

Hydrogen technologies — Methodology for determining the greenhouse gas emissions associated with the production, conditioning and transport of hydrogen to consumption gate

Annex G

Hydrogen Production Pathway – Auto Thermal Reforming (with Carbon Capture and Storage - CCS)

© ISO 2023

All rights reserved. Unless otherwise specified, or required in the context of its implementation, no part of this publication may be reproduced or utilized otherwise in any form or by any means, electronic or mechanical, including photocopying, or posting on the internet or an intranet, without prior written permission. Permission can be requested from either ISO at the address below or ISO's member body in the country of the requester.

ISO copyright office
CP 401 • Ch. de Blandonnet 8
CH-1214 Vernier, Geneva
Phone: +41 22 749 01 11
Email: copyright@iso.org
Website: www.iso.org

Published in Switzerland

Contents

Annex G (informative) Hydrogen Production Pathway – Auto Thermal Reforming (with Carbon Capture and Storage - CCS)1

G.1 Process description and overview.....1

G.1.1 Description.....1

G.1.2 Overview2

G.2 Emission sources and inventory2

G.2.1 Emission sources2

G.2.2 Inventory in case of Attributional Approach3

G.2.3 Inventory in case of Consequential Approach.....4

G.3 Emission Allocation.....4

G.3.1 Allocation in case of Attributional Approach4

G.3.2 Allocation in case of Consequential Approach.....5

G.4 Information to be reported6

Annex G (informative)

Hydrogen Production Pathway – Auto Thermal Reforming (with Carbon Capture and Storage - CCS)

G.1 Process description and overview

Sections G.1.1 and G.1.2 provide a description and an overview for hydrogen produced from steam methane reforming with carbon capture and storage.

G.1.1 Description

An auto-thermal reformer is typically considered 'self-heating' as it includes the exothermic oxidation of methane which provides enough heat to support the concurrent endothermic reforming reaction.

In Auto Thermal Reforming (ATR), methane is first partially oxidized to produce hydrogen and carbon monoxide. Contrary to the steam methane reformer, the auto thermal reactor does not require any heat from an external source (although other external heating operations may still be required, such as pre-heaters). The partial oxidation reaction is exothermic and provides the required heat to the concurrent steam reforming reaction, taking place in the auto thermal reactor, in which methane and steam reacts to produce carbon monoxide and hydrogen in the reformer fixed catalyst bed. The syngas stream is then fed to the water-gas shift reactor(s) to further convert the carbon monoxide and excess steam into hydrogen and CO₂.

Oxygen required for the partial oxidation reaction is separated from air in an air separation unit (ASU). The partial oxidation reaction occurs in the top section of the auto thermal reformer. The top section is fitted with a burner where methane and oxygen are mixed in a diffusion flame.

In practice, there are a number of configurations in which ATRs can be deployed, including in combinations with other reformers. These arrangements can help to optimize hydrogen yields while minimizing flue gas heat losses. Possible configurations include: using a fired tubular reformer in series with a heat exchange steam reformer (HSER), working as a gas-heated pre-reformer; using an HSER in series with an ATR to form a two-staged configuration; or deploying an ATR followed by a gas heated reformer, where the counter-current heat exchange with a product syngas from the ATR provides the heat for the endothermic reforming reaction.

Whereas steam methane reforming typically requires post-combustion CO₂ capture, in ATR CO₂ capture can typically be achieved entirely through process CO₂ capture from the hydrogen product stream. This may be conducted before or after the hydrogen purification step, using chemical solvent absorption or membrane and cryogenic separation. The CO₂ can then be compressed and dehydrated for export.

Depending on the available data of the natural gas used, the emission factor of the used gas (as energy or feedstock) (kgCO₂e/MWh_{LHV}) can be taken from (i) a well-documented emission factor of the gas purchased or if not available (ii) calculated by developing the upstream system as described in 4.3.2.4.3.

