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Authors		
Name	**Organisation**	**E-mail**
Diana Iruretagoyena	ICL	d.iruretagoyena09@imperial.ac.uk
Nixon Sunny	ICL	nixon.sunny13@imperial.ac.uk
Niall Mac Dowell	ICL	niall@imperial.ac.uk
Nilay Shah	ICL	n.shah@imperial.ac.uk
Federico d'amore	ICL	f.damore18@imperial.ac.uk
Karin Treyer	PSI	karin.treyer@psi.ch
Rahul Anantharaman	SINTEF	Rahul.Anantharaman@sintef.no
Brage Rugstad Knudsen	SINTEF	brage.knudsen@sintef.no
Julian Straus	SINTEF	Julian.straus@sintef.no
Daniel Sutter	ETH	sutter@ipe.mavt.ethz.ch
Mijndert Willem van der Spek	ETH	mijndert.vanderspek@ipe.mavt.ethz.ch
Robert de Kler	TNO	robert.dekler@tno.nl

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Executive Summary
The following document describes the component model specifications for the modelling tool-kit as part of work package 4 (WP4) of the ERA-Net ACT ELEGANCY project. The purpose of this document is to provide details on the dynamic unit operations within the modelling tool-kit. The document includes an overview of the hydrogen production process via steam reforming with carbon capture and storage (CCS). Each unit operation is described in terms of input and output streams, and main design parameters.

TABLE OF CONTENTS

1 INTRODUCTION

1.1 General overview and purpose of this specification

ELEGANCY will enable the evaluation of integrated H_2-CCS chains with respect to their performance trade-offs, operability and environmental impact, and will apply all its research findings to five national case studies including The Netherlands, Switzerland, The United Kingdom, Germany and Norway. To this end, work package (WP4) will develop an open-source modelling package to design and simulate H_2-CCS systems.

In particular, the aims of WP4 are the following:

- Develop an open-source systems modelling framework with a steady-state (multiperiod) design mode and a dynamic operational mode.
- Develop multiscale models and an integrated modelling approach for the chain components incorporating results from WP1 and WP2.
- Apply the methodology in conjunction with the case studies in WP5 with respect to (i) the potential time evolution of the system and (ii) integrated assessments of the proposed designs.

The operational tool of WP4 is focused on assessing the dynamic behaviour of the designed system (i.e. a fixed network) including intermittent operation and exploring how such transient behaviour propagates through the system and what mitigation strategies may be required (e.g. design reinforcements through storage). The operational envelope of the system and key components are established by the user using a design basis. Upon which, the simulation tools can be used to quantify of a range of key system variables such as flowrate, temperature, pressure and impurity profiles that can be realistically tolerated by the processes. The operational performance and system capabilities will be subject to dynamic demand and market price fluctuations that are typically experienced in end-use sectors. The operational tool is developed using the open-source modelling software, OpenModelica, and with its accompanying documentation.

The purpose of this document is to provide relevant information of the key operation units of the H_2-CCS systems, including design and operational parameters, and input and output streams of material and energy. The ranges of important variables involved (e.g. flow rate, temperature, pressure and impurities that can be tolerated) is also given based on surveys of literature. Comments on the document can be sent to Diana Iruretagoyena (d.iruretagoyena09@imperial.ac.uk).

1.2 Background

Hydrogen is one of the most important raw materials for the chemical and refinery industries worldwide. In addition, during the last decades the continuous increase in the demand of energy and environmental concerns have promoted interest in the use of hydrogen as energy carrier for stationary and mobile applications, as it is a zero-carbon energy vector.

The economics of hydrogen production are determined by several factors such as the price and quality of the feedstock, along with cost of capital and many other factors. Over 95% of the feedstock used in the production of hydrogen are fossil-derived, i.e. natural gas, fuel oil and coal. Currently, steam methane reforming (SMR) is the leading technology for H_2 production from natural gas or light hydrocarbons.

Table 1: Main components of an SMR plant with CCS

Components
• Feedstock pre-treatment
• Pre-reformer
• Reformer
• Water gas shift section
• Pressure swing adsorber
• CO_2 capture section
• CO_2 compression and dehydration
• CO_2 transportation and storage

