ACT Project Number:
271498

Project acronym:
ELEGANCY

Project full title:
Enabling a Low-Carbon Economy via Hydrogen and CCS

ERA-Net ACT project

Starting date: 2017-08-31
Duration: 36 months

D4.1.1
Technical Specification

Issue 1

Date: 2018-03-04

Organization name of lead participant for this deliverable:
Imperial College London

ACT ELEGANCY, Project No 271498, has received funding from DETEC (CH), FZJ/PtJ (DE), RVO (NL), Gassnova (NO), BEIS (UK), Gassco AS and Statoil Petroleum AS, and is cofunded by the European Commission under the Horizon 2020 programme, ACT Grant Agreement No 691712.

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Dissemination Level		
PU	Public	X
CO	Confidential, only for members of the consortium (including the Commission Services)	

Deliverable number:	D4.1.1
Deliverable title:	Technical Specification
Work package:	WP4
Lead participant:	Imperial College London (ICL)

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Keywords

Modelling tool-kit, Technical, Model, Architecture, Metrics

Executive Summary

The following document describes the technical specifications for the modelling tool-kit as part of work package 4 (WP4) of the ERA-Net ACT ELEGANCY project. The purpose of this Technical Specifications Document (TSD) is to provide technical 4details of the modelling tool-kit such as model development requirements and system architecture. The TSD also includes environmental, economic and process metrics relevant to the H_2-CCS system. This document is an "evolving" document and it will be updated periodically throughout the project to reflect any changes in user expectations.

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1 INTRODUCTION

1.1 Document overview

This document describes the technical specifications for the modelling tool-kit as part of work package 4 (WP4) of the ERA-Net ACT ELEGANCY project. ELEGANCY will enable the evaluation of integrated H_2-CCS chains with respect to technological and economic efficiency, operability and environmental impact, and will apply all its research findings to five national case studies including The Netherlands, Switzerland, The UK, Germany and Norway. To this end, WP4 will develop an open-source and physical model-based H_2-CCS whole systems chain evaluation tool-kit. WP4 will incorporate results from WP1 and WP2, and will apply the methodology in conjunction with the case studies in WP5.

The purpose of this Technical Specification Document (TSD) is to provide technical details, architecture and metrics of the modelling tool-kit platform including input and output requirements, user cases, scenarios and network designs involved. This is an 'evolving' document and will be updated periodically throughout the project. Comments on the document can be sent to Nixon Sunny (Nixon.sunny13@imperial.ac.uk), Diana Iruretagoyena (d.iruretagoyena09@imperial.ac.uk), Niall Mac Dowell (niall@imperial.ac.uk) and Nilay Shah (n.shah@imperial.ac.uk).

1.2 Background

In the 21st century, global warming is considered to be one of the most important challenges affecting people across the world. The term "global warming" refers to an increase in the average global temperatures as a result of increasing levels of "greenhouse gas" emissions worldwide [1]. Gases such as methane, water vapour, carbon dioxide and nitrous oxide are considered as greenhouse gases due to their contribution towards the greenhouse effect [2]. The greenhouse effect refers to the ability of a greenhouse gas to trap heat from escaping Earth's atmosphere. This is a key climate mechanism, which has allowed many living species including ours, to thrive on planet Earth. However, recent years have seen an increase in the atmospheric concentration of greenhouse gases such as carbon dioxide (CO_2). This can mainly be attributed to a rise in anthropogenic CO_2 emissions that has resulted in additional warming effects, which subsequently led to a measurable increase in average global temperatures [3]; such temperature rises have significant consequences. Some of the anticipated, undesirable consequences of global warming includes sea level rise, droughts, storms, heat waves, etc [4]. These events combined with possible unknown indirect effects, could have significant adverse impacts on the quality of our daily lives. Therefore, it is important to limit the emission of greenhouse gases and mitigate against climate change.

A significant proportion of CO_2 emissions worldwide arises from the energy and industrial sectors [5]. Emissions from the energy sector mainly arise as a result of power generation from feedstocks such as coal, gas, etc. Industrial sectors generally use fossil fuel-based

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resources as feedstock to produce manufactured goods as well as for both heat and electricity production. The carbon intensive nature of these resources, when combined with the scale of industrial operations, often results in significant quantities of CO_2 being released during its processing. This leads to several large and concentrated emission sources of CO_2 which can be potentially mitigated with the use of low-carbon technologies such as Carbon Capture and Sequestration (CCS).

Currently, CCS is viewed as a retrofit type technology where an existing industrial facility can be retrofitted with a CCS unit that can potentially capture up to 90% of its CO_2 emissions [6]. One of the major advantages of utilising CCS as a low-carbon technology in the energy and industrial sectors is that CO_2 emissions from conventional, more stable power sources (gas, coal, etc.) can be reduced significantly whilst allowing them to be operational in the future. In the energy sector, this will reduce the burden placed on renewable technologies as a coal or gas fired power station can respond more readily to changes in demand. CCS technologies have not enjoyed the same level of commercial implementation as other low carbon technologies, and this is mainly due to a lack of a feasible business model. Nevertheless, CCS can play an effective role as a climate change mitigation technology, provided that a sustainable framework is developed that includes economic, environmental, legal and social considerations. This is highly important since the problem of global warming and climate change is a multi-faceted problem which requires such considerations.