Autothermal reforming system

An ATR production plant is typically composed of the following subprocesses:

- A gas pretreatment / Sulfur removal unit

- An autothermal reformer (optionally a pre reformer if the feed contains higher hydrocarbons) where the feedstock is reformed in Syngas composed of Hydrogen and CO. The main chemical reaction is $\text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2$
- A Water Gas Shift where the CO in the Syngas is “Shifted” to CO_2 and H_2 through the following chemical reaction: $\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$
- A Pressure Swing Adsorption unit (PSA) to purify the hydrogen
- A Carbon Capture Unit

For the ATR system, the co-products are carbon dioxide and, steam. Steam can be used to produce electricity, if there is associated power generation, e.g. combined heat-power or cogeneration applications, or to provide heat for any application.

G.1.2 Overview

An example of a process diagram for hydrogen produced from auto thermal reforming with carbon capture and storage is presented in Figure G.1 —.

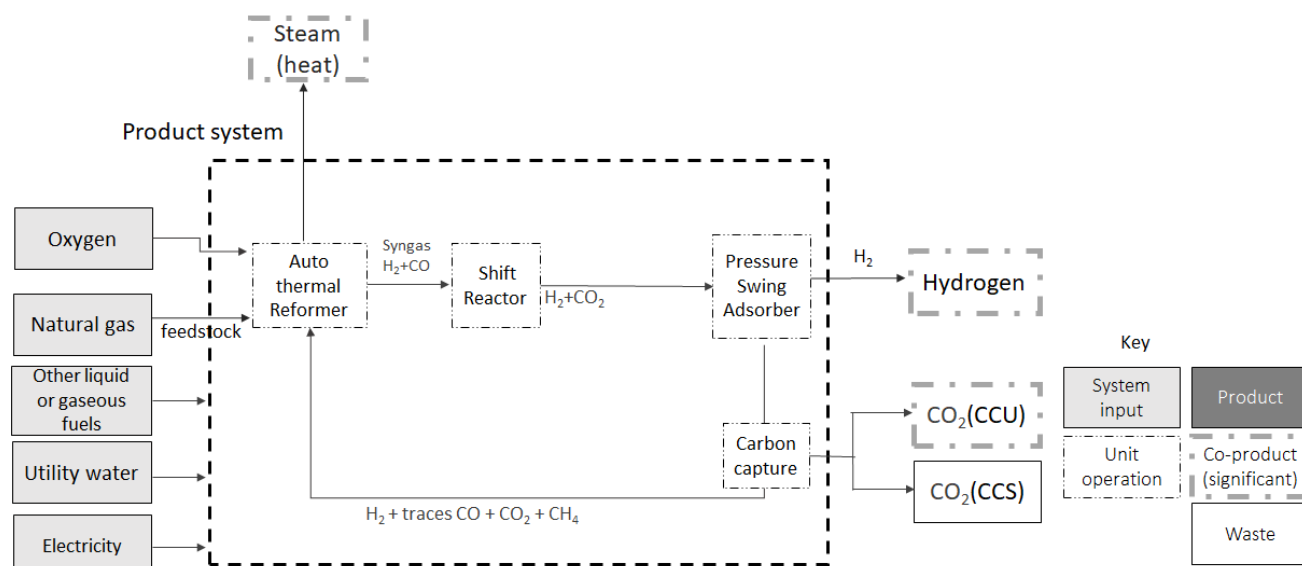


Figure G.1 — Example of process diagram for hydrogen produced from ATR/CCS

G.2 Emission sources and inventory

Sections G.2.1, G.2.2 and G.2.3 provide information on emission sources and inventory for hydrogen produced from auto thermal reforming.

G.2.1 Emission sources

For auto-thermal reforming with CCS, the main source of GHG emissions include GHG leakages, separation and capture of CO_2 , CO_2 compression and transport for CCS.

Each process unit or stage in the ATR process contains unique emissions sources as outlined in Table G.1.

