NETL Life Cycle Inventory Data
Process Documentation File

Process Name: H2 from Coal gasification

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 representative coal gasification (CG) facility that processes and reacts coal to produce >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 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.

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_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 that are associated with a representative coal gasifier configured to primarily produce hydrogen. Coal gasification 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 particular configuration 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. The facility modeled 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 (CG). CG, and gasification in general, is a multistep process to convert solid fossil fuels to hydrogen. Like steam methane reforming (SMR), there are two key reactions and unit processes included in a conventional CG facility. Coal feedstock is reacted with oxygen in the gasifier to produce mostly hydrogen and carbon monoxide (syngas), and the syngas is later converted to additional hydrogen and carbon dioxide via the water-gas shift reaction. CG requires several units that aren't necessary in SMR facilities due to higher levels of particulates, sulfur, mercury, and other contaminants in coal. Particulate removal, a syngas scrubber, mercury control, a Claus plant, and slag handling are all necessary system components in a CG facility and included in the model which informed the data included in this technology profile.

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 that operate at 615 psia. The Shell gasifier was selected for modeling due to the flexibility it can offer for the feedstock used. While gasification itself doesn't produce much CO_2 (in fact, very little at all), the water gas shift reaction does, and it is required to maximize H_2 yield. Particulates are removed from the syngas using a cyclone separator. HCl that enters as a constituent of coal is removed using an ejector-type venturi scrubber, and the blowdown must be sent to a process water treatment system before it is reused. In the current configuration, mercury is removed using a conceptual design for a sulfur-impregnated, activated carbon bed adsorption system that must be replaced every 18 to 24 months. Lastly, a modified Claus process was included in the system modeled for the removal of sulfur compounds.

There are several byproducts of coal gasification 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.

Inputs and outputs have been scaled to a reference flow of 1 kg of gaseous hydrogen 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

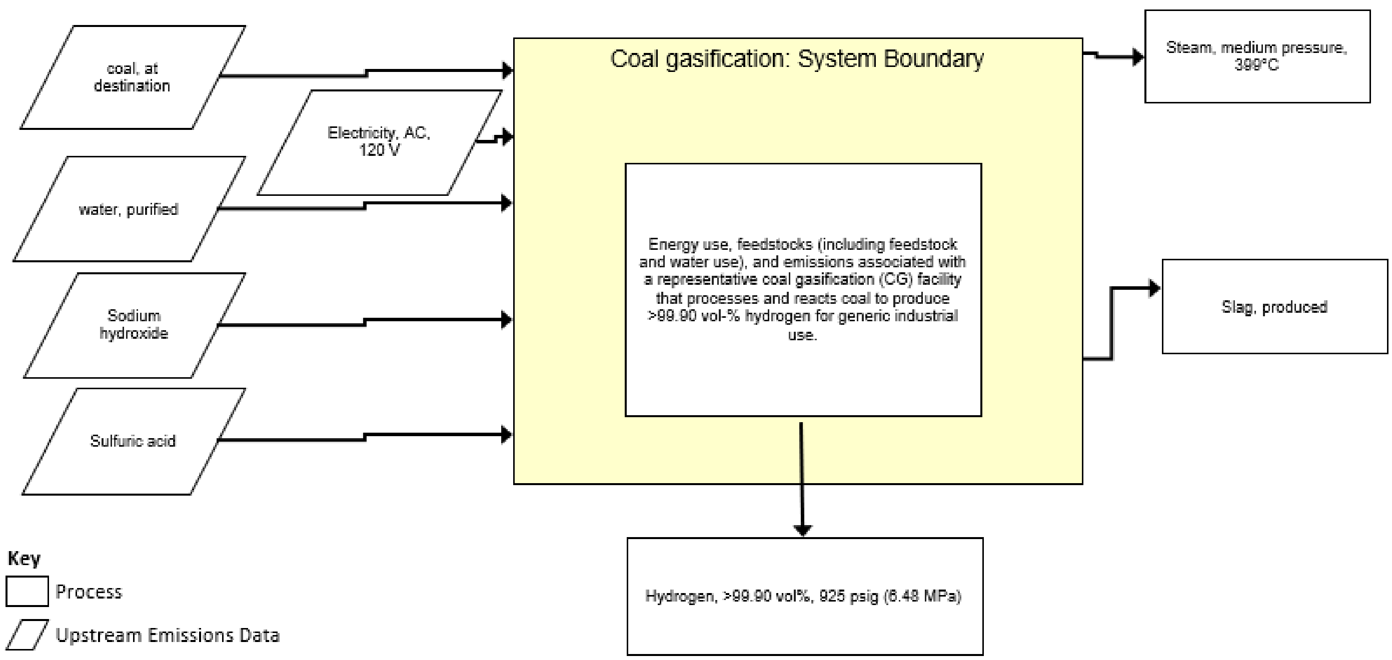

Table 1: Parameters

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_credit_pct	1.00	0	1	%	Percent 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 26, 2021

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None.

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Section IV: Disclaimer