In the power generation sector, there are a variety of available options for generating low carbon electricity such as renewable sources. However, in industrial and transportation sectors, the number of options is limited. In particular, industries which rely on carbon-based feedstocks in the form of fossil fuels will find it increasingly difficult to reduce their emissions using conventional feedstocks and fuel in the future. It is important to note that CCS can be of great value to these industries such as the refining and chemicals industry.

Hydrogen (H_2) is an energy carrier and it is an important feedstock for several industrial processes. It can be produced from almost all forms of energy and it is a clean fuel that produces water as the sole product from combustion. This is an attractive feature that makes it ideal for use as fuel in power stations or in transportation. Globally, H_2 is produced largely from fossil fuels without CCS and only approximately 5% of H_2 is produced using electrolysis of water using electricity [7]. However, a continuation of this statistic is not sustainable in the future due to the aforementioned reasons. In countries such as the UK and Germany, where a substantial proportion of the domestic heating infrastructure is developed on a natural gas network, conversion into a H_2 based network with CCS can potentially result in great reductions in overall emissions [8]. These considerations highlight the opportunities for synergies between large scale H_2 and CCS networks. The successful implementation of a large scale H_2-CCS chain network, based on low-carbon H_2 from natural gas, will provide

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opportunities for Europe to showcase its technical excellence whilst making valuable contributions towards the challenges associated with global warming.

To aid commercial implementation of a H_2-CCS network, there needs to be extensive analysis on its technical feasibility in conjunction with an integrated assessment under multiple criteria. This immediately highlights the requirement for an information generation tool that can analyse various potential applications for H_2-CCS chains, whilst being able to assess its performance under multiple performance criteria. The primary focus of ELEGANCY WP4 is to address this need and provide the necessary tools and techniques for analysing large scale H_2-CCS chain networks in the form of a modelling tool-kit. Large-scale applications, such as the case studies from WP5, are often too complex to have an obvious or an intuitive solution. In such scenarios, optimisation tools and methods are empowering due to their capability for utilising the decision variables to improve upon various performance criteria. The objective can either be a single criterion such as cost or an array of multiple criteria such as cost and environmental impact amongst various others, in the case of a multi-objective optimisation model. The multitude of available techniques and options makes this a valuable tool in decision-making.

1.3 Project aims

ELEGANCY aims at investigating and maturing promising technologies for H_2 production from different carbon-containing fuels (natural gas, biogas, coal and biomass) while providing storage-ready CO_2. ELEGANCY postulates the CO_2-emission-free production of H_2 for both centralised (from natural gas) and decentralised applications (road transport, residential heating and small/medium industrial processes). It aims to explore technical options that can be deployed at different scales (i.e. large, mid- and small-scale), and address the technical barriers that have to be overcome for deployment of the selected technologies.

In particular, the aims of WP4 are the following:

- Develop an open-source systems modelling framework with a steady-state 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.

WP4 forms a link between the research done in WPs 1,2 and 3 and the case studies performed in WP5.

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1.4 Purpose of this specification

The technical specification document (TSD) describes the components of the modelling tool-kit of WP4, including methodology and architecture. It provides the baseline to develop the first prototype of the whole chain design and simulation tool and also determines the overall design and operational specifications of the toolkit.

The following descriptions are created for the platform developers:

- An operational overview of the modelling platform
- The platform building blocks and their relationships, including output/input relations and operation in the form of pseudo-code algorithm descriptions
- The platform use and development requirements

The TSD also includes environmental, economic and process metrics relevant to the H_2-CCS system.

2 MODEL DEVELOPMENT AND USE REQUIREMENTS

The open-source model-based tool developed in the WP4 will be central in the national case studies (the Dutch, Swiss, British, German and Norwegian cases) within ELEGANCY (an early version will be available by month 18, M4.2), and will further be available for more widespread use e.g. by government agencies. It will consist of a multiscale, open-source modelling framework, with reduced order models used to couple different levels of detail including linear approximations of thermodynamic models. The tool will apply consistent model assumptions, e.g. thermo-dynamics and handling of impurities, and a methodology for uncertainty estimation and will consider the different opportunities for H_2 use; the latter also influences chain decisions. To this end, the chain tool will make use of the reduced order models developed in collaboration with WP1 for the H_2 production and CO_2/H_2 separation technologies investigated. Further, advantage will be taken of existing component models and of frameworks for infrastructure design. The framework will be designed to study cost- and risk-effective as well as environmentally sustainable regional H_2-CCS value chains and support the development of time-phased master plans for different regional economies with a view to supporting the timely emergence of such value chains.

2.1 Aims and requirements for prototype development

- A division of the outlined components into a prioritization for development at three levels: necessary for operation, ‘must to have’ and ‘nice to have’.
- The prototype should be operable on a high-end 64-bit computer based on a model for a specific sector under the phases of the ELEGANCY project.
- The prototype is going to be operated from a command line or programming interface, where data is extracted directly and subsequently translated manually into visuals. In

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the subsequent phase, the model is going to be expanded with user interfaces as defined in the functional specifications.