Table G.1 — Key life cycle GHG emission sources in hydrogen production by ATR

Process unit/stage	Key emissions sources	Other emissions sources
Natural gas recovery	<ul style="list-style-type: none"> Electricity and/or fuel combustion for natural gas extraction and transport to a processing plant Fugitive methane and/or carbon dioxide from natural gas extraction and transport 	- Flaring and venting
Natural gas processing	<ul style="list-style-type: none"> Electricity and/or fuel combustion for separating heavier components of recovered gas (e.g., natural gas liquid) or acid gases (e.g., CO₂) from pipeline-quality natural gas Fugitive methane and/or carbon dioxide from natural gas processing 	
Gas transport	<ul style="list-style-type: none"> Electricity and/or fuel combustion for gas transport Fugitive methane emissions 	
Heat recovery and electricity generation	<ul style="list-style-type: none"> No significant emissions other than those covered under common emissions sources 	
Auxiliary Heating Processes	<ul style="list-style-type: none"> Electricity and/or fuel combustion to provide auxiliary heat, e.g. in pre-heaters 	
Air separation	<ul style="list-style-type: none"> Electricity and/or fuel combustion to separate oxygen from air to feed reformer 	
CO ₂ and hydrogen purification	<ul style="list-style-type: none"> Electricity and/or heat for operation of the relevant purification units 	Exhaust CO ₂ due to sulphur removal of exhaust gases (where applicable)
Hydrogen enrichment	<ul style="list-style-type: none"> Electricity and/or heat to supply water gas shift reactions occurring as part of hydrogen enrichment (if required) 	
CO ₂ capture and separation	<ul style="list-style-type: none"> Electricity and/or heat for relevant separation units Residual CO₂ which is not captured for permanent storage 	
Compression and transport of CO ₂	<ul style="list-style-type: none"> Electricity for compression of CO₂ Electricity and/or fuel combustion for pipeline transport Fuel combustion for motive transport Fugitive carbon dioxide emissions 	
Storage of CO ₂	<ul style="list-style-type: none"> Electricity/fuel use for compression and injection 	Fugitive CO ₂ from permanent storage location ¹
Hydrogen compression and storage	<ul style="list-style-type: none"> Electricity for compression and storage maintenance 	
Disposal of waste products (where not valorized)	<ul style="list-style-type: none"> Electricity and fuel combustion for transport of waste products 	

G.2.2 Inventory in case of Attributional Approach

The emission inventory is performed across the life cycle stages from cradle to gate.

¹ These are not accounted for as part of the standard emissions calculation.

Upstream / Indirect emissions:

Upstream indirect GHG emissions are evaluated based on relevant data available for the Natural Gas (and/or other Feed Gas / Fuel Gas) and electricity supplied in the considered geography.

They are taken into account from the well to the inlet meter of the production plant and are evaluated based on relevant data available for the Natural Gas (and/or other Feed Gas / Fuel Gas) supplied in the considered geography.

Direct emissions at production:

The quantity of CO₂ released into the atmosphere during the production lifecycle stage is determined by the carbon balance within the boundaries of the plant. The total carbon input is determined from the quantity and characteristic of the feedstock. It corresponds to the total carbon output which is the sum of the carbon in the CO₂ emitted + the carbon in the CO₂ non-emitted (used or stored) + other possible carbon containing species, such as CH₄, VOC, etc.

Note: in case of SMR, other possible carbon containing species in the emissions may be considered as negligible.

Emissions from capital goods:

As per Article 4.2.1 the quantification of CAPEX emissions shall be provided for information.

G.2.3 Inventory in case of Consequential Approach

In case of a consequential approach, the inventory may be performed across life cycle stages extending beyond the production unit. The goal of the LCA should define the boundaries to take into account for consideration of the consequential emissions.

For instance the goal of the LCA may include:

- the emissions occurring during the usage phase of hydrogen coproducts such as CO or CO₂
- the emissions resulting from other means to produce the co-products (substitution methods)

G.3 Emission Allocation

Several co-products may exist for an ATR/CCS system. In addition to hydrogen, steam, and CO₂ are introduced as examples, but exact coproducts depend on specific designs.

G.3.1 Allocation in case of Attributional Approach

As described at para 4.3.2.8, the first step for the emission allocation is to subdivide the process.

