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Executive Summary

The following document describes the functional and architecture specifications for the modelling tool-kit as part of work package 4 (WP 4) of the ERA-Net ACT ELEGANCY project. The purpose of this Functional Specifications Document (FSD) is to detail user expectations for the modelling tool-kit functionality. This FSD serves to inform stakeholders about the purpose of the modelling tool-kit and provide a clear basis for its application. It offers examples of some typical use cases that a potential user may wish to test, using the modelling platform. Furthermore, it provides an overview of the timeline for tool-kit development whilst also providing the scope for each deliverable during the development phase. In addition, an outline of model insights and outputs is presented in the document. The FSD will serve as the precursor to the Technical Specifications Document (TSD), whilst summarising the inputs and outputs from the modelling tool-kit. 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 functional and design specifications for the modelling tool-kit as part of work package 4 (WP 4) of the ERA-Net ACT ELEGANCY project. The modelling tool-kit will be developed to address all the various national case studies from WP 5 of the project. The motivation behind the development of the tool-kit is to deliver important insights in relation to the feasibility of an optimised H_2-CCS chain network for various national applications in Europe. The main purpose of this Functional Specification Document (FSD) is to detail user expectations for the modelling tool-kit. Furthermore, it provides an overview of model architecture, including high-level descriptions of the modelling components. It aims to inform the project stakeholders on the usability and purpose of the modelling tool-kit as well as highlight any limitations in its application. This FSD also plays a key role as a precursor to the Technical Specifications document. It further informs the data collection strategy, and allows for the definition of data specifications for application of the modelling tool-kit prototype. The document draws on inputs from collaborative discussions between the various WP teams during the designated workshop in the ELEGANCY Kick-off meeting. The FSD is an "evolving" document and it will be updated periodically throughout the project to reflect any changes in user expectations. Any comments/ inputs can be sent directly to Nixon Sunny (nixon.sunny13@imperial.ac.uk) and Diana Iruretagoyena (d.iruretagoyena09@imperial.ac.uk).

1.2 Project Aims

The ELEGANCY modelling tool-kit will enable the evaluation of an integrated H_2-CCS chain network with respect to technological efficiency, economic viability, operability and environmental impact. For this purpose, an open-source systems modelling framework, containing a steady state design mode accounting for uncertainty, and a dynamic operational mode, will be employed. The tool-kit will incorporate results from WP 1 and 2 to provide an integrated modelling approach.

The primary objective of the modelling tool-kit is to gain a quantitative understanding of the performance of H_2-CCS networks, when considering various performance metrics. A multi-scale modelling approach will be used, whereby a user will be prompted to provide parameters for the various interacting, scale-specific models to effectively undertake a whole-systems analysis of the H_2-CCS chain networks. A potential user can utilise steady state models, which can be used to design H_2-CCS chain networks and further evaluate CO_2 emissions, for risk assessment and quantification of environmental burdens based on life cycle assessment (LCA). Furthermore, dynamic models will enable a user to establish an operational envelope, determine the performance flexibility and understand the transient behaviour of the system.

Throughout its three-year development timeframe, a number of modelling tools will be made available for use in the form of deliverables within WP 4. Furthermore, an early version of the complete modelling tool-kit will be made available as a prototype by month 18. Following this release, the development team will make modifications based on user input until the final version is released in month 36, with complete documentation and training material made available to all users.

1.3 Document Structure

The FSD is structured as follows:

- **Introduction** – A brief introduction into the aims of the ELEGANCY project. It outlines the use of an open-source systems modelling framework to describe the optimal time-phased development of a H_2-CCS network. It describes the role of the FSD in capturing user expectations whilst providing an overview of model architecture.
- **Model Purpose –** Provides the user with a short overview of the motivation behind the development of the modelling tool-kit as well as the relevance of the physical systems under consideration. It further highlights examples of typical use cases for the modelling tool-kit so that users can understand and influence its development.
- **Model Scope & Development –** This section describes the various deliverables related to WP 4 and the development phases leading up to the final modelling tool-kit. It provides a short overview and scope for each of the four modelling-based deliverables. This is linked with their corresponding deadlines to show the interactions between various deliverables throughout the development timeframe of three years.
- **Tool-kit Architecture** – The section introduces the modelling framework behind the development of the tool-kit. It also describes the high-level model architecture which enables a user to understand the various elements in the tool-kit and their interactions to form a complete network. A short description of both the design and the operational mode are also given here.
- **Model Insights –** This section presents a detailed overview of user insights that can be obtained from the application of modelling tool-kit. In addition, the advantages of using the tool-kit for decision-making and analysing future projects are summarised here. The section also contains a list of common questions that a user may have from an insight generation standpoint.
- **Model Outputs –** This section contains a preliminary list of model outputs along with a brief description of performance criteria. An exhaustive list of performance metrics can be seen in Deliverable 4.2.1 of ELEGANCY. The use of uncertainty analysis in testing the robustness of the generated solutions, and its corresponding implications on use cases are also summarised here.