- The prototype is developed using a flexible, modular and comprehensive architecture of concepts, so that expansive functionality can be built, and local city-regions can provide tailored performance indicators for model use.
- The prototype code will be developed with a series of standard programming conventions to ensure readability and maintainability of the code, within the modular framework.
- The prototype will be developed using a version control system to enable collaborative development and to ensure transparency and accountability, security of backups, roll-back possibilities, and effective development. Datasets are to be assembled in a similar manner with sufficient security.
- The software components should comply with open source initiative standards, such that the long-term goal of free of end use is maintained.

2.2 Tool-kit modes

1) Design mode: Steady state model where the user can explore the evolution of system design (e.g. choice, scale and location of key technologies and network structure for H_2 and CO_2) as a means of enabling design optimisation of integrated H_2-CO_2 value chains. This will use higher-level models for the system elements based on abstractions (meta-models) of the detailed models. The time phasing and risk management approach will be based on real-options methods and identify low-regret near-term investigation options. H_2 production using different feedstocks, technologies and scales will be included, based on WP1 data and associated reduced order models. The designs can take advantage of existing or planned related investments such as industrial and power CO_2 sources and transport infrastructure. Similarly, we anticipate the development of injection and storage hubs, which might be shared between CO_2 originating from NG reforming and from other sources. The tool will be able to establish the pros and cons of such integration. We will develop the steady state models using ***Python*** and particularly ***Pyomo*** for optimisation purposes. The advantage of using Pyomo is that in an open source-tool where its modelling objects are embedded within a high level programming language with a rich set of supporting libraries.

2) Operational mode: Dynamic behaviour of the designed system (i.e. a fixed network) including intermittent operation and explore how such transient behaviour propagates through the system and what mitigation strategies may be required (e.g. at the injection and storage end). The operational envelope of the system and key components will be established. This quantifies the ranges of key system variables such as flowrate, temperature, pressure and impurity profiles that can be tolerated. The ability to blend different CO_2 streams to meet

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operational requirements is included. The operational performance and system (dynamic) capabilities also will be subject to long- and short-term market price dynamics experienced in the different end markets where the produced H_2 is being utilized, be it in relevant chemicals (e.g. ammonia), fuels or power production. Ammonia market price development or required inertia of the E-grid could result in different load requirements on the total chain as an example of short-term dynamics. Longer-term dynamics include integration of the H_2-CCS system with the wider regional de-carbonization (e.g. integration with post combustion capture) to optimize the economic performance. Hence, the tool, particularly in design mode, will also include the ability to integrate other key CO_2 sources into the infrastructure and show how the H_2-CCS infrastructure may be biased by such other point sources. We will develop these using open-source Modelica modelling software ***OpenModelica*** (i.e. an optimization platform for the design model and a dynamic simulation platform for the operational model) and make the models and their documentation available.

The first iterations of these tools will be available by month 18 (M4.2) to evaluate on the national case studies. We will use the case study results for iterative refinement.

2.3 Key issues that the modelling tool-kit will answer

1. What will an optimised evolving European H_2-CCS infrastructure look like?
2. How will the H_2 production infrastructure best be integrated with related system elements such as other H_2 and CO_2 sources, downstream H_2 user markets, and the transport and distribution infrastructure?
3. What will be the key economic, environmental impact, safety and operability metrics?
4. How can these metrics be optimised and what trade-offs exist at this level?

2.4 Component prioritization

The prioritization of components development is split into three types: the components which are necessary for operation, 'must have' components that are essential for demonstration of functionality, and those that are 'nice to have' which provide for more advanced capabilities:

Table 1. Overview of prototype components development prioritization

No.	Component	Type of requirement for demonstration
• 1	• Code execution environment	• Necessary
• 2	• Database environment	• Necessary
• 3	• Model testing engine	• Necessary
• 4	• Spatial allocation	• Necessary
• 5	• Built environment entities mapping	• Necessary
• 6	• Process to entity allocation	• Necessary
• 7	• Exogenous demand initialization	• Necessary
• 8	• Weather patterns	• Necessary

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• 9	• Transport process operation	• Must have
• 10	• Market exchange/Price development	• Must have
• 11	• Process operation decisions	• Nice to have
• 12	• User decision inventions	• Must have
• 13	• Key performance indicators	• Must have

2.5 Prototype usability for demonstration of functionality

The development of the prototype platform serves to demonstrate its functionality and value for the five national case studies within ELEGANCY.

The usability is set to provide for:

- The representation of a particular case study in the modelling platform, its physical input requirements and resulting in outputs provided over time.
- The representation (potentially at quite a conceptual level) of network sector including aspects such as resources, infrastructure, technologies, etc.
- The change of the infrastructure over time in terms of the defined performance metrics.
- To examine a number of example user decisions/interventions and their impact on key performance indicators.

At the end of the ELEGANCY project, for the demonstration of functionality, a baseline scenario will be developed for the sector based on only current decision interventions as they are already in place. On top of this a series of 3-4 input scenarios (i.e. decision intervention) are to be defined and their impacts are to be established, as expressed by the key performance indicators.

In the prototype stage, the functionality is demonstrated by creating and operating the platform by the WP4 team from a command line interface. User decisions are to be entered directly as model source code and/or data files and the model is subsequently operated. Results are then extracted as raw data-files. For purposes of the demonstration, the results are manually summarized into appropriate visuals, a presentation summarizing results, and associated reporting with scenario comparison and interpretation.

