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

Annex E

Hydrogen Production Pathway – Coal Gasification (With Carbon Capture and Storage - CCS)

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Annex E
(informative)

Hydrogen Production Pathway – Coal Gasification (With Carbon Capture and Storage - CCS)

E.1 Process description and overview

Sections E.1.1 and E.1.2 provide a description and an overview for hydrogen produced from coal gasification with carbon capture and storage.

E.1.1 Description

Coal is removed from coal seams using either open-pit or underground mining depending upon the depth of the coal seam. These operations consume electricity for conveying to and from storage areas and through the crushing and washing facilities.

The coal is transported to a processing facility via ships, trucks and trains. Loading and unloading steps typically employ electricity driven stackers/reclaimers and associated conveyors. Transport vessels use diesel, fuel oil or electricity for motive power.

To produce hydrogen gas, coal is mixed with oxygen and steam in a reactor (a gasifier). The basic gasification reaction is:

$$C\ (carbon, \text{in}\ coal) + H_2O\ (\text{ste}am) + heat \rightarrow CO\ (carbon\ monoxide) + H_2\ (hydrogen) \quad \text{(E1)}$$

The reaction takes place at high temperatures and some of the coal is oxidised by the oxygen to produce the energy needed to drive the reaction:

$$C + O_2\ (oxygen) \rightarrow CO_2\ (carbon\ dioxide) + heat \quad \text{(E2)}$$

The oxygen used in the gasifier is generated in an air separation unit. Oxygen is used in preference to air, to prevent nitrogen diluting and contaminating the hydrogen. Air separation technologies include cryogenic distillation, pressure-swing adsorption, and membrane separation. All consume large quantities of electricity. In addition to oxygen and nitrogen, crude argon may also be produced in smaller quantities (argon constitutes about 0.93% of air)[i]. Pending the scale and valorisation of these outputs, they may be considered as co-products and allocated emissions.

A gasifier is a high temperature reactor where coal undergoes partial oxidation and reaction with steam. There are three main types of gasifiers that can be used to create syngas, each varying in the method it uses to generate heat, to contact the reactants and the physical state of the residue it produces. These are fixed bed (e.g. Sasol-Lurgi gasifiers), fluidised bed (e.g. Winkler gasifiers) and entrained flow (e.g. Koppers-Totzek gasifiers)[ii,iii] . These different gasifiers have their advantages and disadvantages but at a macro level perform the same function. They have common inputs (coal, oxygen and water) but can produce syngas with varied properties, also subject to the properties of the coal, which will impact the configuration of downstream processing activities.

This unit also produces ash and/or slag as waste products.

Waste heat recovery units are typical for coal gasification processes, reflecting the high temperature operation of coal gasification processes and the requirement for cooling of syngas products for subsequent processing. Regulation of the gasifier temperature is managed through a heat exchanger which can be used to raise steam and generate electricity. Steam may be supplied elsewhere in the plant (i.e. steam use in regeneration of acid gas removal (AGR) absorption systems) or exported out of the product system boundary. Electricity may be generated from this steam and used elsewhere in the plant such as to drive the air separation process, or exported beyond the product system boundary.

Any exported steam and/or electricity is considered a co-product and should be allocated a share of emissions.

Syngas conditioning

The output of the gasifier is a stream of raw syngas, which may contain a number of contaminants, including particulate matter and heavy metals. In addition, this stream contains significant CO gas. To maximise the quantity of hydrogen produced, syngas from the gasifier is sent through to another reactor where the carbon monoxide is reacted with water to yield additional hydrogen. This is known as the water-gas shift (WGS) reaction, as follows: $CO+H_2O \rightarrow CO_2+ H_2+heat$. This is a reversible reaction, with an equilibrium established between CO and CO_2, subject to the reaction conditions. Low temperatures favour the formation of CO_2. As the conversion of CO to CO_2 generates heat, there are often several water gas shift reactors in series with coolers between them (including high temperature and low temperature stages). Typically, iron-chromium and copper-zinc catalysts are used to facilitate the reaction at high and low temperatures, respectively (Pal, Chand, Upadhyay, & Mishra, 2018). High temperature WGS may include conversion of sulphur compounds to hydrogen sulphide (H_2S), for removal in the acid gas removal (AGR) stage.

