NETL Life Cycle Inventory Data
Process Documentation File

Process Name: Autothermal Reforming with CCS

Reference Flow: 1 kg of Hydrogen, >99.90 vol%, 925 psig (6.48 MPa)

Brief Description: Energy use, feedstocks (including water use), and emissions associated with a representative autothermal reforming facility with carbon capture (ATR + CCS) that converts natural gas to 1 kg of >99.9 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.

Tracked Input Flows:

natural gas, delivered

[Technosphere] Amount of natural gas used as a feedstock for reforming process.

Electricity, AC, 120 V

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

Water, purified

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

Tracked Output Flows:

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

[Reference flow]

Carbon dioxide, captured product

[Technosphere] Mass flow rate of the captured carbon dioxide, 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_Autothermal Reforming_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 that are associated with autothermal reforming coupled with post-combustion carbon capture. Autothermal reforming is a variant of steam methane reforming that uses the exothermic partial oxidation reaction to supply the energy needed to drive the reforming reaction. This configuration includes a methyl diethanolamine (MDEA) system for pre-combustion CO_2 capture, which achieves an overall capture rate of 94.5% (defined as one minus the percentage of carbon in the stack relative to the total carbon). The reaction occurs in a refractory-lined vessel consisting of a partial oxidation section and a fixed bed catalytic reforming section. This configuration does not require supplemental natural gas for heating, and also does not generate excess steam or electricity. The reference flow of this unit process is: 1 kg of >99.9 vol-% hydrogen at 925 psia.

Boundary and Description

This unit process provides a summary of relevant input and output flows associated with autothermal reforming with CCS (ATR w/ CCS). ATR w/ CCS is a two-step process that converts methane or natural gas to concentrated hydrogen using a ratio of oxygen and steam. Natural gas feedstock is first supplied to the autothermal reformer (ATR), where both the oxidation and reformation of methane occurs. The difference between ATR and steam methane reforming (SMR) is that ATR combines partial oxidation of methane with reformation of methane in a way that eliminates the need for an external heat source. Like with SMR, the syngas produced by the ATR reaction is then fed to a water-gas shift reformer, where steam further reacts with carbon monoxide to produce additional hydrogen and carbon dioxide. ATR w/ CCS includes only pre-combustion carbon capture, which removes 94.5% of the carbon dioxide generated by the system, in this configuration. The system boundaries also include CO_2 compression and drying, where captured CO_2 is treated to meet pipeline export specifications. No excess steam or electricity is produced by the system.

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 is a refractory-lined vessel with a partial oxidation section and a fixed bed catalytic reforming section that is configured to produce 27,500 kg/hr, or 274 MMSCFD, of >99.90 vol-% hydrogen suitable for generic industrial use. A refrigerated methyl diethanolamine (MDEA) system was used to model pre-combustion CO_2 capture from the shifted synthesis gas stream. Secondary post-combustion capture of CO_2 is not needed for ATR. Data on CO_2 compression is based on model characteristics of an eight-stage front-loaded integrally geared centrifugal compressor.

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

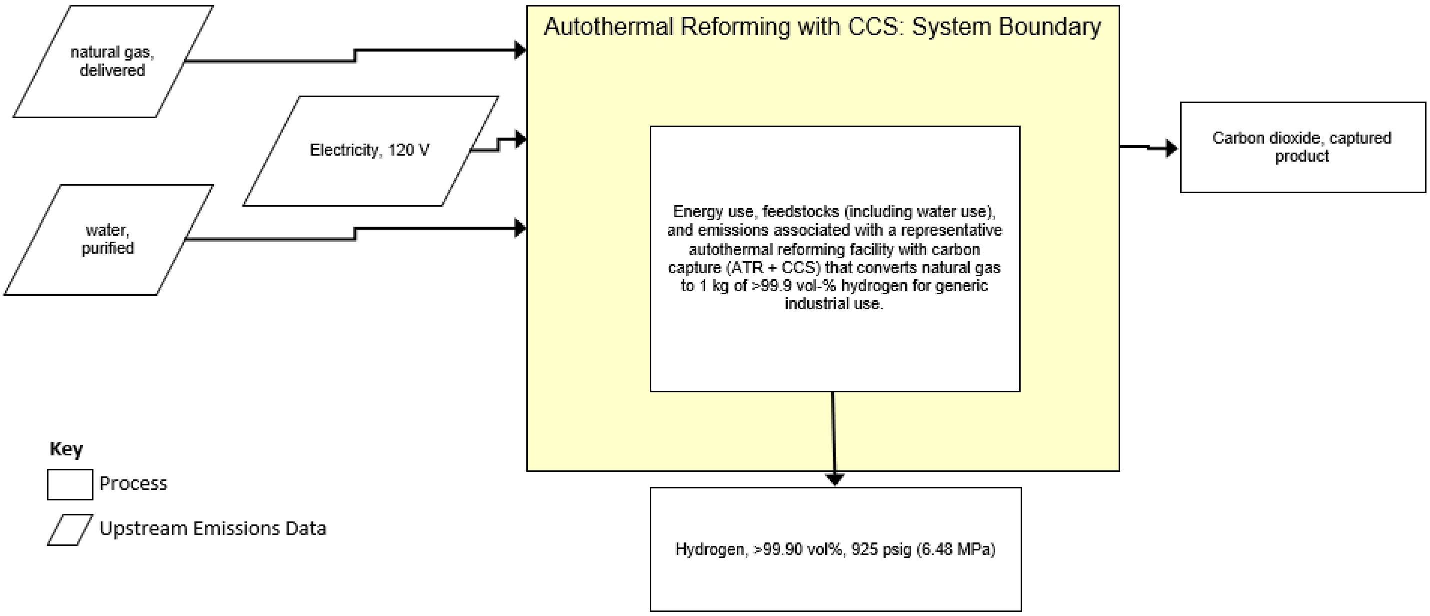

Table 1: Parameters

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.

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 29, 2021

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Revision History:

None.

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

NETL (2022). NETL Life Cycle Inventory Data – Unit Process: Autothermal Reforming 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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