2 MODEL PURPOSE

2.1 Context

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 dubbed 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 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 against 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 are 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 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 there to be 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 WP 4 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 WP 5, are often too complex to have an obvious or an intuitive solution. In such scenarios, optimisation tools and methods are largely empowering due to its 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.

2.2 Model Objectives

The modelling tool-kit has several key objectives. They are discussed in greater detail in the subsequent sections. Nevertheless, they can be summarised as follows:

- A multi-scale modelling framework which interlinks various industries and sectors on a national scale, which can subsequently be incorporated into a larger Europe-wide network.
- An approach which is effective in the evaluation of a proposed design under various performance criteria and not simply from an economic standpoint. This must include

societal and political challenges and should be developed with a long-term perspective.

- The free supply of knowledge and insight generation tools so that potential users are not disadvantaged in any way/ means. This implies that open-source/ open access software must be utilised for modelling without any significant performance limitations.
- A decision-making aid/ tool for the industrial partners along with the five national case study teams. It must provide important insights in relation to tailored use cases and applications.

2.3 Use Case Examples

2.3.1 Mr. S – H_2 production facility within an existing industrial region

The optimal design of a process facility for the production of H_2 whilst considering intra-seasonal variations in demand for the product as well as supply variations pose a significant challenge. The question on optimal utilisation of existing infrastructure in industrial areas whilst enabling new and continued links with natural gas suppliers requires considerable analysis. The choice of location to build new production facilities for H_2 is not trivial. The following use case can give an insight into how the modelling tool-kit will aid a user in decision making in such scenarios.

Mr. S is designing a facility to produce clean H_2 using natural gas as feedstock. He has proposed that this facility should be incorporated into an existing industrial region so that it is tactically placed with access to an unconstrained supply of natural gas. Mr S has a site plan to check for spatial requirements and understands the various constraints within the system. He would like to find out whether it's economically viable to place this facility at the proposed location. Furthermore, he would like information on sizing and throughput requirements for the facility so that it is possible to meet consumer demands at various locations. Since Mr. S negotiates directly with H_2 consumers, he needs this information to reach vital trade agreements. Table 1 shows sample inputs that Mr. S will need to provide along with a sample of some expected outputs from the modelling tool-kit, which will help him formalise his business model.

Table 1: Sample input-output analysis for Mr. S's production facility case.

Model Inputs	Model Outputs
• Downstream purity and quantity demands for H_2. • Spatial constraints. • Supply limits on natural gas and other feedstocks.	• Location-specific details for plant design, including access to CCS infrastructure. • Size of the plant, the average production rate of H_2 (long time horizon), and peak production rates.

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• Existing infrastructure. • Time scale of interest.	• Type of production, purification technologies combined to produce H_2. • CO_2 production and transportation rate for transportation and storage. • Total costing of the plant. • Residual emissions from the plant.

These outputs provide key performance metrics that Mr. S could use to identify whether it is a sensible investment or whether an alternative strategy may be more beneficial. This will allow comparisons to be made with the proposed solution and alternative reference designs that may have been suggested to Mr. S. Furthermore, he will also be able to determine how the designed facility is able to cope with variations in supply and demand over the course of shorter time periods such as weeks or days. This allows him to determine intermediary storage requirements and analyse the potential for the designed system to meet peaks in demand. There is also an option for Mr. S to check for the uncertainties in decision-making, using the tools as described in Section 6.3. This allows him to understand the likelihood of an alternative scenario being selected as the optimal solution and the criteria upon which this might occur.

2.3.2 Ms. A – Design of an energy network development case

This particular use case is used to study and analyse the design of a synergistic H_2-CCS system, based largely on existing infrastructure with significant focus on a few applications. Ms. A works in a non-profit research organisation focused on providing sustainable solutions to key technical challenges within the energy and industrial sectors. She would like to propose the development of a large scale H_2-CCS chain network, as a means for reducing CO_2 emissions from domestic heating and industrial sectors in her country. For this purpose, she would like to understand the optimal design of a full-scale H_2-CCS chain network in her country. She has collected data across the whole chain which includes spatially dependent data on H_2 demand profiles, expected CO_2 sources, storage opportunities and infrastructure routes. She would like to use the modelling tool-kit to study and analyse the economic, environmental and energy outputs from the model as a result of her data inputs. Furthermore, she would like to study how this type of infrastructure could support further industrial decarbonisation in many areas in the country. She would also like suggestions on the optimal time-phased development of the network instead of a myopic solution at a certain time to avoid any excessive costs/ investments upfront. Finally, Ms. A would like to understand the utilisation potential of existing natural gas infrastructure within her country in order to minimise the overall investments required.