2.6 Computational performance

The prototype simulation will cover ultimate targets for CO_2 reductions in the Region for 2030 and 2050. Since the model includes substantial parameter uncertainty, a large number of complete calculations across this time period are required to provide for a confidence interval of outcomes (“sensitivity analysis”). An early estimate is that an approximate one hundred of such model runs are necessary to capture the range of possible outcomes.

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The model should be able to:

- Run routine calculations on a high-end 64 bit workstation.
- Support multiple simulations of different parameter values (e.g. Sensitivity analyses or various scenario analyses).
- Carry the necessary multiple simulations within a time-frame of a number of days up to a week on a single machine, and with linear speedup on parallel machines/nodes.

2.7 Software interface requirements

The prototype at the end of the project will be at the level of a software interface in the form of a simple command line interface to demonstrate model functionality. This interface is designed to be used by a developer at this stage rather than the intended user of the final product. To this end, a development toolkit is to be incorporated, which selection depends on the chosen programming language(s) as part of the platform design specifications.

The command line interface provides for:

- The ability to provide data entry to the platform.
- To execute a model run with a given set of parameters.
- To export raw data files in an appropriate format.

2.8 Manageability/Maintainability

The model code is to be assembled such that it can be easily modified and maintained by more than one person, as well as easily read and understood by other programmers. For this purpose a number of programming conventions are to be adopted for keeping track of code interpretation, cleanliness and future code expansion. After selection a style-guide is to be followed since it provides for a structured way to deal with a number of issues, including:

- **Standardized naming** of classes, methods, variables, parameters and other entities, using the principle of long names for global entities and shorter names for local entities. To keep track of naming a centralized listing and definitions.
- **Separation of words** for names composed of multiple words, either through underscores or capitalization of second and/or third words, as dependent on the conventions of the used programming language.
- **Indentation and spacing**, the maintainability and readability of code is greatly improved with the appropriate number of horizontal spaces and blank lines (sparse). In principle the standard for the used programming language is utilized (often embedded within the development environment), and otherwise another standard convention is to be taken.

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- **Breakdown of functions/methods**, into smaller methods based on hierarchical sub-model decomposition that provide for one function, which can then be modularly used into other functions, as opposed to building large more error prone blocks.
- **File naming** in a standardized way and based on a standardized set of locations using a naming convention in relation to the modular structure.
- **Code Comments,** to be provided in a standardized way for each variable and function/method as well as complex code structures within these blocks of code to provide for i) markers outlining incomplete items or opportunities for code improvement, ii) summaries of what the code should do, and what it at present does is (as part of code development), and iii) external references where applicable, such as that this function is based on an algorithm that is explained in a particular reference work or project document.

2.9 Security

The model code is to be developed internally within Imperial College London and other partner computer servers plus updated into a secure version control repository. The repository provides for both a secured cloud copy of the code as well as a possibility for code roll-backs and efficient collaboration within the development team. To this end a repository is to be selected in the platform design and implemented within a private setting for the prototype development.

All datasets are developed and stored in three locations, as csv/excel files on internal computer servers, as part of the Imperial College London database environment, and in a stored version as csv files within an online repository including periodic updates.

2.10 Standards compliance

The aim is to make the fully scaled model available publicly free of end use, in line with the principles as defined by the open source initiative. This should be done as soon as a viable product is available for release, which at present is envisioned. To keep in line with this goal the used software should in principle comply with the licenses as approved by the open source initiative, which includes over several dozen licenses including the common GPL and LGPL licenses. The main restrictions within this constraint are imposed on the external model linear programming solver (e.g. GLPK, scipy), the model database environment, and any external agent-based algorithms which are included. Details on the choice of software and hardware components inclusive of licensing aspects are to be provided in the platform design specification; however CC-BY is a current recommendation.

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3 SYSTEM ARCHITECTURE

3.1 Resource Technology Network (RTN) framework

As described in the functional specification document, the design of the modelling architecture is largely based on the Resource Technology Network (RTN) framework [9]. RTNs are mixed integer linear programming optimisation models which target to represent the flow and interconversion of resources given specific technological infrastructure via a spatial and temporal approach. The interactions between various agents of the network and their corresponding effects on resource flows, costs and other factors can be captured using this framework. RTN focuses on MILP optimisation models which simulate the spatial and temporal flow of resources when given specific demand constraints, technological infrastructure, etc. This provides the general framework with which the tool-kit will be developed. The use of multiperiod time representation will allow for an effective pathway to be developed and will help avoid any myopic solutions. Similarly, the use of spatial discretisation allows for specific spatial effects to be captured. The design mode will allow for more tailored applications by giving users the capability to introduce local specifics as well as modify the existing parameter sets and datasets. In addition, users who wish to modify the algorithm for their use will be able to do so. Figure 1 shows a schematic representation of the key elements of the RTN modelling framework.