- 1st Step: Process subdivision:

The process is subdivided in 2 parts:

The Unit process is subdivided into 3 sub processes:

- Sub process 1 - The Auto Thermal Reformer reactor. This sub process has Natural Gas or other Hydrocarbon as inputs, Syngas and Steam as co products. The Syngas is mainly composed of Hydrogen, CO, some traces of CO₂ and other impurities such as N₂ and unreacted methane.
- Sub process 2 - Water Gas Shift: This sub process has Syngas as input and Hydrogen as output. In case of CCUS, it also has CO₂ as a coproduct (CCU) or waste (CCS)

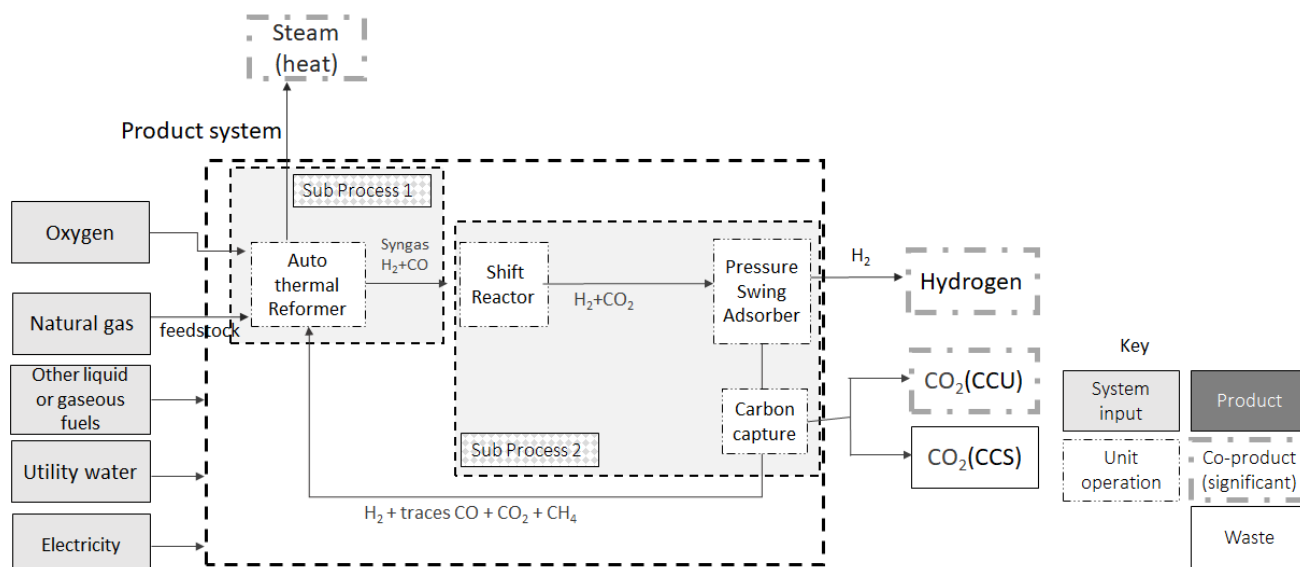


Figure G.2 — Example of ATR plant block diagram – Subdivision in sub processes

- **2nd Step: Allocations:**

Sub Process 1 – ATR Reactor:

The Feed (Natural Gas or other Hydrocarbon) is allocated to Syngas and Steam *prorata* their energy content (LHV² or, in case of the steam, the enthalpy difference between steam and the steam condensate). The steam Partial Carbon footprint results from the allocation of the combustion emissions of the NG allocated to it.

The Syngas is fully allocated to the sub processes 2 Water Gas Shift.

Sub Process 2 – Water Gas Shift

The emissions from Sub Process 2 are determined as described at para F3, and allocated to Hydrogen from WGS.

G.3.2 Allocation in case of Consequential Approach

In case of a consequential approach, the goal of the LCA should define the boundaries to take into account for consideration of the consequential emissions.

Under a consequential approach, the allocation of emission to coproducts may be avoided by applying substitution / system expansion with displacement as provided for at article 4.3.2.8.

² LHV is more commonly used over HHV in situations where water vapour can't be recovered.

G.4 Information to be reported

Table G.2 — presents the information to be reported for hydrogen produced from autothermal reforming with carbon capture and storage.