This type of modelling activity includes inputs and outputs as stated in 2.3.1. In addition, it offers an in-depth analysis on the ability of the designed infrastructure to support further industrial decarbonisation by quantifying storage limits. The tool-kit will provide quantifiable values on:

- Number, size and location of H_2 production plants in the country as well as CO_2 infrastructure during the timeframe of interest.
- The state of the existing infrastructure at a certain point in time.
- Capacity for expansion for both H_2 and CO_2 infrastructure, based on various factors.
- A comprehensive costing for the designed network, including CAPEX and OPEX at plant level. A corresponding level of investment required by funding authorities over a given time horizon will be provided.
- Robustness of the designed network and a portfolio of alternatives using uncertainty analysis.
- The environmental footprint of the designed network and infrastructure.
- Ability of the optimised network to cope with seasonal and more frequent variations in supply and demand – Operational flexibility.

These outputs will utilise both modes of the tool-kit and it will allow Ms. A to form a structured proposal for the design of a large-scale H_2-CCS network.

2.3.3 Ms. L – Operation of the H_2-CCS Network

Ms. L works as a piping and infrastructure engineer in a country which is a large exporter of natural gas. Ms. L would like to use the modelling tool-kit to determine the opportunities for H_2 or H_2 enriched natural gas to meet demands from transport and industrial sector customers from abroad. This is important for them to ascertain since it allows them to decide whether they should continue to export natural gas or whether they should produce H_2 and transport it to their consumers, whilst storing the CO_2 formed locally. An important result that Ms. L would like to establish is whether it is more economically feasible to export H_2 as liquified H_2 or as H_2 enriched natural gas to her international customers. Furthermore, she would like to obtain some specific technical details such as H_2 transportation velocities through pipelines at peak demand periods. Similarly, Ms. L would like to gather information on the necessary technology and infrastructure requirements for the capture and storage of CO_2. She needs to provide her management team with details on economics, safety, reliability and environmental impacts of the project.

Ms. L will benefit greatly from the use of both the design tool and the operational tool. She will initially obtain one of the following decisions – a) Continue exporting natural gas; b) Export H_2. In the former decision, she will largely obtain details on infrastructure requirements for capacity expansion, if needed. Whereas, in the latter case, she will be provided with insights into the joint-infrastructure requirements for H_2 transport, CO_2 transport and storage. Further decisions will help her identify whether CO_2 should be stored near the production facilities, storage sites or even transported to the consumers.

The design mode will provide valuable insights into the economic viability of H_2 transportation via various transportation methods. Moreover, she will be able to provide her managers with a detailed breakdown of total costs associated each of the processing steps. This will eventually, equip them with insights into the most “profitable” physical forms of H_2. Furthermore, with the aid of the operational mode, Ms. L will be able to compute H_2 transport velocities through the pipelines, to check for compliancy with safety and operability standards. This will further assess the technological feasibility of the proposed solution and provide a basis for experimentation and prototyping.

3 MODEL SCOPE & DEVELOPMENT

3.1 Phased Development Trajectory

The overall modelling-toolkit development for the ELEGANCY project is part of a three-year development plan with several key deliverables in the process. The overall modelling tool-kit will be available as an open source modelling tool, containing models which describe a steady state design mode and a dynamic operational mode. The steady state design mode contains multi-scale models with optimisation capabilities. The dynamic operational mode will enable a detailed assessment of the transient behaviour of the designed system at plant/ component level. The overall development timeline is summarised below in Table 2.

Table 2: WP 4 Deliverables, its corresponding descriptions and due dates in months.

ID	Deliverable Title	Description	Due
4.1.1	Functional and Architecture Specification	Describes the key requirements that the modelling tool-kit must meet in terms of the project as well as for the individual case studies in WP 5. It contains three key documents – User Requirements Specification (URS), Functional Specification (FSD) and Technical Specification (TSD).	M3
4.2.1	Performance Metrics	Defines a list of performance metrics that are required to compare the designed network with alternative reference cases.	M3
4.3.1	Component Models	Detailed models to describe the various operations within the H_2-CCS chain, including software for thermodynamic property calculations.	M15
4.4.1	Reduced Order Component Models	Models which are suitable abstractions of the original, more detailed component models in order to generate the higher-level system/ network optimisation model.	M18
4.5.1	First Prototype	A first prototype of the whole chain design and simulation tool with accompanying user documentation to kick-start WP 5 analysis.	M18
4.5.2	Final Modelling Tool-kit	Final version of the design and operational tool-kit, with accompanying documentation and training material.	M36

This document belongs to the first deliverable – Deliverable 4.1.1 and builds on the URS. In this FSD, we discuss the functionality aspects relating to the deliverables starting with Deliverable 4.3.1.

3.2 Component Models Scope – D4.3.1

In this deliverable, both simple static and dynamic models of each element in the H_2-CCS chain will be developed. The development work associated with each of the elements will include specification of the type of element, implementation, followed by testing and verification of model performance. It is important to note that the dynamic models developed in this deliverable will be well suited for individual simulation but will be too detailed for the high-level analysis in design mode. The following lists the functional specifications and scope for Deliverable 4.3.1.