ELGANCY investigates maturing, and promising technologies for H_2 production from different carbon-containing fuels (natural gas, biogas, and biomass) emphasising SMR, while providing storage-ready CO_2. The main components of a SMR plant coupled with CCS are given in Table 1, and a schematic representation is presented in Figure 1. It is worth mentioning that the CO_2 produced could be captured from three areas of the plant: (1) the reformer flue gas, (2) the shifted syngas and (3) the PSA tail gas. It is also possible, in principle, to have combinations of CO_2 removal from these different streams. Each of these capture points have their associated benefits (i.e., lower cost) and drawbacks (i.e., higher pollutant concentrations) and the ideal system would be designed to meet the goals of the user. It is worth highlighting that capturing from both flue gas and the shifted syngas (location 1) is the only option capable of delivering CO_2 reductions of 90% or greater.
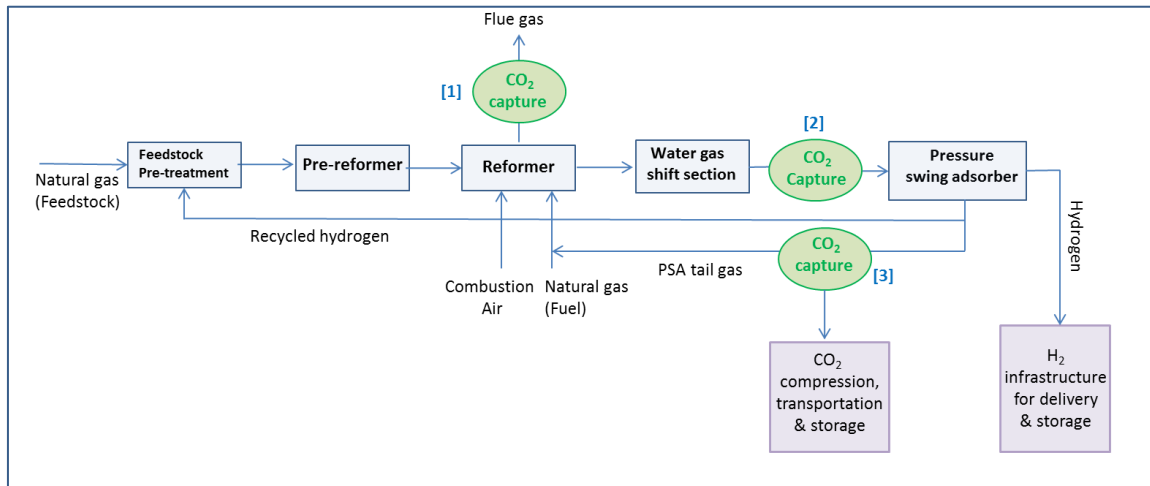
Figure 1: SMR plant with integrated CO_2 capture

2 DESCRIPTION OF UNIT OPERATIONS

2.1 Feed specifications

The composition of natural gas is not uniform, and the precise composition can have significant implications on the optimal performance and design of the plant. In particular, it is important to consider the presence of sulphur compounds, non-methane hydrocarbons and hydrocarbon liquids. Table 2 gives a representative range of natural gas composition.

Table 2: Natural gas composition, mole %

Components	Normal range
Methane	87.0 - 96.0
Ethane	1.8 - 5.1
Propane	0.1 - 1.5
iso-Butane	0.01-0.3
n-Butane	0.01-0.3
iso-Pentane	trace - 0.14
n-Pentane	trace - 0.04
Hexanes and higher	trace - 0.06
Nitrogen	1.3 - 5.6
Carbon Dioxide	0.1-1.0
Oxygen	0.01-0.1
Hydrogen	trace - 0.02
Mercaptan	4.9 mg/m^3
Water	16-32 mg/m^3
Hydrogen Sulphide	4 ppmv
HHV, dry, MJ/m^3	36.0 - 40.2

2.2 Feed desulphurisation

The first stage of the SMR process involves the pre-treatment of the feedstock to remove sulphur compounds, which poison the reforming catalysts. The main elements of this section are presented in Figure 2. The feed is introduced to a flash drum where, if required, the liquid phase components are removed. A slip-stream of hydrogen (recycled) from the PSA unit is introduced to the gaseous feed for use in downstream hydrogenation processes. The pre-heated feedstock is further heated up to ~343°C and then sent to a desulphurisation unit where the organic sulphur compounds are hydrogentated releasing their sulphur as H_2S. In the same reactor, the H_2S produced is adsorbed in a zinc oxide bed reacting to form zinc sulfide, which is then removed as a solid waste.