The syngas now includes large quantities of CO_2 in addition to other impurities including sulphur compounds (such as H_2S) and heavy metals (such as mercury). These components must be removed from the syngas. Particulate matter can be removed using a water scrubber. Mercury and other heavy metals can be removed by via adsorption, particularly using activated carbon beds. Drying (water removal) is also required (Higman, 2008). Sulphur compounds may be removed using lime. CO_2 and sulphur compounds can also be removed together. The capture of CO_2 and removal of these sulphur compounds simultaneously is discussed below.

Whilst configurations for syngas conditioning vary, the key inputs and outputs (electricity, heat) are largely common.

Hydrogen compression and buffer storage

Common to hydrogen produced via coal gasification, electrolysis, and any other means is the requirement for compression of the dry, high purity hydrogen product. This is particularly important given the low density of hydrogen gas. Subject to the nature of downstream hydrogen storage, transport and use, there will be different requirements for hydrogen compression. Common to the coal gasification, electrolysis and steam methane reforming pathways, there are four main approaches to hydrogen storage: compressed gaseous hydrogen, liquid hydrogen and materials-based storage technologies (either physical or chemical).

With regards to hydrogen compression and storage, it is important to be clear about the boundary for certification. Where storage is required for the delivery of the functional unit (i.e. hydrogen under the specific boundary conditions) this must be included within the system boundary. However, where the hydrogen is processed (for storage or otherwise) in such a way as to provide additional functionality (e.g. the liquefaction of hydrogen for delivery to customer to meet their preferences) this should be treated using a module (or annex, yet to be developed) covering hydrogen energy carriers. Different forms of storage are briefly described below but their inclusion within the defined system boundary is subject to the considerations noted above.

Compression refers to the storage of hydrogen in its gaseous form at higher pressures. This includes pressurisation of hydrogen within steel cylinders but also includes large-scale and longer-term storage in locations such as salt caverns and depleted gas fields, and the storage of hydrogen in existing natural gas pipelines (line packing) (Makridis, 2016).

E.1.2 Overview

An example of a process diagram for a coal gasification upstream system is presented in Figure E.1 —. Likewise, an example of a process diagram for hydrogen production from coal gasification with carbon capture is presented in Figure E.2 —