- Provide an in-depth understanding of the various components in the H_2-CCS chain with respect to various performance metrics.
- Identify the performance limitations of a single component along with the interdependence between various types of technologies. For example, limitations on production rates, purity of products, incompatibility of a separation process route for H_2 due to the type of production technology used.
- Simulate the various technologies used for the production, purification, transportation and storage of H_2 and CO_2 separately, and together to identify optimal operating configurations; noting the need for integration of component elements.
- Explore how various component elements affect overall system performance. For example, the effect of the solvent type on CO_2 absorption rate in an absorption column, and its subsequent effects on process efficiency and total costs.

3.3 Reduced Order Component Models Scope – D4.4.1

In Deliverable 4.4.1, component models from Deliverable 4.3.1 will be abstracted to form simpler models that are well-suited for analysis and optimisation using the design mode. The model elements will include – H_2 production, H_2 transport and intermediary storage, CO_2 capture, CO_2 purification, transport, compression and storage processes along with its underpinning thermodynamics. The following points summarise the functional specifications and scope for Deliverable 4.4.1.

- Provide a high-level overview of the interaction between various elements in a network and allow for the specification of constraints, to enable pathway development based on feasible combinations of technologies.
- Establish suitable abstractions of detailed component models so that an effective steady state optimisation-based design mode can be developed.
- Develop an extensive profile of features related to each technology type. An example could include identifying spatial requirements for a steam methane reforming (SMR)

plant of a specified production rate. Furthermore, additional processing requirements due to specific by-product formations from that production route must be quantified.

3.4 Prototype Scope – D4.5.1

The prototype is an integrated high-level system model which contains all the reduced order component models developed in Deliverable 4.4.1. In addition to design and operational analysis, this modelling tool-kit prototype will also be able to perform uncertainty analysis on key system parameters. The following points summarise the functional specifications and scope for Deliverable 4.5.1.

- Determine the optimal development strategy for H_2-CCS chain over time in a system with well-defined boundaries and, simulate its transient behaviour when subject to supply/ demand variations.
- Evaluate the robustness of the designed network by allowing the most sensitive or uncertain system parameters to vary.
- Establish the key operating components which influence the overall performance of the H_2-CCS chain under the various performance criteria.

3.5 Final Tool-kit Scope – D4.5.2

Deliverable 4.5.2 is the final deliverable in the development of the tool-kit. All the above mentioned functional specifications will apply to this deliverable and this final version of the tool-kit will be made available as an open-source modelling framework with accompanying documentation for users. The figure below shows the timeline of model development and interactions between the various deliverables, between month 0 and month 36 of the project.

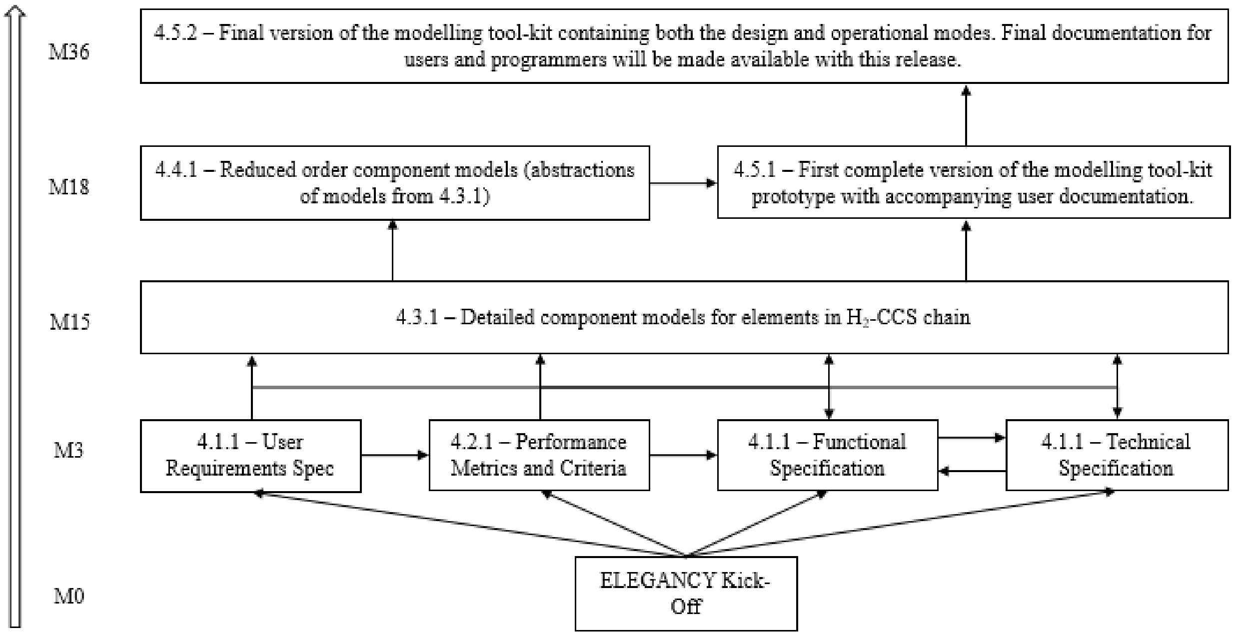

Figure 1: WP 4 deliverables and their interactions on a timeline, shown on the vertical axis.