Table 3: Operating parameters for pretreatment equipment

Component	Parameter	Baseline
Feed stream	Temperature	21 °C
	Pressure	20 bar
Flash tank	Temperature	21 °C
	Pressure drop	-0.5 PSI
H_2 recycle stream	Temperature	38 °C
	Pressure	20 bar
	Flow rate	Set by design specification to assure 2% H_2 in the reagent stream
Compressor	Outlet pressure	30 bar
Reactor	Isentropic efficiency	0.72
	Temperature	343 °C
	Pressure drop	-25 psi
	Effectiveness	The reactor is assumed to achieve equilibrium concentrations
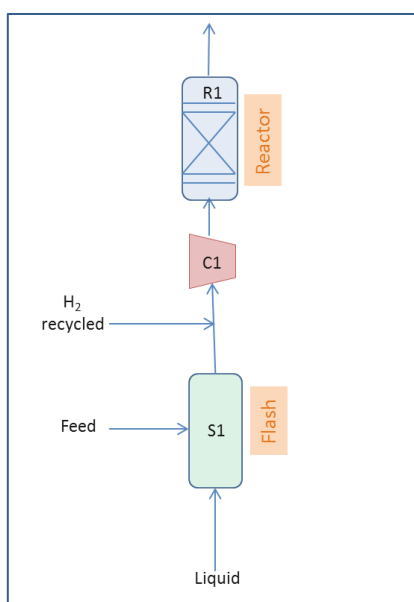
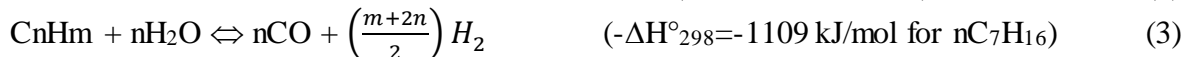**Figure 2:** Pre-treatment desulphurisation system

2.3   Pre-reforming and reforming

The treated (purified) feed gas that leaves the desulphurisation unit is then mixed with a high pressure superheated steam in order to maintain a fixed overall steam-carbon molar ratio of ~2.8. The stream then enters to the pre-reformer, which is an adiabatic reactor that is mainly responsible for converting any heavy hydrocarbons in the feed to CH_4 and other co-products (i.e. CO_2, CO and H_2). The temperature of the pre-reformer is ~ 510 °C. The temperature of the stream reduces by ~52 °C in passing through the pre-reformer due to the endothermic reactions that take place.

It is necessary to operate the steam reformer with an outlet temperature around 800 to 950°C to achieve reliable conversion. The reaction is highly endothermic and heat has to be supplied to the process. Several reforming technologies can be used for heat provision. These technologies can be differentiated by the means of heat transfer, which rank in increasing intensity based on: convective heat transfer, radiative heat transfer and internal combustion. The operating conditions for the pre-reforming and reforming sections are given in Table 4.

The main reactions involved are:

$$CH_4 + H_2O \Leftrightarrow CO + 3H_2 \qquad (-\Delta H°_{298}=-206 \text{ kJ/mol}) \qquad (1)$$
$$CO + H_2O \Leftrightarrow CO_2 + H_2 \qquad (-\Delta H°_{298}=41 \text{ kJ/mol}) \qquad (2)$$
$$CnHm + nH_2O \Leftrightarrow nCO + \left(\frac{m+2n}{2}\right) H_2 \qquad (-\Delta H°_{298}=-1109 \text{ kJ/mol for } nC_7H_{16}) \qquad (3)$$

Table 4: Operating parameters for pre-reforming and reforming sections

Component	Parameter	Baseline
Steam feed	Temperature	510 °C
	Pressure	30 bar
Desulfurized feed to pre-reformer	Temperature	510 °C
	Pressure	28.5 PSI
Pre-reformer	Temperature	510 °C
	Pressure drop	25 psi
	Effectiveness	The reactor is assumed to achieve equilibrium concentrations
Pre-reformer feed to primary reformer	Temperature	650 °C
	Pressure	27 bar
Reformer	Temperature	815 °C
	Pressure drop	25 psi
	Effectiveness	The reactor is assumed to achieve equilibrium concentrations
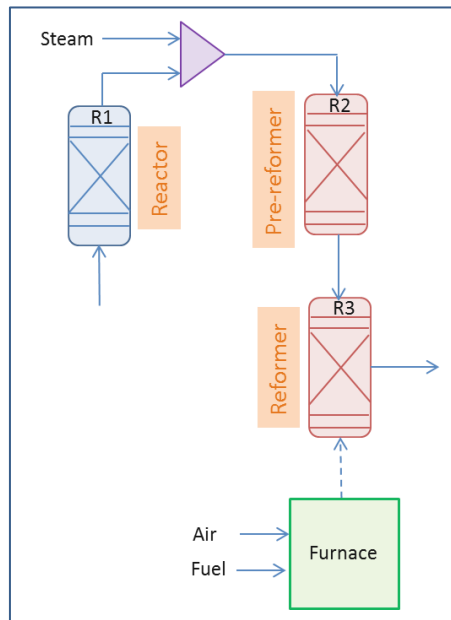
Figure 3: Pre-reformer and reformer

