NETL Life Cycle Inventory Data
Process Documentation File

Process Name:	H2 from Coal Gasification with CCS
Reference Flow:	1 kg of Hydrogen, >99.90 vol%, 925 psig (6.48 MPa)
Brief Description:	Energy use, feedstocks (including feedstock and water use), and emissions associated with a coal gasification facility with a two-stage Selexol capture system (CG + CCS) that converts coal to >99.90 vol-% hydrogen for generic industrial use.

Section I: Meta Data

Geographical Coverage: United States **Region:** Midwest

Year Data Best Represents: 2021

Process Type: Basic Process (BP)

Process Scope: Gate-to-Gate Process (GG)

Allocation Applied: No

Completeness: All Flows Captured

Flows Aggregated in Data Set:

☒ Process ☒ Energy Use ☐ Energy P&D ☐ Material P&D

Relevant Output Flows Included in Data Set:

Releases to Air:	☒ Greenhouse Gases	☒ Criteria Air Pollutants	☒ Other
Releases to Water:	☐ Inorganic Emissions	☐ Organic Emissions	☐ Other
Water Usage:	☒ Water Consumption	☒ Water Demand (throughput)	
Releases to Soil:	☐ Inorganic Releases	☐ Organic Releases	☐ Other

Adjustable Process Parameters:

groundwater_pct

[%] Percent of water supply sourced from groundwater

potw_pct

[%] Percent of water supply sourced from publicly-owned treatment works.

slag_credit_pct

[%] Percentage of slag produced that is credited as a coproduct. Customizable parameter for the user's specific system configuration. It should be set to one if and only if the plant designers have a confirmed use-case for all of its slag throughout the lifetime of the project.

Tracked Input Flows:

coal, at destination

[Technosphere] Mass flow rate of coal entering the facility. Coal is used as both feedstock and heat source. Mass flow rate is based on assumption of Illinois No.6 coal, with an as-received HHV of 27,113 kJ/kg.

Electricity, AC, 120 V

[Technosphere] Auxiliary grid electricity required to operate the full CG + CCS facility.

Water, purified

[Technosphere] Water filtered to acceptable purity by water treatment train.

Sodium hydroxide

[Technosphere] Sodium hydroxide input, scaled to the reference flow.

Sulfuric acid

[Technosphere] Sulfuric acid input, scaled to the reference flow.

Tracked Output Flows:

Hydrogen, >99.90 vol%, 925 psig (6.48 MPa)

[Reference flow]

Steam, medium pressure, 399°C

[Technosphere] Steam available for export, scaled to the reference flow. Default for coal gasification is zero.

Carbon dioxide, captured product

[Technosphere] Mass flow rate of the captured carbon dioxide, scaled to the reference flow.

Slag, produced

[Technosphere] Mass flow rate of co-product slag generated, scaled to the reference flow.

Section II: Process Description

Associated Documentation

This unit process is composed of this document and the data sheet (DS) *DS_O_H2_from_Coal_Gasification_with_CCS_2022.01.xlsx*, which provides additional details regarding relevant calculations, data quality, and references.

Goal and Scope

This unit process provides a summary of relevant input and output flows associated with a representative coal gasifier with CO_2 capture (CG + CCS) that has been configured to primarily produce hydrogen. Coal gasification (CG) is a method to convert solid coal into synthesis gas (CO and H_2). The syngas can then be shifted to mainly hydrogen and carbon dioxide via the water-gas shift reaction. This design utilizes two Shell dry feed, pressurized, up-flow, entrained, slagging gasifiers operating at 615 psia, and is based on the gasification of Illinois No. 6 coal with an as-received higher heating value of 27,113 kJ per kilogram. A two-stage Selexol process is used to remove the CO_2 from the flue gas, which includes a sulfur adsorber like conventional CG, followed by a second adsorber that removes the CO_2. The facility requires supplemental electricity from the grid for auxiliary systems but does not require an external fuel source for the gasification reaction. The reference flow of this unit process is: 1 kg of >99.90 vol-% hydrogen at 925 psia.

Boundary and Description

This unit process provides a summary of relevant input and output flows associated with coal gasification with carbon capture (CG w/ CCS). The plant configuration for CG w/ CCS is nearly identical to that of CG -- a multistep process to convert solid coal feedstock into gaseous hydrogen. There are two principal reactions that occur in a CG w/ CCS facility, along with a two-stage acid gas removal unit that processes the acid gas and removes sulfur and CO_2. Coal feedstock is first reacted with oxygen in the gasifier to produce mostly hydrogen and carbon monoxide (syngas), and the product is then converted to additional hydrogen and carbon dioxide via the water-gas shift reaction.

The material, energy, and emissions reported in this unit process are based on the NETL publication, Comparison of Commercial, State-of-the-Art, Fossil-Based Hydrogen Production Technologies (2022). The plant modeled consists of two Shell dry feed, pressurized, up-flow, entrained, slagging gasifiers, and it produces 27,498 kg H_2 per hour (274 MMSCF per day). The Shell gasifier was selected for modeling due to the flexibility if can offer for the feedstock used. Carbon dioxide is mainly generated by the water-gas shift reaction, and it is captured from the hydrogen stream using a two-stage Selexol unit. The first stage of this unit removes sulfur from the acid gas stream, while the second separates the carbon dioxide. Both steps utilize absorbers. The captured carbon dioxide is then treated to meet pipeline export specifications using an eight-stage front-loaded integrally geared centrifugal compressor, along with dehydration using a triethylene glycol desiccant. Other contaminants that must be removed include particulates, HCl, mercury, and miscellaneous sulfur compounds.