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4 TOOL-KIT ARCHITECTURE

4.1 Model Architecture

The architecture used for modelling a wide variety of outputs for users are detailed in this section. The design of the modelling architecture is largely based on the Resource-Task Network (RTN) framework, with multiple nodes linking the resources and technologies. 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. The RTN framework can be utilised in Mixed Integer Linear Program (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 upon which the tool-kit will be developed. The use of multiperiod time representation in this framework allows for an effective pathway to be developed and helps to 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. A high-level overview of the modelling architecture can be seen as follows:

- **Resources** – consists of 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 resources in the modelling tool-kit.

- **Infrastructure** – supports the conversion from resources such as natural gas to H_2 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 development or capacity expansion of current infrastructure 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 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 typically 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 at the same scale as industrial combustion units.

- **Demand** – defines a user input which is 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. The demand for a particular physical form of H_2 will affect the transportation, storage and distribution modes of the network. Spatial and temporal variations in demand for H_2 will also impact the optimum infrastructure layout.

Figure 2 shows a stage-wise schematic on how the main elements mentioned above will feature in the modelling tool-kit in the form of a specific route of production, transportation and storage. In 1, natural gas represents one of the primary resources/ feedstocks that are required for the design of the network. A traditional SMR is used as the H_2 production technology, with amine-based absorption of CO_2 in combination as shown in 10. The stream passing 10 to 12 encompasses the various steps that are involved in capture, transport, injection and storage of CO_2 where there are multiple storage possibilities such as saline aquifers, depleted gas fields, etc. Two separate possible routes (2-4-6-8, 3-5-7-9) with various pathways are used to represent the movement of liquid H_2 and compressed gaseous H_2 within the network.

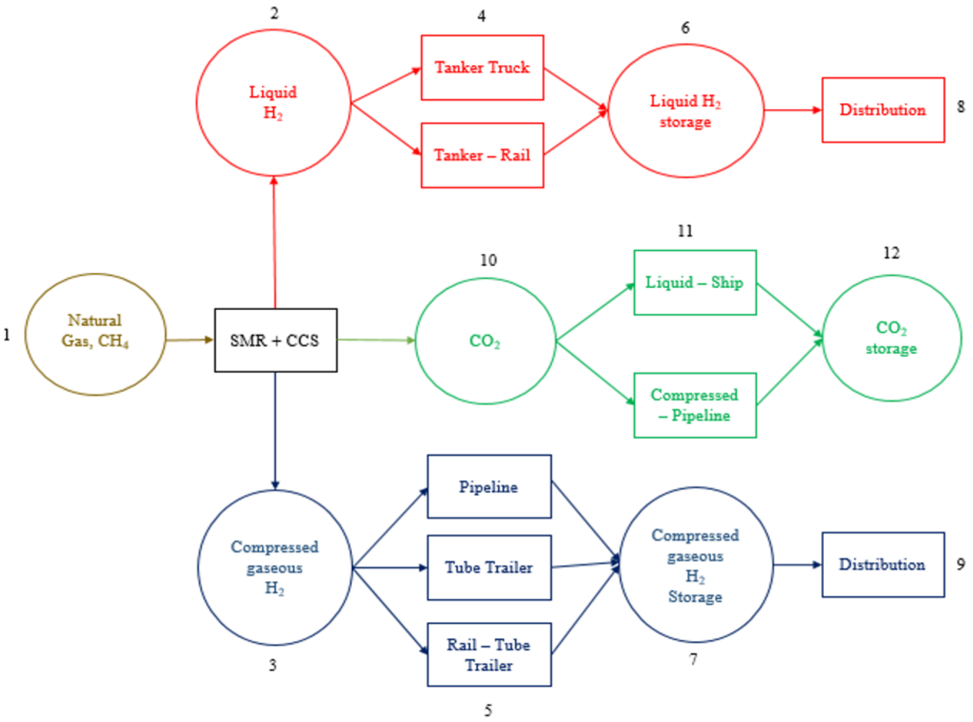

Figure 2: Possible routes to identify the conversion of natural gas to usable H_2.

4.2 Tool-kit Modes

The tool-kit architecture applies to both available modes, although optimisation capability is limited to the design mode. The characteristic features of both modes are as follows:

- **Design** – Uses a simpler steady state model where the user can explore the long-term evolution of system as a pathway with structural changes over time (where the time scale of interest is a user input). Many of the elements mentioned above will feature to a greater extent in the design mode as opposed to the operational mode, although both rely on the same modelling architecture.
- **Operational** – Enables a user to simulate the dynamic behaviour of the designed system with a fixed structure. It will use 1-dimensional (1-D) models to simulate the network so that it is possible to determine how intermittent operation and transient behaviour propagates through the system. It's important to note that this will allow for the operational envelope of the system to be identified along with key operational elements.