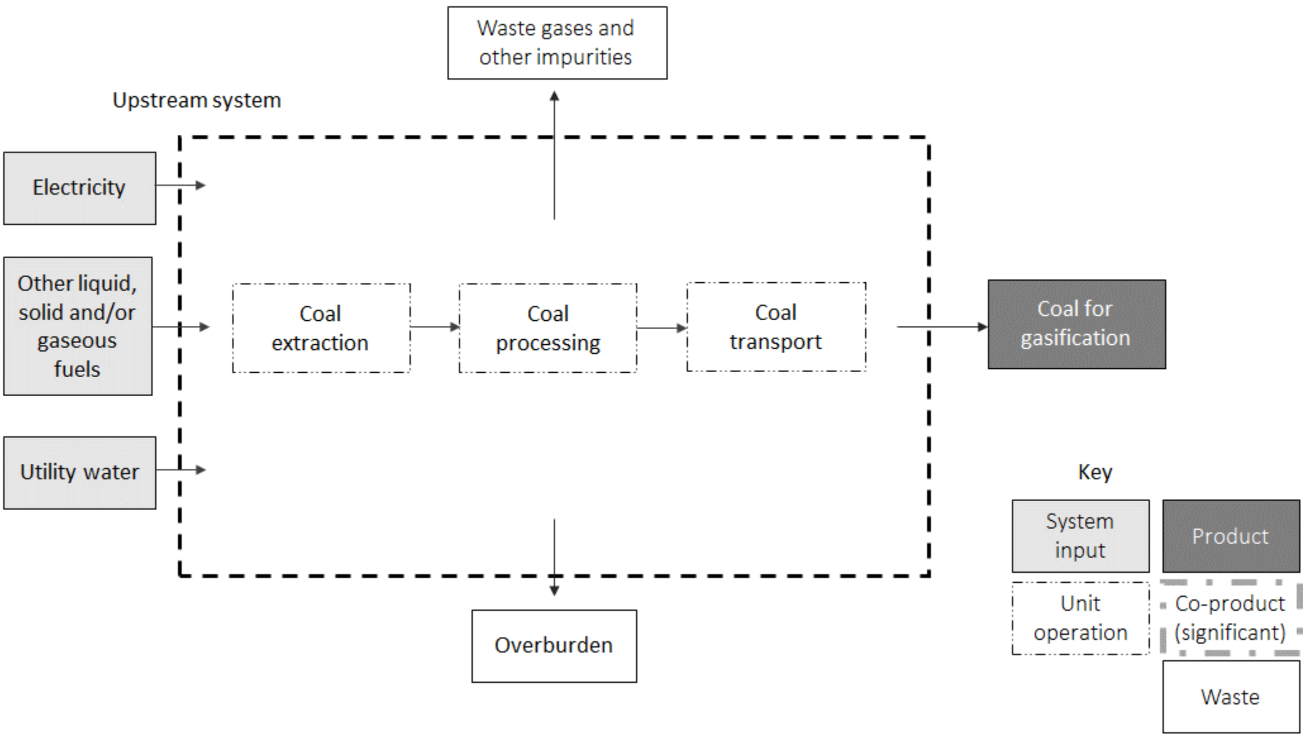

Figure E.1 — An example of coal gasification upstream system

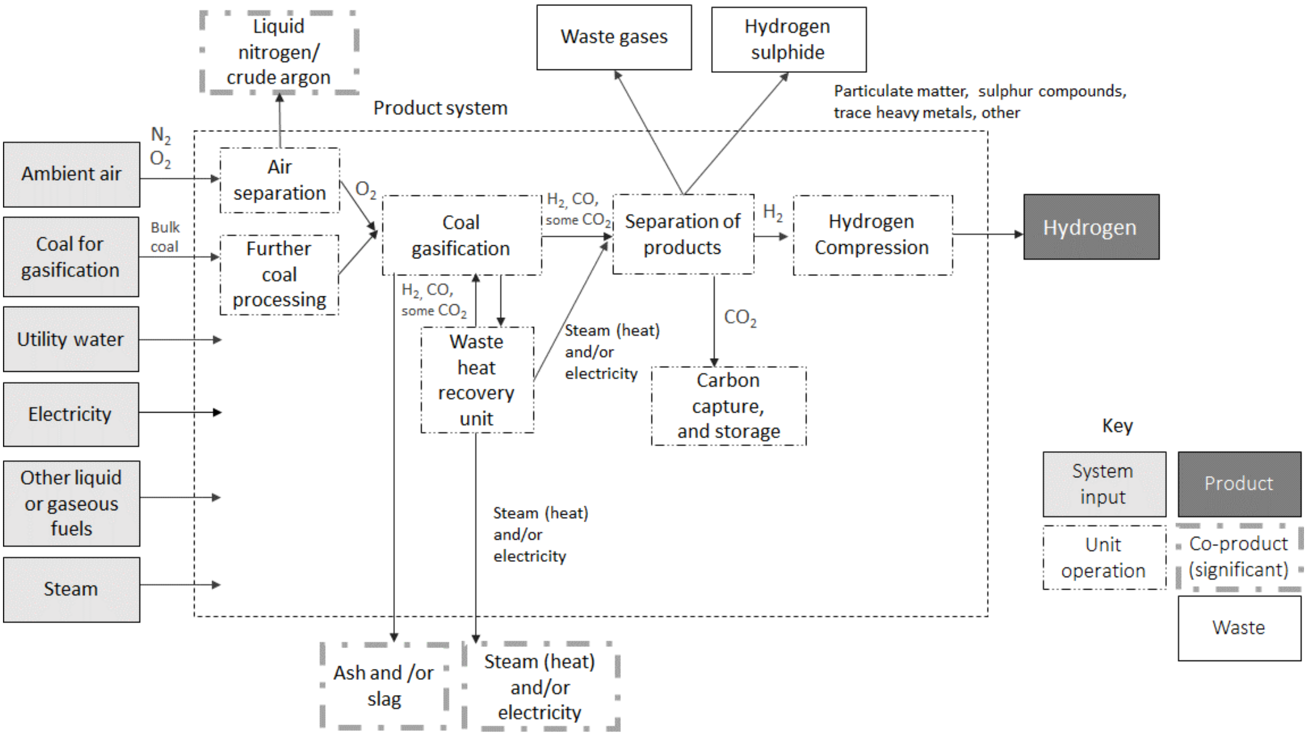

Figure E.2 — An example of hydrogen production from coal gasification system with carbon capture

E.2 Emission sources and inventory

For coal gasification with CCS, the main source of GHG emissions is the conversion of carbon in coal to CO_2. Other significant emissions sources include the emissions of grid electricity used for air separation (including air compression and oxygen compression), CO_2 removal, CO_2 compression for CCS, coal processing (size reduction and cleaning) activities and fugitive methane emissions associated with coal mining.

Each process unit or stage in the coal gasification process contains unique emissions sources as outlined in Table E.1 – GHG emissions summary for coal gasification /CCS.

Table E.1 – GHG emissions summary for coal gasification /CCS

Process unit/stage	Key emissions sources	Other emissions sources
Coal mining and processing	• Electricity and/or liquid fuel combustion for materials extraction and movement • Fugitive methane and/or carbon dioxide from coal extraction	Explosives for coal extraction
Primary coal processing	• Electricity for loading and unloading of coal • Electricity for coal size reduction, washing and separation	Chemical usage for coal processing
Coal transport	• Electricity and/or liquid fuel combustion for materials movement	
Further coal processing	• Electricity for additional size reduction	Electricity and/or liquid fuel combustion for materials movement
Air separation	• Electricity for air compression	
Gasification	• Combustion of coal within the gasifier • Gasification of coal within the gasifier • Steam for gasification (if purchased from third party rather than self-generated)	
Heat recovery and electricity generation	• No significant emissions other than those covered under common emissions sources	
Hydrogen enrichment	• Water gas shift reactions occurring as part of hydrogen enrichment	
Syngas purification	• Electricity and/or heat for operation of the relevant purification units	Exhaust carbon dioxide due to sulphur removal
CO_2 capture and separation	• Electricity and/or heat for relevant separation units	
Compression and transport of CO_2	• Electricity for compression of CO_2 • Electricity and/or gaseous fuel combustion for pipeline transport • Liquid and/or gaseous fuel combustion for motive transport	

	• Fugitive carbon dioxide from CO_2 transport	
Storage of CO_2	• Electricity for injection or transformation	Fugitive carbon dioxide from permanent storage location
Hydrogen compression and storage (if in the production boundary)	• Electricity for compression and storage maintenance	

E.3 Emission Allocation

The coal gasification production pathway has been divided into distinct modules to facilitate application of emissions accounting analysis through system expansion. For coal gasification, analysis is performed across three distinct modules, as presented in Figure E.3 —:

