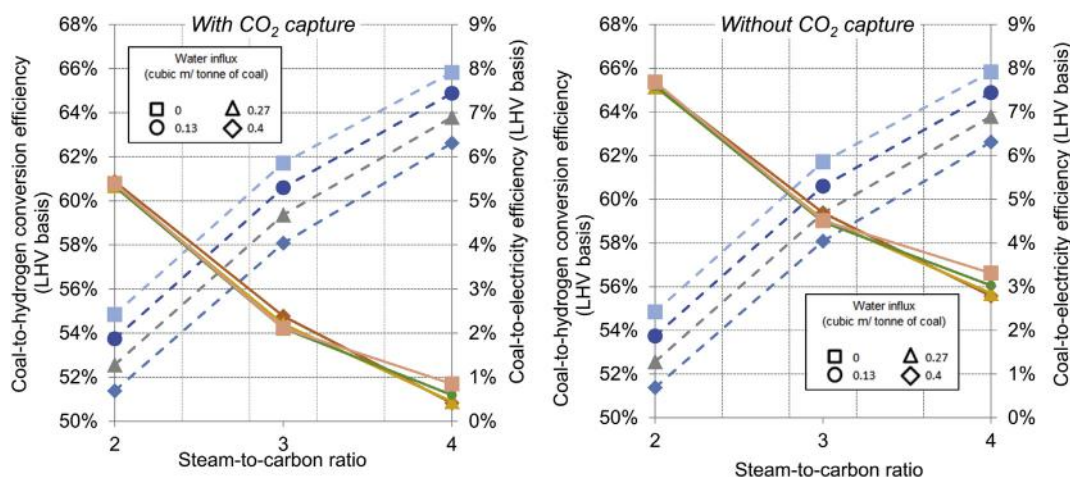


Fig. 5 – The effect of the steam-to-carbon ratio on η_h and η_e in H_2 production from UCG with CCS with different ground water influx rates and a fixed H_2O -to- O_2 injection ratio of 2. Dash lines represent η_h and solid lines represent η_e .

production well of the UCG plant. For a ground water influx of 0.4 m^3 per tonne of coal, with an increase in the steam-to-carbon ratio from 2 to 4, η_h increases from 51.4% to 62.6%. This is because a higher flow of steam is favorable for converting CH_4 into H_2 in SRR and CO into H_2 in WGSRs, ultimately increasing the net H_2 output. It is important to note that this trend is identical in both plant configurations – H_2 production with and without CCS – because the unit operations and their conditions are the same until H_2 separation and transport (see Fig. 1).

However, there is a counter effect on η_e with an increase in the steam-to-carbon ratio. With an increase in steam flow to the SRR, the unconverted CH_4 concentration decreases, and the CO_2 flow rate increases in the product gas downstream of WGSRs. These increases result in a lower heating value of the purge gas after CO_2 removal and H_2 separation in the PSA and ultimately lower GT power output. Additionally, the amount of heat recovered from the WGSRs decreases with an increase in steam flow, resulting in lower ST power output. Overall, the gross power output decreases with an increase in steam flow. However, the power required to remove and compress CO_2 for sequestration increases because of the increased CO_2 flow rate. Overall, the net power output decreases with an increase in the steam-to-carbon ratio. For a fixed ground water influx rate of 0.4 m^3 per tonne of coal, with an increase in the steam-to-carbon ratio from 2 to 4, η_e decreases from 5.4% to 0.4% in H_2 production with CCS, whereas the decrease in the magnitude of η_e ranges from 7.6% to 2.8% in H_2 production without CCS.

It is interesting to note that for a fixed steam-to-carbon ratio, η_h decreases with an increase in ground water influx in the UCG reactor (see Fig. 5). This stems from the fact that with a rise in ground water influx, the CH_4 content in the syngas obtained from the production well increases, whereas its H_2 content decreases. As a consequence, the steam consumption in the SRR unit rises in order to maintain the fixed steam to carbon ratio, thus compensating for the shortfall in H_2 content of the syngas. The aggregate effect of this amounts to a slight drop in the H_2 output as shown in Fig. 5. On the other hand, the rise in CH_4 content of the syngas results in a

small appreciation in the value of η_e . The reason for this trend is two-fold. First, the increase in CH_4 content of the syngas results in an increase in the total flow of the purge gas. At the same time, due to increased steam consumption, the heat duty requirement in the SRR unit also rises. Since a greater portion of the purge gas is burned in a combustor to satisfy this heat requirement, the flow of the purge gas fed to the GT is only slightly increased. As a result, only a small increase in the GT power output is observed. Second, the rise in the steam consumption imposes a penalty in the power output of the ST.