The operational performance and system capabilities will also be subject to long and short-term market price variations. Variations in prices will inevitably lead to variations in demand for H_2 and hence, it is necessary to determine the load requirements of the total chain.

5 MODEL INSIGHTS

This section details the key insights from the application of the modelling tool-kit. This is the realisation of model purpose, after incorporating the user expectations from the modelling tool.

5.1 Decision-making Aid for Users

The design mode is used to provide a user with insights on network development as a whole. It will focus on the optimum use of established technologies to form a large scale H_2-CCS chain network which enables the user to develop plans within their national framework. The operational mode will focus more on the technical aspects of operation such as flexibility in plant operation. It will further enable an in-depth overview of the overall operation of the designed system so that a potential user can use it to make informed decisions.

The time horizon for the design mode will typically be an input that the user may decide but most commonly, 5 – 50 years is used. The main outcomes of the model are generated based on the detail provided for inputs such as:

- Current and future demand for H_2 at a local, regional, national and international level.
- Natural gas and feedstock availability at each location at a national level as well as regional and local levels.
- Currently installed technologies, potential conversion and end-use technologies as well as infrastructure, “projects in the pipeline”.
- Planning limitations and constraints due to various factors including socio-economic and political opposition.
- Limits on residual emissions in a particular region due to environmental regulations and other factors.
- Spatial restrictions due to planned development of alternative technologies.

From a decision maker’s perspective, the model provides valuable outputs as it offers a number of potential solutions to challenges in various locations and indicates the robustness of these solutions. It will define the proposed solution for a spatial scale suggested by a user – sector, regional, national or international. This may allow a user to compare the optimum strategies for regions/ countries facing a similar issue and this could spark some mutually beneficial relationships between interested parties. Various model runs with different input scenarios can be compared to identify best and worst-case scenarios. This will provide the user with the knowledge of key criteria upon which an optimum portfolio of technologies is selected over another. This is particularly valuable in decision making, since this can allow for a user to identify an optimal solution based on their insights into factors affecting these criteria.

One of the many benefits of using this sort of approach is that a user will be able to compare mid- to long-term effects of certain input scenario assumptions; and the effects of various input decisions on the model outputs when compared to a “reference” scenario. This supports informed decision-making amongst all the stakeholders who intend to use the model. A range of technology portfolios allow users to have access to alternative solutions which may be easier to implement. For example, in a country with substantial public support for solar technology, it may be easier to implement H_2 production from electrolysis of water using solar electricity. Although it may not be selected as optimum, this highlights the opportunities arising from a variety of solutions that are generated for given regions/ countries. These functionalities will be available in the modelling tool-kit prototype from Deliverable 4.5.1. Additionally, they will be enhanced for use in Deliverable 4.5.2 to accommodate for any further user requirements after application of the prototype to the case studies in WP 5.

The ability to make informed decisions when faced with societal challenges is considered to be extremely useful. The optimum solution from the H_2-CCS modelling tool-kit may represent an ideal solution, rather than one which may be easily implemented. It may not be possible to implement this ideal solution due to various factors including a lack of political and financial support, more stringent environmental legislations, etc. In situations such as this, the tool-kit is still valuable due to its ability to determine the optimal solution given any additional constraints at any given time. This means that although the initial implementation plans may change, it is still possible for users to re-run a scenario and determine the optimum solution and hence, make the best possible decisions, given the circumstances. The economic implications of particular constraints can also be explored. Another significant advantage of the tool-kit is that it provides a platform for effective collaboration with various partners in the H_2-CCS chain network. This can provide an opportunity for stakeholders from various organisations to network and suggest methods to ensure that technologies in consideration are deployed efficiently.

5.2 Analysis of Future Developments

One of the most pertinent applications of the modelling tool-kit will be to analyse planned developments or “projects in the pipeline” as an input scenario. This will enable the user to analyse a scenario where there are multiple constraints on future development opportunities for H_2-CCS infrastructure in a spatial element. This may be due to planned developments for alternative technologies or simply due to an area being unavailable for use. A scenario such as this can be compared with the results from an unconstrained scenario to provide key outputs to decision-makers. This enables them to understand the wider impacts of their decision-making on future projects as well as obtain an evolving snapshot of the system, starting with its initial layout. Further ideas to include in such analysis may incorporate variations in H_2 market prices, technological improvements, new technologies, introduction of new nation-wide policies, etc. These changes can have tremendous impacts on the nature of the solution obtained so users should understand the significance of incorporating the highest level of detail that they possibly can.

In the tool-kit, such internal and external changes can be incorporated by creating user defined input scenarios for a select number of changes. This can be captured as absolute data values for entries related to future, i.e. a unique input for a distinct time point in the future.