2.4 Water gas shift section

The synthesis gas from the reformer is rich in H_2 and CO. The shift reaction, $CO + H_2O \leftrightarrow CO_2 + H_2$, can be used to increase the H_2 content. Equilibrium for this reaction favors the products at low reaction temperatures, but high temperature is required to achieve a practical reaction rate. This trade-off is normally addressed through the use of a two stage shift system. In the first stage, a high temperature is required, typically 350 °C reactor inlet temperature. The temperature will increase in the reactor due to the exothermic nature of the shift reaction. At this temperature, the reaction is promoted by a low cost iron-based catalyst and reduces the CO concentration to a few percent. In the second stage of shift, a lower temperature is used (190 – 210 °C) to increase the equilibrium concentration of H_2. A more expensive, copper-based catalyst is required to achieve equilibrium at a reasonable rate. These catalysts are sulphur intolerant and require operation above the gas dew point. Alternatives to the two stage shift might be preferred for some installations. These include a single-stage high temperature shift or a single-stage medium temperature shift. These options result in higher CO concentrations in the product gas. Figure 4 shows a schematic representation of the water gas shift stage.
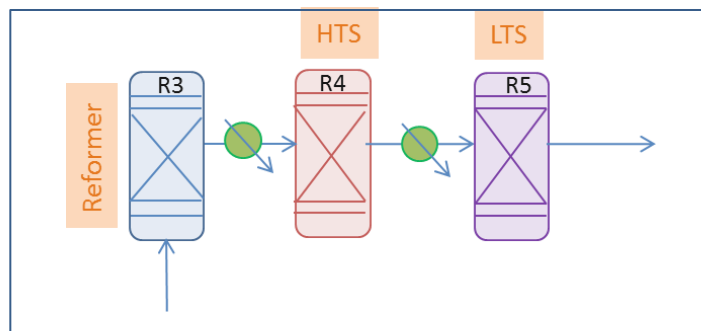
Figure 4: Water gas shift reaction stage

Table 5: Operating parameters for conversion section equipment

| Component	Parameter	Baseline
Reformed gas	Temperature	816 °C
	Pressure	19.5 bar
Cooled gas feed to high temperature shift	Temperature	350 °C
	Pressure	19 bar
High temperature shift	Outlet temperature	427 °C
	Pressure drop	15 psi
	Effectiveness	The reactor is assumed to achieve 90% CO conversion
Cooled feed to low temperature shift	Temperature	200 °C
	Pressure	18 bar
Low temperature shift	Outlet temperature	213 °C
	Pressure drop	15 psi
	Effectiveness	The reactor is assumed to achieve 90% CO conversion
Shifted gas to purification	Temperature	213 °C
	Pressure	17 bar

2.5 Pressure swing adsorber

The shifted synthesis gas has a high concentration of H_2, but it also includes a high concentration of CO_2 and H_2O, as well as residual methane and small amounts of carbon monoxide and nitrogen. To produce a high quality hydrogen product as required for fuel cell applications, the gas is purified by removal of CO_2 in a MDEA process, removal of moisture by condensation and drying, and removal of other contaminants in a PSA (pressure swing adsorption) unit. These processes are complicated, requiring a complex model of their own for complete representation. A simplified scheme of the process is presented in Figure 5, and a list of the purification section operating parameters is given in Table 6.

The hot, hydrogen rich stream from the low temperature shift is cooled against a feedwater stream in a heat exchanger to a temperature of ~93°C. Further cooling to 38 °C may be accomplished with quenching in the condenser. The cooled gas is treated in a MDEA chemical absorption system for removal of CO_2. The highly concentrated hydrogen stream from the MDEA is treated in the PSA unit to achieve hydrogen purity of up to 99.99%. The PSA waste gas stream includes unrecovered hydrogen, CH_4, CO, and other contaminants. This stream is valuable as a process fuel and is used in the reformer furnace to reduce overall fuel requirement.

Table 6: Purification section operating parameters

Component	Parameter	Baseline
H_2-rich gas from low temperature shift	Temperature	213 °C
	Pressure	17 bar
Cooled gas from feedwater heater	Temperature	93 °C
	Pressure	16.5 bar
Condenser quench	Temperature	38 °C
	Pressure drop	5 psi
MDEA	Temperature	38 °C
	Pressure	16 bar
	CO_2 recovery	95%
PSA	H_2 recovery	90%
	Contaminants in H_2 product steam	Assumed to be 0.001% of product stream
	Fuel gas composition	calculated
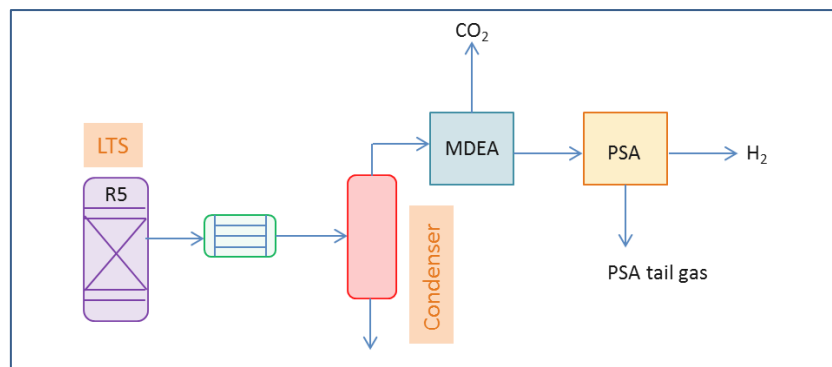
Figure 5: Purification system