The effect of H_2O -to- O_2 injection flow ratio on η_h and η_e

Stability of the UCG operation in relation to the quality of the syngas can be achieved by controlling the H_2O -to- O_2 injection ratio [28]. At the same time, the H_2O -to- O_2 ratio was found to have a significant influence on the product gas composition [27]. Clearly, it is imperative to appreciate and analyze the sensitivities of variable H_2O -to- O_2 injection ratios on H_2 production from UCG-based syngas. Fig. 6 shows the effect of the H_2O -to- O_2 injection ratio on η_h and η_e in H_2 production from UCG with and without CCS. Again, due to the uncertainty of the ground water influx in the UCG reactor, the sensitivity of the H_2O -to- O_2 ratio for different influx rates is investigated. For the same reasons mentioned in the above section, η_h increases as ground water influx increases. Other parameters remain the same. At the same time, the effect of ground water influx on η_e is negligible.

However, with an increase in H_2O -to- O_2 ratio, η_h decreases. This is mainly due to an increase in CH_4 content and a decrease in H_2 content in the product gas after UCG, resulting in a lower H_2 flow rate for the same flow rate of steam in the SRR and the WGSRs. The findings of the effect of the H_2O -to- O_2 ratio on the product gas composition provided by the present model – FUNNEL-EGY- H_2 -UCG – are found to be consistent with a simulation study done for a similar type and depth of in situ coal gasification by the authors in Ref. [27]. Overall, the η_h decreases from 58.1% to 54.4% as the H_2O -to- O_2 ratio is increased from 2 to 3 for a fixed ground water influx rate of 0.4 m^3 per tonne of coal. Contrastingly, η_e increases

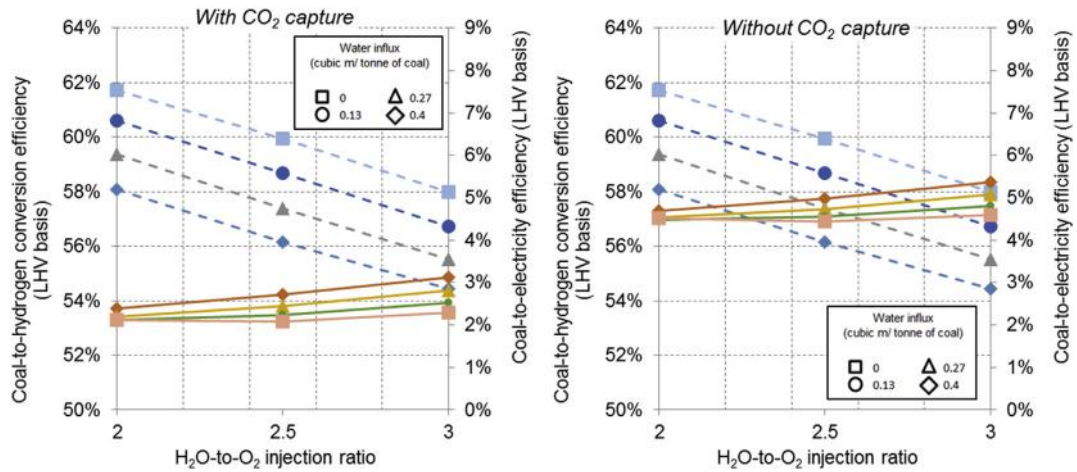


Fig. 6 – The effect of the H₂O-to-O₂ injection ratio on η_h and η_e in H₂ production from UCG with CCS with different ground water influx rates and a fixed steam-to-carbon ratio of 3. Dash lines represent η_h and solid lines represent η_e .

marginally with an increase in the H₂O-to-O₂ ratio, with values ranging from 2.1% to 3.1% and 4.4%–5.4% for a range of ground water influx rates (0–0.4 m³ per tonne of coal) in H₂ production with and without CCS, respectively. This counter effect is justified by a slight increase in net power output by the GT due to an increase in the CH₄ flow in the purge gas on increase in the H₂O-to-O₂ injection ratio.

Sensitivity analysis

Fig. 7 depicts the sensitivity analysis done for H₂ production from UCG with CCS, wherein the ground water influx rate is 0.4 m³ per tonne of coal and the H₂O-to-O₂ ratio is 2. It is important to mention that the same trend is observed when the analysis is conducted for H₂ production without CCS; the only difference is in the absolute values of electrical

efficiencies because there is no CO₂ compressor power requirement in this plant configuration.