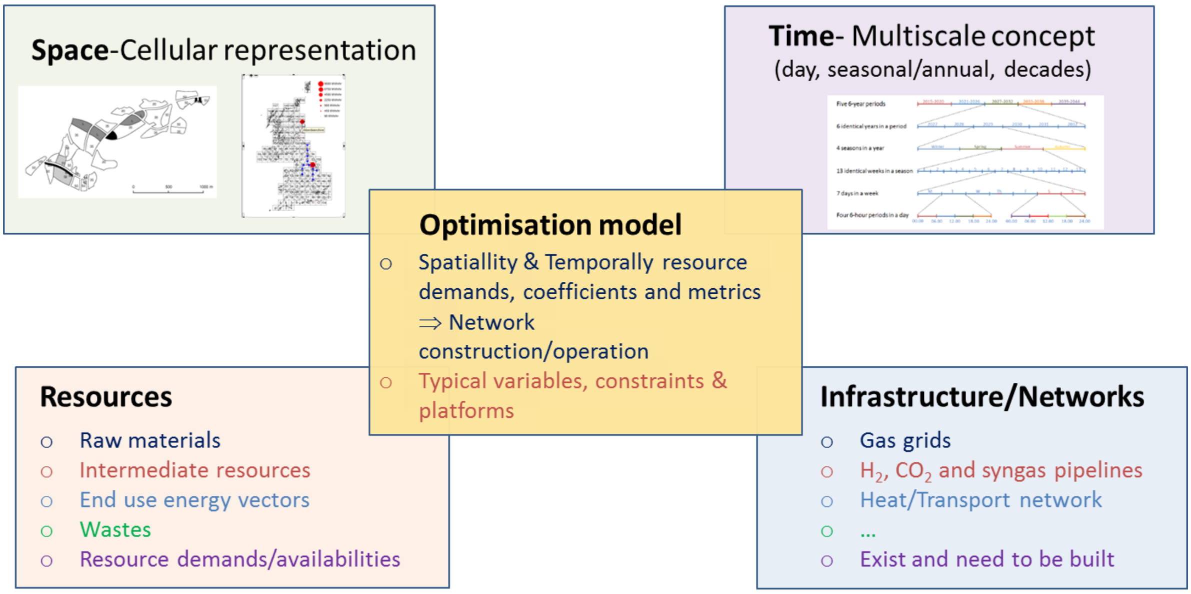

Figure 1. Key elements of RTN modelling framework

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3.2 Elements of the modelling architecture

- **Resources** – renewable and non-renewable resources that are available within a particular location. Spatial resolution of resources should be as high as possible but it is dependent on the mode of application of the tool-kit. Primary raw materials and energy sources include biomass, natural gas, petroleum and sunlight. End use energy vectors such as power, heat, transport fuel and waste products are also characterised as a resource in the modelling tool-kit.
- **Infrastructure** – supports the conversion from resources such as natural gas to hydrogen and further allows for linkage with process blocks. A well-constructed infrastructure enables new processes to be integrated into the network so that an adaptable nation-wide network is developed over time. Infrastructure can refer to many things – transport network for primary resources, power grid, gas grid, heat network, H_2 and CO_2 pipelines, etc. This modelling tool will report infrastructure requirements mainly surrounding transport networks for primary resources, H_2 transport, CO_2 transport, etc. It's important to note that infrastructure can be presented in two forms in the model – existing or recommended infrastructure. Therefore, optimal solutions may suggest infrastructural changes or capacity expansion of current networks to aid optimal development of H_2-CCS systems.
- **Process** – represents the aggregate effects of all the processes by which the resources are converted into the end products that are of useful value to an economy. This element characterises the material and energy inputs/ outputs at each stage of material conversion. Some examples of process technologies are feed transportation, processing, reaction, separation, compression, etc. These technologies are used to interconvert the resources and they can vary in scale. They normally vary based on the mode of application or the end use of the product. For example, boilers used in domestic heating applications do not operate with the same scale as industrial combustion units.
- **Demand –** defines a user input which is also a key constraint that could have significant influences on the objective function. The demand profile impacts the selection of technologies that are being employed at any given time. The demand for H_2 is dependent on its physical form – liquid H_2 or compressed gaseous H_2. In addition to demand, this will affect the transportation, storage and distribution modes of the network. Spatial and temporal variations in demand for H_2 will also have impacts on the optimum infrastructure.

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4 MODEL OUTPUT METRICS USED TO ASSESS H_2-CCS SYSTEMS

4.1 Introduction

In addition to delivering the modelling tool-kit, a key outcome of this work will be provided in terms of a reported assessment of the H_2-CCS system (relevant to the region of interest) in terms of environmental, economic and operability metrics, and of its comparison to alternative options.

A metric, in the context we are using here, is defined as “a standard of measurement” [10]. The two most common groups of metrics are those dealing with economics (costs and values of inputs, outputs, and processes, including capital and operating costs) and performance (mass conversion, energy efficiency, and generally speaking, energy and mass balance derived parameters).

Economic and performance metrics are needed to be able to compare and/or screen various components of the technologies involved in ELEGANCY from different perspectives or points of view. It is important to have available as wide a set of metrics as possible, because, at different stages of development, there are usually gaps in the information available; varying from technology to technology, such that not every metric can be evaluated for each. The metrics developed here are applied to H_2-CCS systems considered in WP4 for beneficial use involving environmental, economic, market and risk-safety metrics, Figure 2.