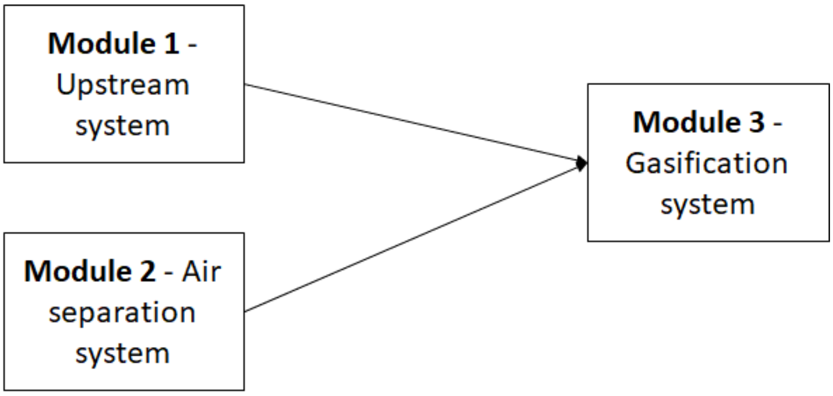

Figure E.3 — coal gasification production pathway

Module 1 (Upstream system) – covers upstream activities associated with the extraction, processing and delivery of the coal feedstock (Figure E.1). This system is taken out of the process as a separate module to allow treatment of this system in different ways (i.e. collection of primary and secondary data[1] to derive a local or regional emission factor, or use of an indirect emission factor that should at a minimum be country specific[2]). As this system has a single product, no emissions allocation approaches are required and all emissions are attributed to a single output, coal for gasification. That is, all emissions associated with this system are allocated to the intermediate product: coal. These emissions are carried with the coal (as upstream emissions) into the gasification system (module 3). Where applicable assessment of module 1 may be by-passed via use of an appropriate indirect emissions factor covering coal supply.

Module 2 (Air separation system, example in Figure E.4 —) – covers the supply of oxygen for the coal gasification process. For module 2, there are two potential co-products (nitrogen and crude argon) associated with the system in addition to the intermediate product: oxygen[3]. This system has been scoped

1 As per the GHG Protocol Standard "primary data are data collected from specific processes in the studied product's life cycle" and "secondary data are defined as data that are not from specific processes in the studied product's life cycle"

2 Note this treatment is likely dependent on the availability of data. For an integrated system where the hydrogen producer extracts and processes coal, it is reasonable that they might wish to collect primary and secondary data to assess the upstream emissions and derive an upstream emission factor for their coal. However, if the coal is simply bought from a supplier this supplier may provide an upstream emission factor for this coal or in some cases a default upstream emission factor for coal may be identified in appropriate life cycle databases.

3 Some waste heat may also be produced as the electricity is consumed.

out for allocation as, unlike the remainder of the gasification system (module 3), it cannot be resolved using methods to avoid allocation[4].

The nitrogen stream will be significant given its abundance relative to oxygen in air and the oxygen demands of an industrial gasifier. The argon stream will be much smaller, reflecting the low argon concentration in air (approximately 0.93%). One or more of these co-products may be captured and sold noting that they have a variety of common uses. Where these co-products are valorised they may be allocated some share of emissions. The priority approach is to allocate on the basis of physical relationships. Databases of Life Cycle Inventories of Chemicals outline approaches for allocation of emissions across the three products on the basis of the heat of vaporisation and heat capacity of the three products assuming that the thermodynamic efficiency of the cooling and liquefaction process is the same for all three gases (Althaus, 2007). This results in an allocation factors of 22.2% for oxygen, 76.9% for nitrogen and 0.9% for crude argon.