η_h is most sensitive to H₂ separation efficiency in the PSA unit. A 10% reduction in the H₂ separation efficiency would result in a decrease of η_h from 58.1% to 52.3%, while η_e would increase from 2.4% to 4.4% because of increased GT power output. Conversely, a 10% increase in the H₂ separation efficiency would result in a rise of η_h from 58.1% to 63.9% and a decline in η_e from 2.4% to 0.4%. All the other variables, namely heat exchanger efficiency, GT inlet temperature and pressure ratio, CO₂ compressor isentropic efficiency, and H₂ and CO₂ pipeline transportation distance, have no effect on η_h . However, a temperature decrease in the UCG reactor has a marginal effect on η_h . The greater the temperature decrease in the UCG reactor, the lower the η_h . This is mainly because of increased CH₄ content in the produced gas after the UCG process [19,46].

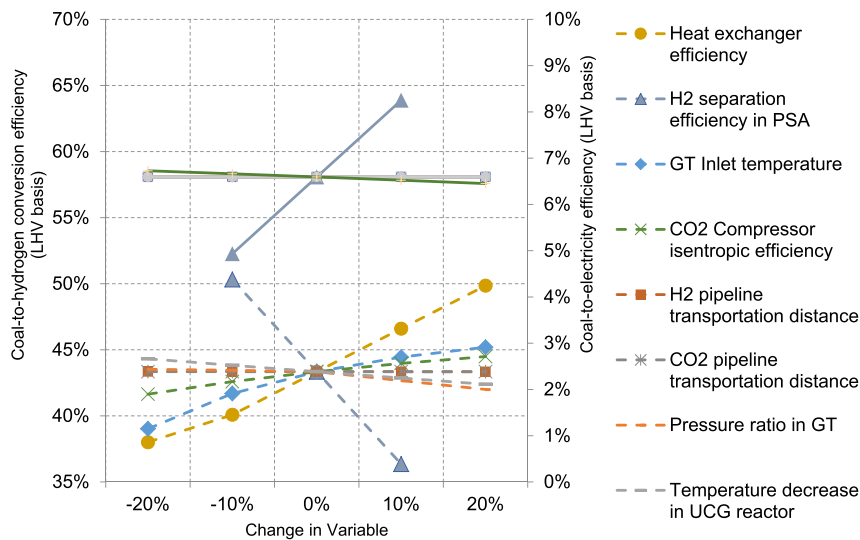


Fig. 7 – Sensitivity analysis for H₂ production from UCG with CCS. The H₂O-to O₂-ratio is 2, and the ground water influx rate is 0.4 m³ per tonne coal. Dash lines represent η_e , and solid lines represent η_h .

The sensitivity of the heat exchanger efficiency on η_e can be appreciated; because of an increase in total heat available in the HRSG, steam production increases, ultimately resulting in increased ST power output, and vice-versa. η_e increases from 2.4% to 4.2% with a 20% increase in heat exchanger efficiency. Conversely, η_e decreases from 2.4% to 0.9% with a 20% decrease in heat exchanger efficiency. A moderate non-linear increasing trend is observed for η_e with an increase in the GT inlet temperature. This is mainly because of the non-linear relationship between the GT inlet temperature and the power delivered by the GT. All the other parameters have a marginal effect on η_e .

Electricity production from UCG with and without CCS

The present analysis illustrates the use of product gas obtained from the UCG process for H_2 production with and without CCS. Taking into account the immaturity of large commercial-scale UCG technology, the literature on the UCG product gas processing for a variety of end uses, i.e., electricity production, H_2 production, etc., is, therefore, limited. However, the authors in Refs. [14,23,57] predict η_e of a combined UCG-IGCC plant producing only electricity in a range of 36.3%–43% without carbon capture and 28.8%–30% with carbon capture. Prabu et al. [26] estimated a net coal-to-electricity efficiency of 32.3% for an integrated UCG–SOFC–CCS plant. But none of these studies evaluates η_h . If the same set of assumptions employed in this paper is applied, and the PSA unit is removed from the H_2 production pathway, it becomes easy to derive a plant configuration that produces only electricity from the produced syngas of the UCG process. The electrical efficiency in plants producing only electricity is evaluated to be 32.1% with CCS and 38% without CCS. The results from this plant configuration are found to be in close agreement with the numbers reported in existing studies. The decrease of 5.9% in the electrical efficiency for adopting a CCS plant configuration against a non-CCS plant configuration is also found to be consistent with the value of 6% reported in Ref. [23]. This

analysis validates the practicality of the FUNNEL-EGY- H_2 -UCG presented in the paper under the stated set of assumptions for different unit operations of the H_2 production pathway.

