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Executive Summary

This document formally describes the user requirements for the modelling tool-kit as part of work package 4 (WP4) of the ERA-Net ACT ELEGANCY project. The purpose of this User Requirements Specification (URS) is to reflect the requirements of the users in detail, and provide a basis for the development of the Functional and Technical Specifications. The URS will be used by the modelling team to ensure that the development of the modelling tool-kit meets all the required criteria. The intended initial users of the tool-kit are members from the relevant case study teams who will apply the tool-kit to deliver key insights in relation to this project. However, the tool-kit will be designed to be used by a range of expert users interested in the topic of H_2-CCS value chains. This URS has been developed in consultation with all anticipated future users of the modelling tool-kit to ensure that their requirements are captured. These specific requirements are characterised as: requirements by user category; scenarios that the tool-kit needs to be able to address; input and output requirements for the tool-kit; and requirements for the software environment itself.

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TABLE OF CONTENTS

Page No.

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.

1 INTRODUCTION

The main aim of the ELEGANCY project is to accelerate the deployment of Carbon Capture and Sequestration (CCS) technologies in Europe through H_2-CCS chain networks. ELEGANCY will conduct research and provide solutions to the commercial, technical, legal and social challenges associated with rapid deployment of H_2-CCS chain networks. Furthermore, ELEGANCY will develop an innovative, open-source modelling tool-kit containing multi-scale models, that can design the optimal time-phased evolution of H_2 systems with CCS. Subsequently, the research findings, tools and technologies will be applied to five national case studies, to inform the members of the ELEGANCY consortium on the optimal approach to decarbonise a wide variety of sectors.

The ELEGANCY modelling tool-kit will enable the evaluation of an integrated H_2-CCS chain network with respect to technological and economic efficiency, operability and environmental impact. For this purpose, an open-source systems modelling framework, containing a steady state design-optimisation mode and a dynamic operational mode, will be employed. These two modes will require two different software environments and they are currently assumed to be Pyomo and OpenModelica. The rationale behind the selection of these softwares are detailed in the Technical Specification, also part of Deliverable 4.1.1. The tool-kit will incorporate results from Work Packages (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 investigate the performance flexibility as well as the transient behaviour of the system.

The following content details the User Requirements Specification (URS) for the modelling tool-kit in relation to the ELEGANCY project. The URS is intended to define the overall user requirements and provide details of the various types of intended users of the modelling tool-kit. It will give a detailed overview of the input-output analysis that a potential user would require. The URS will serve as a constant reference for the design and development activity by the WP4 team. The user requirements are identified from the ELEGANCY proposal document along with discussions between various work package teams during the Kick-Off meeting. This document will be periodically updated, in particular to reflect developments in WP5 and the needs of the national case studies.

A working prototype of the tool-kit will be made available for use by month 18 of the ELEGANCY project. Following which, it will undergo further developmental reviews to ensure that it adapts to the evolving needs of its users as the project progresses.

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2 USER CATEGORIES

A key result from the process of developing this URS was gaining an understanding of the intended users of the tool-kit. This section describes the anticipated user types and their corresponding requirements. All users will be able to run design optimisation of Mixed Integer linear programming (MILP) model instances through Pyomo (most likely platform) and dynamic simulations through OpenModelica (most likely platform). Although all users will be able to simulate, the functions that are available to each user type are different and they are summarised below. Appropriate training material and documentation will be provided for all users.

2.1 Basic User

A basic 'Engineering-level' user is a user who has very little or no knowledge of the modelling methodology behind the modelling tool-kit but understands how to specify the required inputs and handle the outputs. This type of user would, potentially, require a more developed user interface than an Expert user (discussed below) as much of the detail of the modelling process will be hidden, while still being able to do the same analysis. During the setup of an investigation, a basic user will typically be able to:

- Create and edit various existing cases, which consists of a combination of technologies to represent national H_2-CCS chains and the case study boundary conditions (e.g. hydrogen demand), by selecting from options of available system components.
- Obtain outputs from the simulated cases in a familiar format.

Basic users are not the targeted users of the tool-kit in this project and hence, the modelling tool-kit may require further developments before it is able to meet all the abovementioned criteria.

2.2 Expert User

An expert user is identified as a user who understands the methodology behind the modelling-toolkit as it is used in the modelling process and preferably, has some experience of dynamic and optimisation modelling. This will place them in an ideal position to be able to interact more closely with the modelling process and they will, potentially, require a less developed user interface. These users are the focus of this project's development activity.

During the setup of an investigation, an expert user will be able to:

- Configure new cases by assembling different system elements with tailored parameter specifications for those elements.
- Edit the model equations and parameters describing the behaviour of each element.
- Add a new type of element (an element could be a new production technology, a new storage technology, etc.).

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3 REQUIREMENTS

This section will outline some of the typical use cases and scenarios for the modelling tool-kit, as well as a discussion of the scenario defaults that can be edited by a potential user. It also gives examples of the expected inputs for the model from the relevant case study teams in WP5. More detailed information on functionality and architecture are provided in the Functional and Technical Specifications.