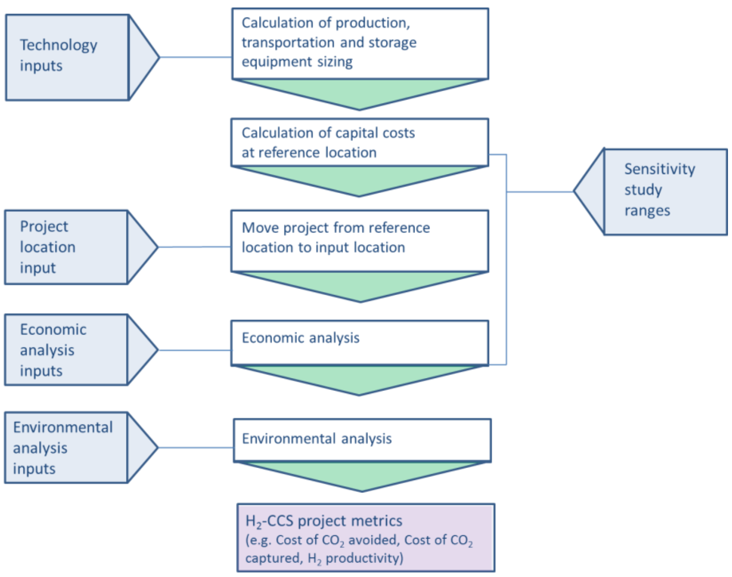

Figure 2. Flowchart of methodology/metrics for H_2-CCS assessments

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4.2 Process metrics

- **Conversion**

The conversion metric corresponds to the conversion of reactants to products in the different stages of the process (e.g. conversion of methane in the steam methane reforming reaction).

- **Selectivity**

The selectivity metric corresponds to the selectivity of the different products for a particular reaction (e.g. selectivity of carbon monoxide in the steam methane reforming reaction).

- **Yield of Hydrogen (and / or H_2 productivity)**

The yield of hydrogen metric corresponds to the yield of hydrogen in a particular stage of the process (e.g. yield of hydrogen in the water gas shift reaction).

- **Rate of reaction**

The rate of reaction metric corresponds to the rate of reaction of a particular reaction involved in the process (e.g. rate of reaction of the water gas shift reaction)

- **Purity**

The purity metric correspond to the purity of H_2 and CO_2 streams at the exit of the purification units.

- **Efficiency**

The efficiency metric corresponds to the efficiency of the different unit operations involved in the process (e.g. efficiency of compression section)

- **Energy consumption**

The energy consumption metric corresponds to the energy consumption of the different unit operations involved in the process (e.g. energy consumption of the purification unit)

- **Gas permeation rate**

The Gas permeation rate metric refers to the permeation rate of hydrogen and carbon dioxide in the storage-transportation pipes.

4.3 Environmental process metrics

- **CO_2 emissions reduction**

The CO_2 emissions reduction metric is the amount of CO_2 emissions reduction per unit amount of H_2 in the new process, relative to that in the reference technology (i.e. traditional methane reforming (SMR) process without CCS). This metric is a dimensionless ratio and should be expressed as a percentage. The greater the value, the greater is the CO_2 emissions reduction.

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$$CO_2\ Emission\ Reduction\ (\%) = \frac{\frac{tonnes}{year} CO_2\ emitted\ in\ existing\ process - \frac{tonnes}{year} CO_2 emitted\ in\ the\ new\ process}{\frac{tonnes}{year} CO_2 emitted\ in\ existing\ process}\ x\ 100 \quad (1)$$

- **CO_2 avoided potential**

The CO_2 avoided potential metric is the amount of CO_2 avoided by the new process, relative to that in the reference technology (e.g. traditional methane steam reforming (SMR) process without CCS) and assumed to offset CO_2 emissions from a user-specified reference CO_2 emitter or plant. This metric is a dimensionless ratio and should be expressed as a percentage. The CO_2 avoided potential is the percentage of the reference plant CO_2 emissions that the new process would avoid producing, when considering the H_2 production process and reference CO_2 emitter within the same envelope.

$$CO_2\ Avoided\ Potential\ (\%) = \frac{\frac{tonnes}{year} of\ CO_2\ avoided\ to\ meet\ H_2\ demand}{\frac{tonnes}{year} of\ CO_2\ emitted\ from\ reference\ plant}\ x\ 100 \quad (2)$$

$$CO_2\ Avoided\ Potential\ (\%) = \frac{\frac{tonnes}{year} CO_2\ emitted\ from\ existing\ process - \frac{tonnes}{year} CO_2\ emitted\ from\ new\ process}{\frac{tonnes}{year} of\ CO_2\ emitted\ from\ reference\ plant}\ x\ 100 \quad (3)$$

- **Carbon intensity**
  - $kgCO_2$/kg product (chemical produced)
  - $kgCO_2$/kW generated (energy generated)
- **Energy intensity**
  - Unit of electric energy per unit mass of product (EEI)
  - Unit of chemical energy per unit mass of product (TEI)
- **Life cycle assessment indicators**

The considered major environmental impacts of an LCA analysis for CCS technology are categorized into environmental mid-point indicators described by characterisation factors:

- Global warming potential (GWP), $kgCO_2$ eqv.
- Terrestrial acidification potential (TAP), kg SO_2 eqv.
- Fresh water eutrophication potential (FEP), kg PO_4^{3-} eqv.
- Photochemical oxidant potential (POCP), kg ethylene-eqv.
- Human toxicity potential (HTP), kg 1,4-DCB-eqv.
- Terrestrial ecotoxicity potential (TETP), 1, 4-DCBeqv.
- Fresh water ecotoxicity potential (FETP), 1, 4-DCBeqv.
- Cumulative energy demand (CED), MJ.