Emissions associated with the intermediate oxygen product can be estimated as follows:

$$E_{liquid\ oxygen} = E_{air\ separation} - E_{liquid\ nitrogen} - E_{liquid\ crude\ argon} \quad (E3)$$

where

$E_{liquid\ oxygen}$	is the emissions associated with liquid oxygen
$E_{air\ separation}$	is the total emissions associated with the air separation module (as calculated in line with the guidance provided for module emissions inventories)
$E_{liquid\ nitrogen}$ and $E_{liquid\ crude\ argon}$	are the emissions associated with the co-products as calculated using the allocation factors referred to above

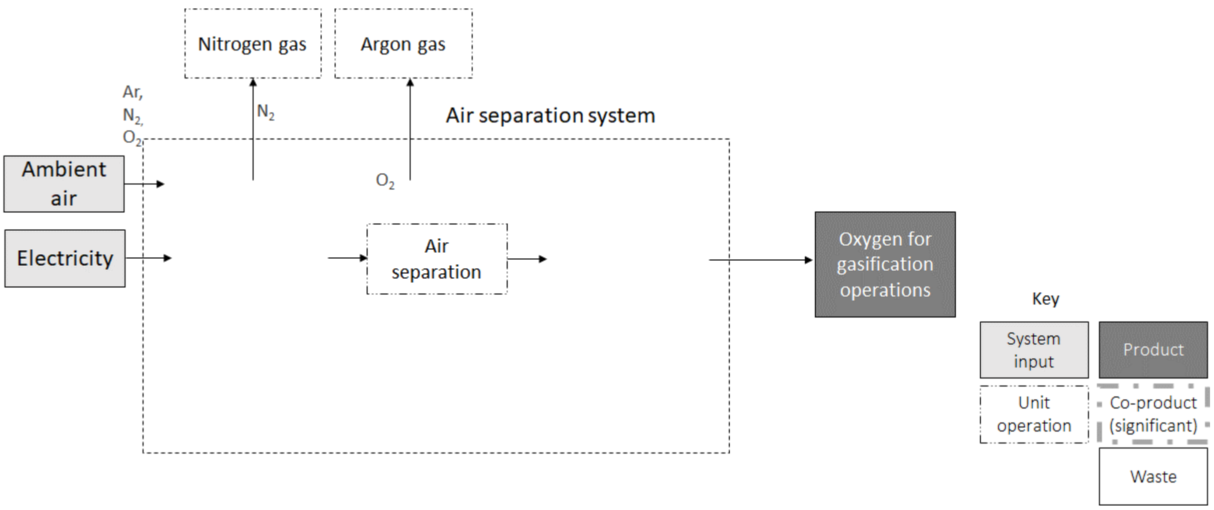

Figure E.4 — An example of air separation system

Module 3 (Gasification system) – covers all remaining processes including further coal processing, gasification, syngas conditioning and waste heat recovery. See Figure E.2)

For module 3, inputs include the intermediate products from modules 1 and 2, which carry an emission factor.

[4] Process subdivision is not appropriate as the process unit cannot be broken down further. Functional unit expansion is not appropriate in the context of this work (as previously noted). System expansion is not appropriate as cryogenic air separation is a typical, system for largescale oxygen supply and a suitable alternative system is not available.

The gasification system includes a range of potential co-products, including electricity and steam, generated via waste heat recovery, ash and/or slag recovered from the gasifier and sulphur recovered via syngas purification. The scale of production for these potential co-products remains uncertain and is likely subject to facility-specific commercial circumstances (i.e. energy costs, grid considerations, plant design and operation).

Where applicable, emissions may be scoped out for the co-products using system expansion. In order to do so, appropriate substitute systems must be identified and appropriate allocation factors established.

Electricity is likely to be an important co-product for the gasification system. Electricity exported from the system could substitute grid electricity (kWh for kWh), and emissions estimated in line with relevant grid emission factors (i.e. local, regional, national). This is a common approach in various carbon accounting schemes. Energy allocation could also be applied to this co-product.