There are several byproducts of CG w/ CCS that have been considered. Slag, a glass-like material formed from the mineral matter embedded in coal, is produced in significant quantities, but is considered to be a waste product that is landfilled by default. Liquid sulfur is a byproduct of the Claus process, and it is commonly stored in a sulfur pit prior to transportation to end users. A complete life cycle assessment should model and include the impacts associated with disposal of the slag and sulfur. This unit process has been developed with a parameter that allows the user to select whether to consider the slag a co-product, and if so, what percentage of the overall output.

Inputs and outputs have been scaled to a reference flow of 1 kg of gaseous hydrogen (>99.90 vol-%) at 925 psia. The facility is assumed to be located at a generic, greenfield plant site in the Midwestern U.S.

Figure 1: Unit Process Scope and Boundary

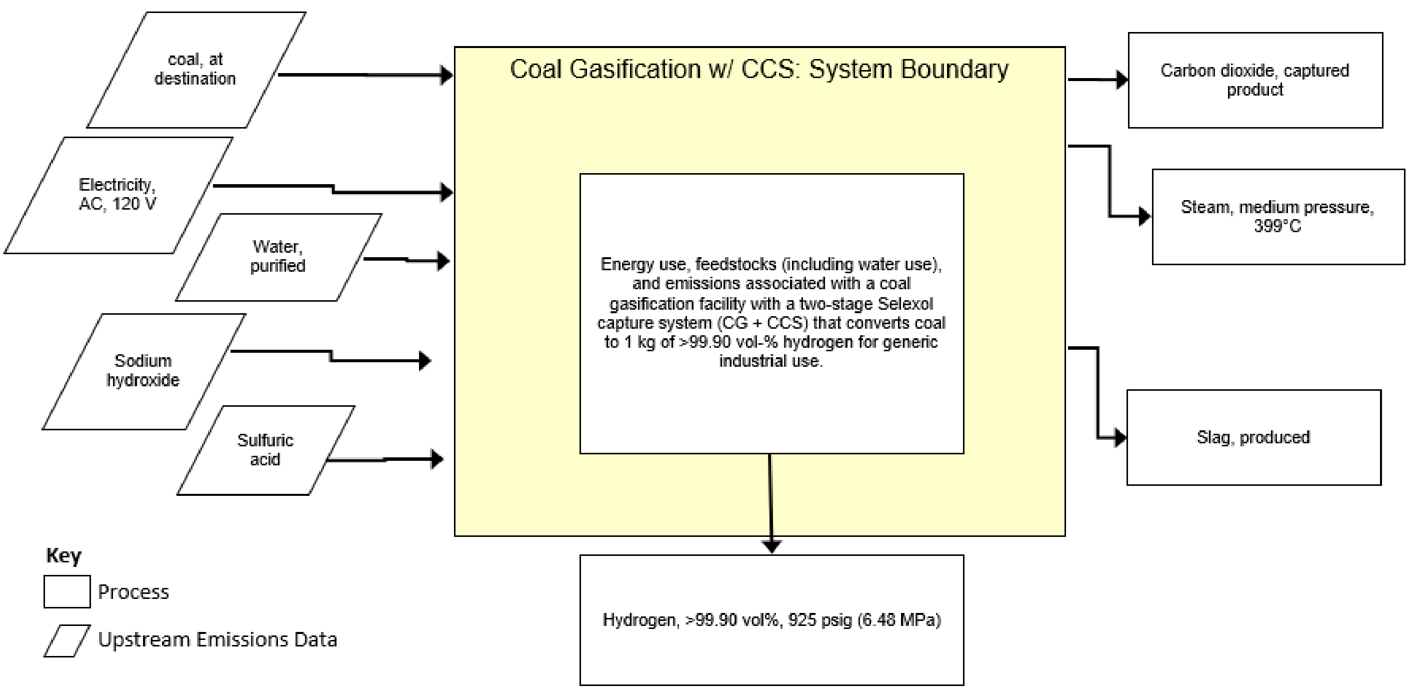

Table 1: Parameters

Parameter Name	Expected Value	Low	High	Units	Description
groundwater_pct	0.50	0	1	%	Percent of water supply sourced from groundwater. The sum of groundwater_pct and potw_pct must equal 1.
potw_pct	0.50	0	1	%	Percent of water supply sourced from publicly-owned treatment works. The sum of groundwater_pct and potw_pct must equal 1.
slag_credt_pct	1.00			%	[%] Percentage of slag produced that is credited as a coproduct. Customizable parameter for the user's specific system configuration. It should be set to one if and only if the plant designers have a confirmed use-case for all of its slag throughout the lifetime of the project.

Embedded Unit Processes

None.

References

Lewis et al. 2022

Lewis, E., McNaul, S., Jamieson, M., Henriksen, M. S., Matthews, H. S., Walsh, L., Grove, J., Shultz, T., Skone, T. J., and Stevens, R. 2022. Comparison Of Commercial, State-of-the-Art, Fossil-Based Hydrogen Production Technologies. DOE/NETL-2022/3241. U.S. Department of Energy, National Energy Technology Laboratory. April 12, 2022. Pittsburgh, PA.

Section III: Document Control Information

Date Created: October 28, 2021

Point of Contact: Timothy Skone (NETL), Timothy.Skone@netl.doe.gov

Revision History:

None.

How to Cite This Document: This document should be cited as:

NETL (2022). NETL Life Cycle Inventory Data – Unit Process: H2 from Coal Gasification with CCS. U.S. Department of Energy, National Energy Technology Laboratory. Last Updated: August 2022 (version 01). www.netl.doe.gov/LCA (http://www.netl.doe.gov/LCA)

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