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  - Human health
  - Ecosystem quality
- **Other environmental impacts that are considered**
  - Leakage of CO_2 within the CCS system
  - Structural changes in the geological formations of the CO_2 underground storage (in collaboration with WP2)
  - Various environmental impacts along process chain as the solvent production and disposal, energy requirements for solvent sequestration or CO_2 transport

4.4 Economic metrics

- **H_2 marketability**

The product marketability metric is the cost to make a unit amount of the desired H_2 relative to its market value. This metric is a dimensionless ratio and should be expressed as a percentage.

$$H_2\ marketability\ (\%) = \frac{\$\ cost\ to\ make\ a\ tonne\ of\ H_2}{\$\ per\ tonne\ market\ value\ of\ H_2}\ x\ 100 \tag{4}$$

- **Cost reduction**

The cost reduction metric is the incremental reduction in cost by the new process over the standard steam methane reforming process without CCS. The unit of this metric are \$ per tonne of H_2. These metric needs to have a positive value to show there is a cost saving to be had in replacing the traditional process.

$$Cost\ reduction\ \left(\frac{\$}{tonne}\right) = (\$\ cost\ to\ make\ a\ tonne\ of\ H_2\ by\ traditional\ process) - (\$\ cost\ to\ make\ a\ tonne\ of\ H_2\ by\ the\ new\ process) \tag{5}$$

- **Cost per tonne CO_2 captured**

The cost per tonne of CO_2 captured metric is the sum of annualised capital and operating costs of the utilisation process relative to the tonnes of CO_2 used. The costs of the process include infrastructure, raw materials, processing, by-product disposal and utilities costs, as well as any other costs. The units of this metric are \$ per tonne of CO_2. This metric is dependent on the maturity or stage of development of the technology or process, and whether the costs are known or can be reasonably estimated.

$$Cost\ per\ Tonne\ CO_2\ captured\ (\frac{\$}{tonne}) = \frac{\sum(annualised\ capital\ and\ operating\ costs, \$/year)}{\frac{tonnes}{year} CO_2 captured} \tag{6}$$

- **CAPEX**

CAPEX (i) = Investment costs of technology *i*

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- **OPEX**

OPEX (i) = Operational costs of technology *i* in the year *a*

4.5 Market metrics

- **Product supply demand**

The product supply demand metric is the percentage of H_2 that can be satisfied with the new process or technology, taking into consideration feedstock or catalyst availability, or other limitations. This metric is a dimensionless ratio that should be expressed as a percentage. The geographic basis for the product market demand should be specified, e.g., Europe, USA, etc.

$$H_2\ supply - demand\ metric\ (\%) = \frac{\frac{tonnes}{year} of\ H_2\ that\ can\ be\ produced}{\frac{tonnes}{year} of\ market\ demand\ for\ H_2}\ x\ 100 \tag{7}$$

4.6 Safety metrics

The relative safety and environmental benefits metric is a composite assessment of the raw materials and processing conditions, including any environmental benefits, of the new process relative to those of any existing process for the same product. The metric assessment is either improved, no change, or reduced.

The relative safety ranking uses the National Fire Protection Association (NFPA) Standard 704 “fire diamond” category hazard values, which range from 0 to 4, with 0 meaning no hazard and 4 meaning severe hazard. The NFPA categories are those of health, flammability, and instability/reactivity. An improved relative safety assessment could be based on reduced reactor temperature and/or pressure, elimination of a hazardous feedstock or catalyst, etc.

5 H_2 END-USE COMPONENTS

They key components of the modelling tool-kit correspond to hydrogen production from a centralised steam methane reforming (SMR) production facility. A brief description of these components is given in Table 2. In addition, a schematic representation of the H_2 production-distribution network and SMR plant are presented in Figures 3 and 4.[11-18]

Table 2 Key components of H_2 production from SMR plant with CCS

Component	Description
• NG pre-treatment	• Required to reduce the sulphur and chlorine present in the NG in order to prevent any poisoning of the catalysts downstream. Sulphur hydrogenation step, typical operating temperature: 350-380 °C. Catalyst: CoMo. Desulphurization step,