2.6 CO_2 capture section

This section provide an overview of a CO_2 capture unit from PSA tail gas using the MDEA solvent. The tail gas from the PSA contains around 51% mol CO_2-wet basis, and is initially compressed from 0.2 MPa to 1 MPa before being fed into the bottom of the absorption column where the CO_2 in the tail gas is removed by contacting with the lean solvent (flowing in counter-current direction). The washed tail gas, containing now 3.5% mol of CO_2 (wet basis) leaves the top of the adsorber column and is pre-heated and expanded to around 0.15 MPa before being fed to the burners of the steam reformer. Whilist, the rich solvent collected at the bottom of the absorber column is fed into the flash drum.

The vapour (flashed gas) released from the flash drum is sent to the burners as additional fuel to the steam reformer. Whilist, the rich solvent leaving the bottom of the Flash Drum is sent to the Lean/Rich Hheat exchanger to be heated by the incoming stream of hot lean solvent coming from the Stripper's reboiler. The hot rich solvent leaving the Lean/Rich Heat exchanger is then fed into the top of the stripper column. In the stripper column, the rich solvent flowing down from the top of the column is stripped of its CO_2 by the vapour generated from the stripper's reboiler.

The stripper's reboiler generates vapour (mainly steam) by re-boiling the lean solvent coming from the stripper bottom. The vapour is then sent back to the bottom of the stripper column and travels upward to strip the CO_2 from the solvent flowing downward. The stripper's reboiler is heated by the LP steam coming from the back pressure steam turbine of the cogen plant. The condensate recovered from the reboiler is sent back to the Hydrogen Plant's BFW system. The overhead gas from the stripper column is then sent to the stripper's condenser where the steam in the overhead gas are condensed, collected and returned as a reflux to the stripper column. The CO_2 rich gas from the stripper's condenser is then sent to the CO_2 compression and dehydration unit.
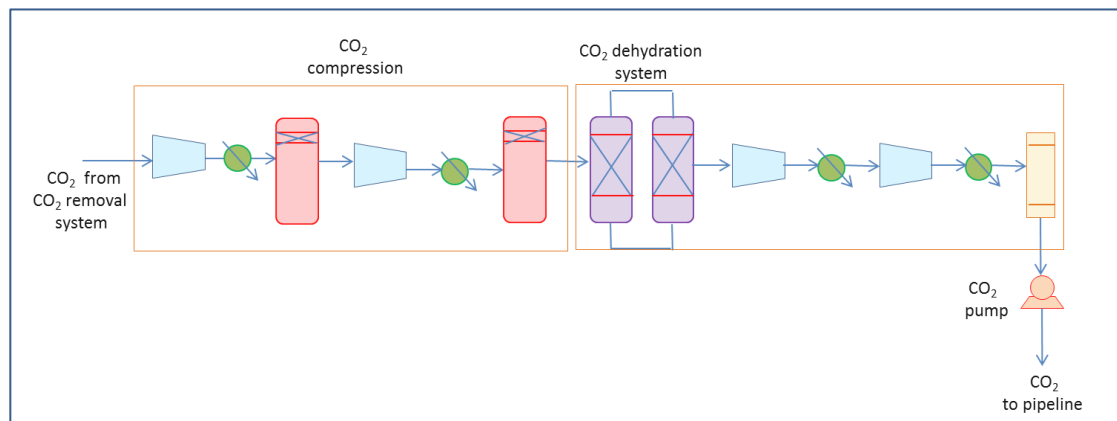
2.7 CO_2 compression and dehydration

The CO_2 compression and dehydration unit includes a compressor, knock out drums, inter-stage coolers, dehydration unit and a liquid CO_2 pump. The overhead gas (mainly CO_2) leaving the stripper condenser is compressed by a single train seven-stage centrifugal compressor. The CO_2 compressor is equipped with anti-surge control, vent, inter-stage coolers, knock-out drums, and condensate draining facilities as required.

There is one inter-stage cooling section installed after each compression stage. Typically large scale cooling towers will be required. Seawater can be used as cooling medium at appropriate locations. The condensed water in the inter-cooler is separated from the gas in the knock-out drum. The gas leaving the final inter-stage cooler is then fed into the dehydration unit.