Steam may also be an important co-product for the gasification system, but this is likely to be highly dependent on the availability of appropriate infrastructure and nearby consumers given the nature of steam supply. Currently the dominant technology for generation of high-grade steam (heat), is via combustion of natural gas within a boiler. As such, steam exported from the system could be estimated in line with the emissions associated with equivalent steam produced in a natural gas boiler of a pre-defined default efficiency (ARENA, 2016).

The ash and slag products are significantly less material. Default allocation factors should be defined here relating to appropriate substitute systems. For ash and slag, these co-products vary in uses from low-value applications such as replacing natural aggregates to high-value applications such as replacing clinker in cement production. A conservative emission factor should be established as the default, but it may be important to include measures which allow and incentivise users of the scheme to seek out higher quality data specific to their value chain.

E.4 Information to be reported

Table E. 2 shows the information to be reported for hydrogen produced from coal gasification with carbon capture and storage.

Table E. 2 – Information to Be Reported for the Coal Gasification /CCS Pathway

Category	**Matters to be identified**
Facility details	• Facility identity • Facility location • Facility capacity
Production	• Production pathway
Product specification	• Hydrogen output pressure • Hydrogen purity • Contaminants • Hydrogen quantity [kg]
GHG emissions overview	• Emissions intensity of hydrogen batch
Batch details	• Beginning and end of batch dates • Batch quantity

Electricity	• Location based emissions accounting
	    • Quantity of purchased grid electricity [kWh]
	    • Location based emission factor used [gCO_2e/kWh]
	
	• Market based emissions accounting
	    • Quantity of purchased grid electricity [kWh]

	- Quantity of contracted electricity [kWh] and/or quantity of associated GOs or RECs - Residual electricity [kWh] - Residual mix emission factor [gCO_2e/kWh] - Type of GOs or RECs - On-site electricity generation - Quantity of on-site generation [kWh] - Emission factor for on-site generation (as applicable) [gCO_2e/kWh]
Other utilities	- Source/s of water - Source/s of steam - Quantity of purchased water [kg] - Quantity of purchased steam [kg] - Quantity of steam exported [kg]
Fuel feedstock	- Types of fuels combusted - Quantities of fuel combusted [L, kg] - Relevant emissions calculation or factors used [$kgCO_2e$/relevant unit of fuel] - Emissions intensity of fuel used, including all emissions associated with fuel extraction, transporting to a processing plant, and processing [e.g. $kgCO_2e/MJ$]
Process	- Coal gasification reactor type - Syngas purification technology - Air separation technology - Sulphur waste gas processing technology (if applicable) - Quantity and type of vented GHG gases [kg] - Quantity and type of flared GHG gases [kg] - Technology for monitoring fugitives from CO_2 storage CO_2 capture rate
Coal feedstock	- Type of coal - Coal composition - Quantity of coal used for gasification reactions [kg] - Quantity of coal used for heating [kg] - Embodied emission factor for coal [$kgCO_2e/kg$] (derived from primary and secondary data, provided by supplier or sourced from relevant source i.e. NGA Factors)[5]
Carbon dioxide treatment	- Type of CO_2 storage - Location of CO_2 storage - Transport type of CO_2 to storage location (if applicable) - Quantity of CO_2 captured [kg] - Quantity of CO_2 stored [kg] - Quantity of fugitive emissions created during injection of CO_2 into the storage location [kg] - Quantity of fugitive CO_2 emissions from storage [kg] (in line with defined timeline)
Waste and/or co-products	- Quantity of ash produced [kg] - Quantity of slag produced [kg] - Quantity of nitrogen produced [kg] - Quantity of crude argon produced [kg] - Quantity of ash sold [kg] - Quantity of slag sold [kg] - Quantity of nitrogen sold [kg]

[5] Note that where upstream emissions are derived using upstream data, there may be a requirement for additional information. This could include items such as coal source.

	• Quantity of crude argon sold [kg] • Quantity of other products [kg]

Bibliography

[i] Althaus, 2007
[ii] Kopp, 2000
[iii] Higman, 2008