An example entry could potentially indicate that the maximum number of H_2 production units in spatial element "X" at 2050, must be less than 5. Alternatively, this can be included as a rate of change relating the rates with which these changes were introduced in the past how they are expected to be introduced in the future. These user inputs are then translated into changes into model parameters which will update its operation so that the optimum solution reflects such change led scenarios. The user can create their own scenarios by combining various input decisions present in the model. It is possible for a user to alter the existence of input decisions affecting network behaviour. Input decisions are used to form the initial picture as well as provide technological solutions and investment decisions at various time points. Furthermore, it can be useful to study the effect of time on the implementation potential for various H_2-CCS technologies.

5.3 User Insights – Key Questions

This tool-kit once applied to a case, should provide its users with the optimal solution to the area under analysis with detailed breakdown on its performance under various metrics. However, a key insight from the tool-kit will be to recognise some of the biggest challenges facing the development of a full-scale H_2-CCS network. Users will obtain a solution and more importantly, they will have the ability to understand the trade-offs which led that particular solution to be optimal. This also highlights the most important issues which needs to be addressed in order to improve the feasibility of alternative technologies. Additionally, it will quantify the barriers to entry for the type of technology. When reference solutions are provided by the user, the optimisation result will highlight the main differences between itself and the reference and indicate opportunities for improving its performance by adjusting some factors under control. The use of the tool-kit to provide information with relation to specific use cases should address various dimensions as shown below:

- How much emissions reduction can be expected from a large-scale H_2-CCS in country X as opposed to using natural gas for the application? What are the cost implications?
- What are the fluid velocities for H_2 in pipelines during peak demand and how does that compare to natural gas?
- How much more expensive is it to use H_2-CCS instead of natural gas for meeting domestic and industrial usage demands? Where are the cost pinch points?
- How much additional NO_x formation can be expected when using natural gas and H_2 blends?
- How scale-dependent are the production technologies for H_2? Is it always cheaper to use SMR or should another technology be used?
- Is it better to produce H_2 centrally and distribute it or is it more feasible to transport natural gas and convert to H_2 using local conversion technologies? Alternatively, should these conversion facilities be placed near CO_2 storage reservoirs for easier

injection and storage opportunities or does the choice of location have negligible effects?

- How much pollution can be reduced from the transportation sector in country Y if everyone used FCEVs and subsequently, what is the investment required for developing the infrastructure to support that?

- Which process technologies are thermodynamically the most efficient and more importantly, are we operating near the maximum possible thermodynamic efficiency? If not, what are the limiting factors?
- How will market price for H_2 in the future affect the type of production technology selected? Will it become cheaper to produce H_2 from large scale electrolysis of water in the future?
- What is the most economical and safe method for intermediate storage of H_2?
- What are the key concerns or technological considerations that need to be addressed when considering joint infrastructure design for H_2 and CO_2?
- Can H_2 be transported more effectively as part of a different compound such as ammonia?
- What are the safety risks associated with large scale deployment and use of H_2-CCS systems? How does it compare with existing natural gas systems?
- Are the same process technologies used to produce H_2 throughout the year or do they vary?
- Which resources need to be stored and how much storage capacity needs to be ensured for these resources?
- How might a greater penetration level by solar PV or other renewable electricity affect the H_2 market? Will this have a noticeable effect on the type and scale of optimum production technologies in the network?
- Which is more expensive – building another production facility at a certain location or building the necessary infrastructure to transport certain quantity of H_2?

It should be noted that further manipulation of output data and results will be required by the user in order to answer several of the questions above. Consequently, these are mainly targeted towards expert users, who are the intended users of the tool-kit. These questions are by no means a conclusive list but the importance is to recognise that they range from system/ network level questions to technical questions at a plant level. This cannot be addressed by single scale modelling and hence, the design and operational modes will be of great importance here. The main benefits of using a multi-scale modelling approach is that a user can combine the insights obtained from various scales to ensure that their confidence levels in decision making is improved.

5.4 Current/ Initial State of the Area

To initialise the modelling tool-kit, a user needs to provide data that is concerned with the list of available resources, infrastructure, etc. Upon initialisation, it's possible to form a visual map of the resources and infrastructure with spatial information to provide a snapshot of the current situation. This is a useful outcome since it is possible to identify clusters of activity without actually running a case on the tool-kit.

Firstly, a geospatial map of resources and infrastructure will be developed where it is possible, so that it is possible to pin point each location at its appropriate spatial resolution. For this purpose, a Geographic Information System (GIS) methodology can be employed. GIS is a very useful approach for identifying relevant infrastructure, scale of the system and the input and output locations such that resource flows can be effectively mapped out and simulated. This has the added benefit of capturing the scale of operations for detailed local/ regional analysis as well as national or international systems. Some of the input data features of a spatial element or a "cell" can be summarised below:

- The spatial coordinates of the elements (normally as two spatial co-ordinates in x and y).
- Demand or expected demand for H_2 at the element/ node at a given time point.
- The type of element – industrial, domestic, service, road, etc.
- Maximum production capacity at an element over time.
- Emissions of CO_2 at the element over time.