The dehydration unit is based on a molecular sieve/activated alumina adsorbent dryer. The dryer is designed to be operated and produce CO_2 product with a dew point temperature of -40°C. The dryer consists of two bed of adsorbents for every train of compressor. During normal operation, one bed is in operation, and the other bed (saturated with water) is regenerated. The bed are regenerated by the dry product gas (ca. 10% taken from the dried product gas after the dryer). The regeneration gas (now saturated with water) is recycled back after the third stage compression.

The final two compression stages downstream of the dehydration unit increases the CO_2 pressure to 8 MPa. This is designed to operate at pressures higher than the critical pressure of pure CO_2 (at 7.4 MPa) in order to prevent any risk of 2 phase flow due to the presence of non-condensable gases. After being cooled, the dried compressed CO_2 (dense phase) is pumped and delivered to the battery limit at a pipeline of 11 MPa.

Figure 6: CO_2 compression and dehydration

2.8 CO_2 transportation and storage

CO_2 are typically transported in two different states: gas, liquid. Commercial-scale transport uses tanks, networks of pressurised pipelines and ships for gaseous and liquid carbon dioxide. The efficacy of each way of transport depends on the quantity of CO_2 and distance from its point of storage or utilisation. Pipelines are considered most promising although transportation via ships are likely to be of increasing importance over long distances. The presence of impurities in the CO_2 stream can significantly affect the thermophysical properties and phase equilibria of the fluid. For CO_2 pipelines, operators have established minimum specifications for composition such as that shown in Table 7.

Gas transportation at atmospheric pressures occupy such a large volume that very large facilities are needed. Therefore, gas is typically compressed and/or liquiefied. Liquefaction is an established technology for gas tranport by ship as liquified petoleoum gas and LNG. These technologies can be applied directly for CO_2 transportation.

Injection of CO_2 in deep geological formations uses technologies that have been developed for and applied by, the oil and gas industry. Well-drilling technology, injection technology, computer simulation of storage reservoir dynamics and monitoring methods can potentially be adapted from existing applications to meet the needs of geological storage.

In areas with suitable hydrocarbon accumulations, CO_2-Enhanced oil recovery (EOR) may be implemented because of the added economic benefit of incremental oil production, which may offset some of the costs of CO_2 capture, transport and injection. Storage of CO_2 in coal beds, in conjuction with enhanced coal bed methane (ECBCM) production, is potentially attractive because of the prospect of enhanced production of methane, the cleaneast of the fossil fuels. This technology, however, is not well developed and a better understanding of injection and storage processes in coals is needed. Carbon dioxide and storage in depleted oil and gas reservoirs is very promising in some areas, because these structures are well known and significant infrastructures are already in place. Nevertheless, relatively few hydrocarbon reservoirs are currently depleted or near depletion and CO_2 storage will have to be staged to fit the time of reservoir availability. Deep saline formations are believed to have by far the largest capacity for CO_2 storage and are much more widespread than other options.

To geologically store CO_2, it must first be compressed, usally to a dense phase known as 'supercritical' state. Depending on the rate that temperature increases with depth (the geothermal gradient), the density of CO_2 will increase with depth, until at about 800 m or greater, the injected CO_2 will be in a dense supercritical state. Geological storage of CO_2 can be undertaken in a variety of geological settings in sedimentary basins. Within these basins, oil fields, depleted gas fields, deep coal seams and saline formations are all possible storage formations. Subsurface geological storage is possible both onshore and offshore, with offshore sites accessed through pipelines from the shore or from offshore platforms.

Table 7: CO_2 quality specifications

| Components	Normal range
Carbon dioxide	Product shall contain at least 95% of CO_2
Water	Product shall contain no free water, and no more than 0.489 m^{-3} in vapour phase
Hydrogen sulphide	Product shall not contain more than 1500 parts per million, by weight.
Total sulphur	Product shall not contain more than 1450 parts per million, by weight.

Temperature	Product shall not exceed a temperature of 48.9 °C.
Nitrogen	Product shall not contain more than 4 mol% of nitrogen.
Hydrocarbons	Product shall not contain more than five mole percent (5%) of hydrocarbons and the dew point of Product (with respect to such hydrocarbons) shall not exceed -28.9 °C.
Oxygen	Product shall not contain more than 10 parts per million, by weight.
Glycol	Product shall not contain more than 4 x 10-5 L m^{-3} of glycol.