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	typical operating temperature: 350-450 °C, catalyst: ZnO
• Pre-reformer	• Adiabatic reactor with a bed of Ni based catalyst, its purpose is to reform a portion of the overall reforming duty and convert any heavy hydrocarbon in the natural gas feed. Typical operating temperature: 500 °C.
• Steam methane reformer	• SMR is a process in which gas or liquid fuel is converted to syngas (steam and methane react to yield hydrogen and carbon monoxide) in an equilibrium limited highly endothermic reaction. Typical operating temperature: 800-950 °C (can vary in range 500-1000 °C). Steam to carbon ratio 2.5-3 (can vary in range 2.5 - 6) and pressure of 20-35 bar. Catalysts: Ni based. High conversion is favoured at high temperature, high S/C and low pressure. $CH_4 + H_2O \rightleftharpoons CO + 3H_2$ $\Delta H = +206 \frac{KJ}{mol}$
• Water gas shift reactors	• WGS is a low exothermic reaction in nature that converts most of CO in the syngas from reformer to H_2 and CO_2. High temp shift (HTS), typical operating temperature: 310-450 °C. Typical operating pressure: 25-35 bar, catalyst: Fe_3O_2/Cr_2O_3. Low temp shift (LTS), typical operating temperature: 210-240 °C , catalyst: CuO/ZnO $\mathrm{CO + H_2O \rightleftharpoons CO_2 + H_2}$ $\Delta \mathrm{H} = -41 \frac{\mathrm{KJ}}{\mathrm{mol}}$

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• Pressure swing adsorption (PSA) unit	• Recovers the H_2 from the shifted syngas, the average recovery rate is about 80 %. PSA is usually carried out in two layered bed adsorption columns using activated carbon for adsorption of CO_2, CH_4 and CO and zeolite in the second layer for N_2 adsorption. Typical operating temperature: 20-50 °C. Typical operating pressure: 10-50 bar.
• H_2 and CO_2 capture and storage elements	• Mainly corresponds to compression units and transportation-storage tanks and gas pipelines.

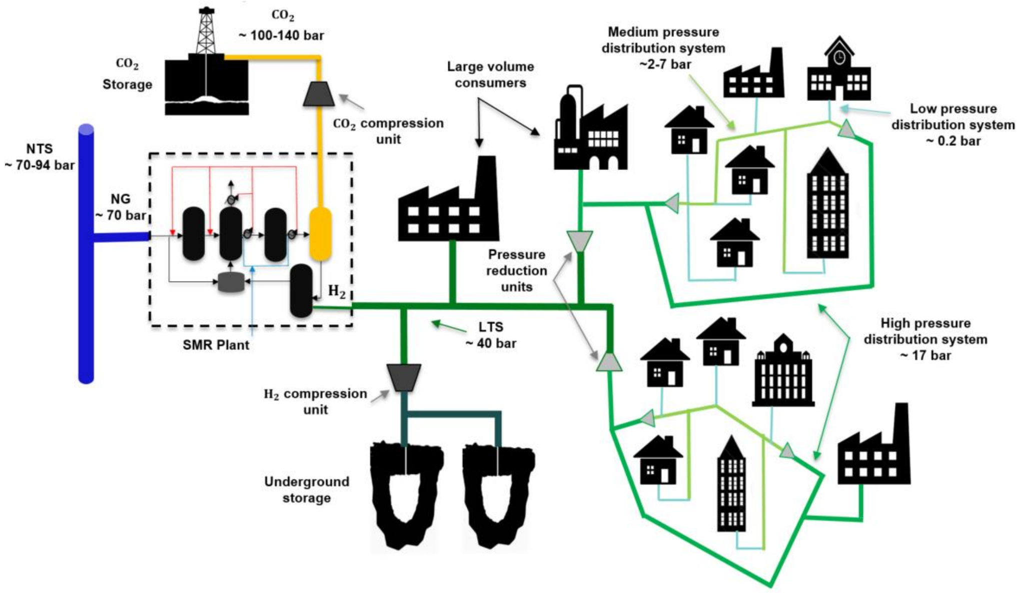

Figure 3. H_2 production-distribution network (to provide heating)

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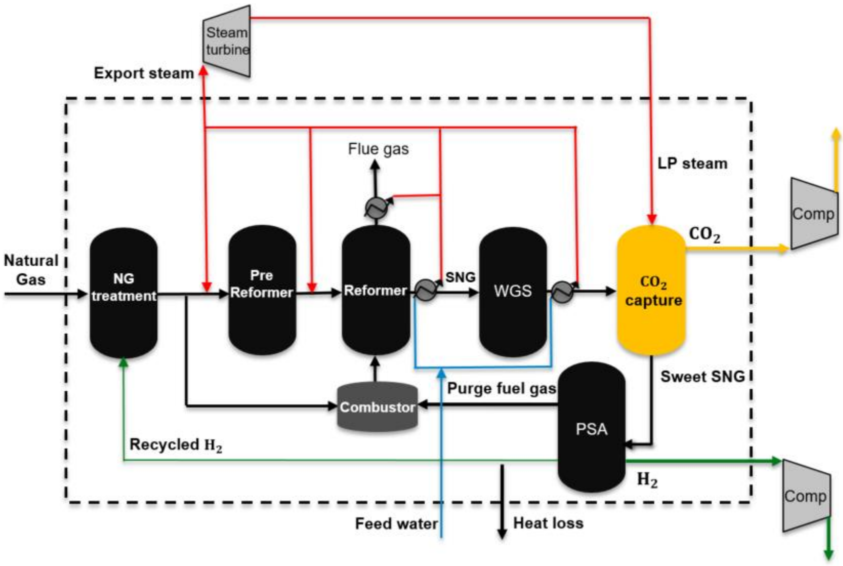

Figure 4. H_2 production from SMR production facility, with CCS

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