Table G.2 — Information to be reported for hydrogen production by ATR

Category	Matters to be identified
Facility details	<ul style="list-style-type: none"> • Facility identity • Facility location • Facility capacity [Nm³/h, t/h] • Capacity Factor [%] • Commencement of facility operation • Main climatic and meteorological data (Atmospheric pressure, average ambient temperature, average relative humidity)
Product specification	<ul style="list-style-type: none"> • Production pathway • Hydrogen produced (kg) • Hydrogen temperature and pressure at the gate • Hydrogen purity level at the gate • Specification of contaminants
GHG emissions overview	<ul style="list-style-type: none"> • Emissions intensity of hydrogen batch [kgCO₂e/kgH₂] •
Batch details	<ul style="list-style-type: none"> • Beginning and end of batch dates • Batch quantity
Electricity	<p>Location-based emissions accounting:</p> <ul style="list-style-type: none"> • Quantity of purchased grid electricity [kWh] • Location based emission factor used [gCO₂e/kWh] <p>Market-based emissions accounting</p> <ul style="list-style-type: none"> • Quantity of purchased grid electricity [kWh] • Quantity of contracted electricity [kWh] and quantity of associated GOs or RECs • Type of GOs or RECs • Residual electricity • Residual mix emission factor [gCO₂e/kWh] <p>On-site electricity generation</p> <ul style="list-style-type: none"> • Quantity of on-site generation [kWh] • Emission factor for on-site generation (as applicable) [gCO₂e/kWh]
Other utilities	<ul style="list-style-type: none"> • Source/s of water • Source/s of steam • Quantity of purchased water [kg] • Quantity of purchased steam [kg] • Embodied emission factor for water [kgCO₂e/kg] • Embodied emission factor for steam [kgCO₂e/kg]
Fuel feedstock	<ul style="list-style-type: none"> • Types of fuels combusted • Quantities of fuel combusted [L, kg] • Relevant emissions calculation or factors used to attribute emissions to fuel combusted [kgCO₂e/appropriate unit of fuel] • Emissions intensity of fuel used, including all emissions associated with fuel extraction, transporting to a processing plant, and processing [e.g. kgCO₂e/MJ] • Credits claimed to evaluate emissions of fuel reformed
Process	<ul style="list-style-type: none"> • Air separation technology and capacity • ATR reactor type and capacity • Syngas purification technology and capacity • Sulphur waste gas processing technology (if applicable) and capacity • Quantity and type of vented GHG gases [kg]

	<ul style="list-style-type: none"> • Quantity and type of flared GHG gases [kg] • Technology for monitoring fugitives from CO₂ storage and capacity • CO₂ capture rate of the unit [%] • CO₂ capture technology
Air separation	<ul style="list-style-type: none"> • Electricity/fuel consumption [MJ, MWh]
Cooling	<ul style="list-style-type: none"> • Electricity consumption [MJ, MWh]
Compression of gases throughout the facility	<ul style="list-style-type: none"> • Electricity consumption [MJ, MWh]
Natural Gas feedstock	<ul style="list-style-type: none"> • Type of NG • NG composition • Quantity of NG used for ATR reactions [kg] • Quantity of NG used for heating [kg] • Quantity of NG used for producing steam [kg] • Embodied emission factor for NG [kgCO_{2e}/kg] (derived from primary and secondary data, provided by supplier or sourced from relevant source i.e. NGA Factors)
Carbon dioxide treatment	<ul style="list-style-type: none"> • Type of CO₂ storage and capacity • Location of CO₂ storage • Transport type of CO₂ to storage location (if applicable) and distance (in km) • Quantity of CO₂ captured [kg] • Quantity of CO₂ stored [kg] • Quantity of fugitive emissions created during injection of CO₂ into the storage location [kg] • Quantity of fugitive CO₂ emissions from storage [kg] (in line with period covered by the reporting)
Waste and other Co-products	<ul style="list-style-type: none"> • Quantity of steam produced [kg] • Quantity of steam sold [kg] • Emissions allocated to steam [kgCO_{2e}/kg] • Quantity of electricity sold (MWh) • Emissions allocated to electricity sold [gCO_{2e}/kWh]