2.9 Alternative technologies for hydrogen production

Partial oxidation (POX)

The partial oxidation reaction (POX) is an alternative route to produce synthesis gas starting from hydrocarbon feedstock. This reaction uses pure O_2 as an oxidant and results in a moderately exothermic reaction. The O_2 to carbon ratio is lower than that required by stoichiometric complete combustion.
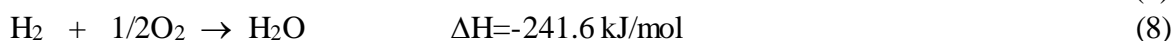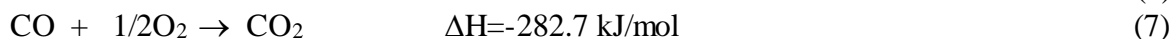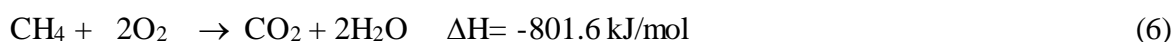
The stoichiometric equation for methane conversion is:
$$CH_4 + 1/2O_2 \rightarrow CO + 2H_2 \qquad \Delta H = -35.6 \text{ kJ/mol} \tag{4}$$
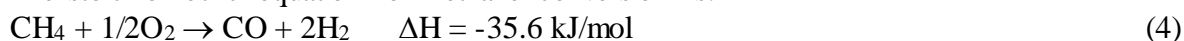
Or for higher hydrocarbons:
$$C_nH_m + n/2O_2 \; nCO + m/2H_2 \tag{5}$$

The theoretical H_2 to CO ratio is lower than that of SMR (about 2/3), as the main oxidant is O_2 instead of H_2O. However, a small amount of water is often added to the reactor feed, to better control reaction temperature and coke formation.

The reactions (4) and (5) are not exclusive routes of the process as other stoichiometric equations are thermodynamically compatible with the mixture composition fed to the reactor. Equations (1), (2) and (3) involved in the reforming process might also occur in partial oxidation. On the other hand, it is necessary to consider that further equations related to several oxidation reactions could occur during fuel conversion:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \qquad \Delta H = -801.6 \text{ kJ/mol} \tag{6}$$
$$CO + 1/2O_2 \rightarrow CO_2 \qquad \Delta H = -282.7 \text{ kJ/mol} \tag{7}$$
$$H_2 + 1/2O_2 \rightarrow H_2O \qquad \Delta H = -241.6 \text{ kJ/mol} \tag{8}$$

POX involves the combustion of hydrocarbon feedstock in a flame with less than stoichiometric ratio of O_2 required for complete combustion, resulting in the production of carbon dioxide (CO_2) and water (H_2O), according to Eqs. (6), (7), (8), which in turn react with the unreacted hydrocarbon to produce CO and H_2. Usually a slightly excess (20-30%) of O_2

with respect to the stoichiometric value required by equations (4) or (5) is fed to the system. The reaction is highly exothermic as the oxidation reaction consumes the available oxygen, and the large amount of thermal energy produced by the combustion is exploited by endothermic reforming reactions. Nevertheless, the POX process remains globally exothermic.

A non-catalytic partial oxidation process based on the above reactions has been largely used for the past five decades for a wide variety of feedstocks, in particular heavy fractions of refinery oils, such as naphtha, vacuum fuel oil, asphalt residual fuel oil, or even whole crude oil. The absence of catalysts implies that the production unit can be operated in a simpler manner but the working temperatures are considerably higher.

A catalytic partial oxidation (CPO) reaction reduces operation temperature and meets the requirements of decentralized applications based on small-scale plants. Coke formation and its deposition on catalyst active sites represent the main barrier to be abated for a practical utilization of CPO in hydrogen production plants.
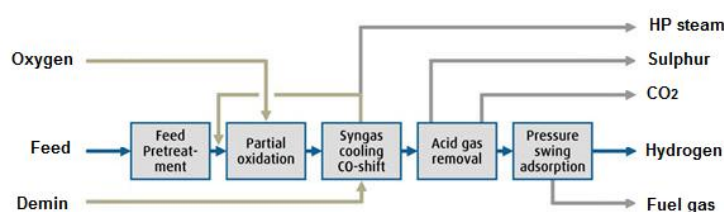

Figure 7: Partial oxidation scheme

Autothermal reforming (ATR)

Autothermal reforming (ATR) uses oxygen, steam and in some cases carbon dioxide, in a reaction with light hydrocarbons such as methane to form raw syngas. ATR combines non-catalytic POX and catalytic steam and CO_2 reforming of de-sulphurised natural gas in a single reactor. ATR uses a lower steam to carbon ratio in the reformer feed as compared to SMR. Such lower S/C ratios lead to lower H_2/CO ratios in raw syngas exiting the ATR. Addition of CO_2 in the feed further reduces the H_2/CO ratio. ATR does not require external heat input as the heat of reaction is provided by internal combustion of hydrocarbon feed with O_2.