Following optimisation, the tool-kit will yield some useful insights including the following:

- Annual production rate of H_2 and capture rate of CO_2 at an element any given time.
- Injection and storage rates of CO_2 at a given element at any given time.
- The number of H_2 production facilities present at an element at time, t.
- If a capture/ storage facility is recommended to be built at that element at time, t.

It is also possible to use GIS as key input information for running cases on the modelling tool-kit. A comprehensive GIS will allow for the extraction of data based on point sources on a geographical map and form distinct entities which are analysed using the optimisation algorithm. The generated results can be easily visualised afterwards to provide insights into the optimum solution that is generated. However, it should be noted that the spatial resolution of the gathered data may not always translate to that used in the model. The design mode will sometimes have spatial elements that are of lower resolution whilst capturing the same details using aggregated values for each of the features mentioned above. This is mainly due to the additional complexities associated with running such a large set of data points.

6 MODEL OUTPUTS

6.1 Performance Metrics

The algorithms used in the design mode will generate a spatial and temporal overview of network performance over long time scales such as 5 – 50 years. The outputs will be categorised under various performance criteria that are relevant to H_2-CCS systems. These performance metrics can be used to assist users in decision-making with regards to the implementation of H_2-CCS systems. The use of existing or familiar performance metrics can provide stakeholders with an improved understanding of the nature of the optimal solution. This allows them to compare the merits of an optimal technology with alternatives and form their own judgement on the quality of these solutions. This can eventually lead to the development of a feasible business model to enhance the deployment of H_2-CCS systems.

The attractive feature in decision-making for users is that it is possible for them to improve on the level of detail presented under each performance criterion or even create their own. Following the release of the prototype tool-kit, users can apply it and identify improvements which can be passed on to the development team. The development team will further ensure that these additional metrics are incorporated before the final release of the modelling tool-kit. If the development team were not able to capture these recommendations to the extent required by a user, then it is also possible for the user to modify it themselves using the user documentation, which contains instructions on the addition of any generic, performance metrics and their computation methods. A detailed specification of various types of performance metrics will be presented in Deliverable 4.2.1.

6.2 Output Decision Variables

A provisional list of output variables from the both design and operational modes will include the following from Table 3.

Table 3: Output variables from both design and operational modes of the tool-kit

Design Mode	Operational Mode
• Total capital expenditure for building a H_2 production or CO_2 capture, storage facility of a certain type within a spatial element. • Annual capture and storage rates of CO_2 in each spatial element at time, t. • Annual transportation rates of CO_2 and H_2 between different spatial elements at time, t. • Decision variables to indicate whether a production, capture or storage facility should be built in each spatial element at time, t.	• Process throughput, consumption rate of resources and energy requirements on a day by day basis. • Thermodynamic efficiencies of all process units designed. • Time series data on temperatures, pressures and flowrates/ velocities of all streams. • Energy and feedstock requirements. • Identification of the operability limits

• Decision variables to indicate which of the existing H_2 production or CO_2 infrastructure should be used. • Decision variables to indicate if existing H_2 production plants should be retrofitted with CCS. • For specific applications of H_2 such as transportation fuel, the number of specific refuelling stations across the studied landscape. • Transportation links that are necessary to establish the network. • Total CO_2 emissions from individual units/ processes and the designed network.	for safe and reliable operation. • Fatality rates and risk analysis. • Process outputs when subject to internal and external disturbances in the system. • Additional control needs and measures required for the process units.

6.3 Uncertainties in Outputs

It is important that users of the toolkit understand the range of uncertainty in the output results. To this end, users must understand that the model elements are developed from abstractions of more detailed models and hence, in reality, the designed process/ unit may not be operating under the conditions that are modelled. The most frequent amongst such variations from the "ideal" case can be expected to occur in process units and in an unpredictable manner. For example, the conversion rates of a SMR unit may be lowered to a value well below the expected rate over the course of a few months of operation due to catalyst deactivation and other issues such as fouling. Many of these effects are difficult to capture in detail in the model due to the complexities that are involved. However, they cannot be ignored. At its best, the random inherent variations within the processes and sub-processes are often harmless and may lead to an increase in total costs as a result of increasing primary resource consumption. At its worst, however, such variations can have tremendous impacts on the overall safety and operation of the infrastructure. Stochastic simulations can be used to improve the accuracy of model predictions and account for such random variability. Stochastic simulations aim to capture the uncertainties which may arise from the nature of these processes at smaller time scales by performing multiple simulations with similar inputs and mapping the outputs. The main benefit of this methodology is that it is possible to infer the variations in output solutions and identify the level of flexibility present in the system. Increasing the number of simulations will improve a user's confidence in model outputs. In addition, it is possible to quantify the likelihood of deviations from an "average" output and inform users on the reliability of model predictions. Furthermore, it is particularly useful for identifying the most important parameters influencing the performance of the system.

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