Comparative analysis: H_2 production from UCG vs SCG vs SMR

In a carbon constrained economy such as western Canada's, where the focus is to move towards clean energy for GHG mitigation, it is important to evaluate the competitiveness of a technology (UCG combined with CCS) that has the potential to recover un-mineable coal and reduce the overall carbon footprint for H_2 production. Table 7 shows typical H_2 plant efficiencies in fossil-fuel based H_2 production pathways (SCG, SMR, and UCG with and without CCS) derived from various studies. Carbon capture technology in most of the listed studies is through physical absorption by Selexol and amines for surface coal gasification and SMR, respectively. The competitiveness of H_2 production of UCG over SCG can be appreciated, given that η_h in UCG ranges from 51.4% to 65.8% versus a range of 44.5%–69% in SCG [2,32,34,35,38,41]. It is evident from the table that there is also a wide range of η_h – 61% to 73% in H_2 production from SMR [34,37,42]. Unarguably, a wide range of efficiency values of H_2 production from SCG and SMR may be attributed to the disparity in the assumptions and the methodology adopted by the authors in the respective studies. Considering the complexity of the H_2 production pathway and the lack of detail in the various studies, it is difficult to outline and justify the dissimilarities that lead to variable outputs [32].

With regard to CO_2 capture efficiency, the value varies from 86.8% to 92% and 85%–90% for H_2 production from surface coal gasification and SMR, respectively. The CO_2 capture efficiency estimated from the current model of H_2 production from UCG (FUNNEL-EGY- H_2 -UCG) – 87%–95.7% – is in close agreement with the values evaluated in various studies for other H_2 production pathways listed in Table 7. Another observation that can be made for H_2 production from surface coal gasification with CCS is the trade-off between H_2

Table 7 – Key performance parameters of H_2 production pathways: UCG, surface coal gasification, and SMR with and without carbon capture.

H_2 production pathway	With or without CCS (CO ₂ capture technology)	H_2 conversion efficiency, %	Electrical efficiency ^a , %	CO ₂ capture efficiency, %	Sources/comments
UCG	With CCS (Selexol)	51.4–65.8 ^b	0.8–5.4 ^b	87–95.7 ^b	Present model
	Without CCS (Selexol)	51.4–65.8 ^b	3.3–7.6 ^b	0	Present model
SCG	With CCS (Selexol)	51.9	1.4	92	[32,38]
	Without CCS (Selexol)	51	4.5	0	[32,38]
	With CCS (Selexol)	44.5	12.8	86.8	[32,35]
	With CCS (Selexol)	57.3	2.8–3.8 ^c	91.1–91.3 ^c	[32]
	Without CCS (Selexol)	57.5	4.2–6.2 ^c	0	[32]
	With CCS (Selexol)	62	2.3	91	[34]
SMR	With CCS (Selexol)	69	–3.7 ^d	90	[34,41]
	With CCS (MDEA)	73	0	85	[34,37]
	With CCS (MEA)	61	–3.9 ^d	90	[34,42]

^a Indicates the amount of electrical energy exported per unit coal energy input.

^b Range of values for different ground water influx rates, steam-to-carbon ratio, and H_2O -to- O_2 injection ratio.

^c The author in Ref. [32] present results for different gasification pressures (7–12 MPa) and syngas cooling modes (quench or syngas cooler).

^d A negative value indicates net import of electricity from the grid.

conversion efficiency, and electrical energy exported per unit coal energy. The higher the H₂ conversion efficiency, the lower the electricity export per unit coal energy. This trend is also true for H₂ production from UCG (see Figs. 5 and 6).

Conclusion

This research provides insight on the energy balances involved in hydrogen production from UCG with and without CCS. In particular, the authors have developed the relationship between key process variables and hydrogen conversion efficiency (η_h) and electrical energy exported per unit coal energy (η_e). For base case assumptions, η_h is calculated to be 58.1% for both plant configurations. In addition to H₂ production, around 2.4% and 4.7% of the coal energy is converted to electricity in H₂ production with and without CCS, respectively. The effect of ground water influx on both η_h and η_e is small. Furthermore, the hydrogen conversion efficiency falls with a rise in the H₂O-to-O₂ injection ratio and increases with an increase in steam-to-carbon ratio. An opposite trend is observed for η_e , where an appreciation of its value occurs with a rise in the injection ratio. However, a decrease in the value of η_e is observed with an increase in steam-to-carbon ratio. In addition, the sensitivity analysis showed that η_e is most sensitive to the efficiency of the heat exchanger and the separation efficiency of the PSA.

Acknowledgments

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Appendix A. Supplementary data

Supplementary data related to this article can be found at <http://dx.doi.org/10.1016/j.ijhydene.2015.06.149>.

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