ATR Reaction using CO_2:
$$2CH_4 + O_2 + CO_2 \rightarrow 3\,H_2 + 3CO + H_2O \tag{9}$$
$$4CH_4 + O_2 + 2H_2O \rightarrow 10\,H_2 + 4CO \tag{10}$$
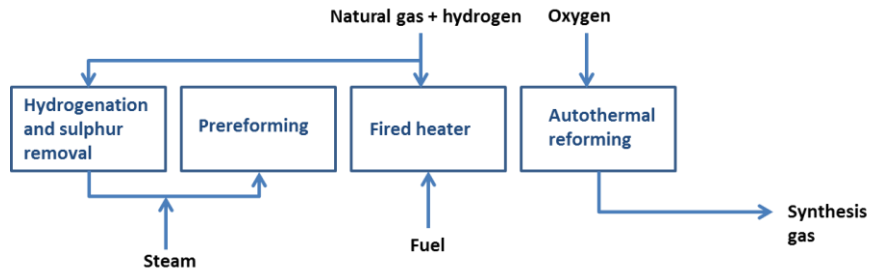
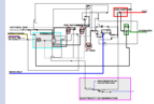**Figure 8:** Autothermal reforming process schematic

Table 8 depicts the comparative trade-offs between the usage of commonly discussed options for the purification of H_2. They can be operated in a manner so as to achieve varying levels of product recovery as well as purity based on the product specifications that are introduced.

Table 8: Purification technologies and attainable purities.

Pressure swing adsorption (PSA)	Permeation membrane	Polybed PSA Systems
Very high purity	High purity	H_2 purity: 99.9-99.9999 %
Up to 90% recovery	Up to 95% recovery	H_2 recovery: 60-90 %
High pressure H_2	Low pressure H_2	H_2 Feed pressure: 6-40 bar g
Tail gas to SR burners	Non-permeate to fuels	H_2 Product pressure: 5-39 bar g
Flexibility	Needs pre-treatment	

3   MODEL INVENTORY

Table 9: Inventory of component models and its implemented software.

Organisation	Model	Software	
ETH	SMR-CCS plant ATR plant CO_2 Compressor train SMR, SR-biogas reactors	Aspen Aspen Aspen Matlab	
TNO	SMR plant CO_2 compressor train MEA –CCS unit Reactor unit	Excel Aspen Dymola Dymola	
ICL	SMR, WGS reactors SE-H_2 systems CO_2 Pipeline model	Matlab Matlab gProms	
RUB	Thermodynamic calculation toolkit (TREND , Excel)		
SINTEF	Reduced order model development		

- H_2 production units are described in the process modelling software, AspenPlus, with all of the unitary operations representing the process. They include the pre-reformer, reformer reactor, water-gas-shift, pressure swing adsorption, compressors, etc.

- The Aspen-MATLAB merge for the production process enables a user to design reactors using equilibrium relations. Therefore, a user can input a desired throughput along with the design specifications/ parameters into the model to evaluate the impact on resource consumption as well as the requisite infrastructure. However, the models do not enable the user to perform any dynamic simulations, principally as there is limited data on the flexible operation of thermal production units.

- The dynamic compressor models enable a user to compute the compression duties for both H_2 and CO_2 depending on the battery limits of the facility at the specific desired specifications. They are implemented in Dymola and AspenPlus, both of which are accessible to the academic audience.

- H_2/ CO_2 pipeline transportation models have been developed in gPROMS, enabling equation-oriented access and control in the modelling domain.

- Tools for thermophysical property evaluation is available as part of the TREND package within Microsoft Excel. Users can access the file directly and perform a range of property evaluations and stability analyses by changing the parameters and species.

4   REFERENCES

- Argonne National Laboratory, 20th Annual International Pittsburgh Coal Conference, September 15-19, 2003, Hydrogen from Steam-Methane Reforming with CO_2 Capture.

- Implementing a Hydrogen Energy Infrastructure: Storage Options and System Design., University of California, 2005.

- J. C. Molburg, R. D. Doctor, Hydrogen from Steam-Methane Reforming with CO_2 Capture, http://www.uxc.com/smr/Library%5CAlternative%20Uses/2003%20%20Hydrogen%20from%20SteamMethane%20Reforming%20with%20CO2%20Capture.pdf

- M. Voldsund, K. Jordal, R. Anantharaman, Hydrogen production with CO_2 capture, Review article, International Journal of Hydrogen Energy, 41, 2016, 4969-4992.

- J. M. Ogden, C. Yang, Implementing a Hydrogen Energy Infrastructure: Storage Options and System Design, https://ideas.repec.org/p/cdl/itsdav/qt4xb940vg.html

- Techno-Economic Evaluation of SMR Based Standalone (Merchant) Hydrogen Plant with CCS, IEAGHG Technical Report, 2017-02, February 2017.

- J.R. Rostrup-Nielsen, Large-Scale Hydrogen Production, CATTECH, 6 (2002) 150-159.

- J. C. Abanades, A Special Report of Working Group III of the Intergovernmental Panel on Climate Change, Carbon Dioxide Capture and Storage, Cambridge University Press, (2005).