3.1 Scenarios and case studies

The following use cases are examples of the type of investigations for which the user would want to use the modelling tool-kit. The tool-kit should be able to provide insights about the trade-offs between different factors and how those trade-offs affect system performance (measured in various ways, see section 3.3 below). The modelling tool-kit will be designed to provide some key insights related to the five national case studies within WP5, as summarised below.

3.1.1 Netherlands

- Large scale production of hydrogen with substantially reduced CO_2 emissions.
- Development of infrastructure for CO_2 storage and reuse.
- Roadmap development for the case study.
- Analysis with regards to sizing and economy of scale in the existing offshore and onshore facilities.

3.1.2 Switzerland

- Decarbonisation of the road transport sector by utilising H_2-CCS chain networks.
- Potential and usability of biomass as feedstock
- Acceleration of the CCS/ geothermal roadmap.
- Understand the safety and economic viability of saline aquifers and targeted geothermal fields.
- Provision of supporting material for the CO_2 storage and CO_2-geothermal field tests.

3.1.3 United Kingdom

- Development of strategies to deal with the inherent uncertainty of complex H_2 – CCS networks, particularly concerning the goals of the H21 Leeds City Gate Project.
- Energy network development for the Leeds area while exploring the system integration issues.
- Industrial feasibility study on the potential for CCUS and H_2 solutions in Grangemouth, Scotland.

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3.1.4 Germany

- Decarbonisation of the existing gas infrastructure as well as an assessment of the potential for new 100% H_2 based networks and corresponding infrastructure requirements.
- Utilisation of infrastructure in Rotterdam region for decentralised CO_2 capture and storage from large point source emissions in Germany, especially the north Rhine region.
- Assessment of the technical challenges associated with the introduction of H_2 via the high-pressure transport grids.

3.1.5 Norway

- Identify the opportunities for H_2-enriched natural gas in the Norwegian industry as well as for exports.
- Determine the nature of an optimal H_2 distribution network within Europe and analyse Norway's role in this network considering its capabilities for H_2 and CO_2 production, transport and storage.

3.2 Default Values and data input

For components of H2-CCS chains and comparative "reference systems", the default values should be based on a set of agreed component elements. It should be possible to select between many predefined elements. The model elements will include production facilities for H_2 as well as storage facilities for both H_2 and CO_2 as well as relatively high-level representations of end-use technologies (in particular capturing purity requirements). It will also consider feed sources, transportation modes and distribution of H_2 and CO_2. The user should be able to edit the defining parameters of such elements by inputting new values. Different user types (Basic or Expert) will be able to edit different levels of data. Potential users will be expected to provide a range of inputs when using the modelling tool-kit. These inputs include, and are not limited to, the following:

- Geographical location and proximity to energy sources within a particular region.
- Demand for H_2 applications with time (overall demand from transport, heating, industrial, etc.).
- Locations, sizes, types of existing H_2 and CO_2 production, transportation and storage facilities within a region.
- Time scales of interest. For example, 2020 – 2035 or from 2020 – 2050 in 5 year intervals.
- "Reference system" or "Business as Usual" scenarios indicating existing infrastructure that is currently used to meet the national demands.

An expert user will have the ability to constrain and set upper and lower limits for sizes of production, transport and storage facilities as well as interact with many of the model

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elements mentioned above. Furthermore, both user types can constrain the system such that hydrogen is produced to meet a desired purity/ specification for use. All other elements of the system will follow the same design procedure, with multiple predefined defaults and the ability to edit values. For multiple scenario runs, the user should be able to define either a table of values to investigate, or define an allowable range of values for each parameter in order to perform sensitivity analysis.

3.3 Outputs

The outputs of the modelling tool-kit are expected to cover a range of formats for different user types. It is expected that the outputs will be written to a database or similar structured file for later interrogation, with some analysis being carried out within the toolkit. This could utilise typical data formats such as CSV or text files so that software such as Microsoft Excel can be used to perform any further analysis that are specific to the case study. Expert users will be able to use the solution reports directly from the utilised software, whereas a basic user will receive outputs via a more developed platform. Expected outputs for each scenario include, and are not limited to:

- Setup information to identify the investigated system.
- Optimal design results, across a range of user-defined objectives (e.g. cost, environmental impact, energy efficiency, etc.).
  - Number, location, type and size of H_2 production, CO_2 capture facilities built in a region at different time scales.
  - Production and transport rates of CO_2, H_2, CH_4, etc. at different times.
- Dynamic simulation results.
  - Transient system response to variations in demand and supply.
- Time series data of key system variables of interest:
  - Temperature, Pressure, etc. for the various components.
  - Input – output flows of all species including H_2, CO_2, H_2O and CH_4.
  - Component efficiencies, production rates, transport rates, etc.

Similarly, the output results mentioned above will contain a wide variety of performance metrics to enable an integrated assessment using a holistic approach. These performance metrics are grouped into the following macroscopic dimensions as shown in Table 3.3.1.

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Table 3.3.1: Performance criteria within the various dimensions.

Economics	Environmental
• Cost metrics – production costs for a unit of H_2 at a desired purity level. • CAPEX and OPEX for design and operation, inclusive of network costs (independent of commodity prices). • Scalability of design. • Industrial competitiveness and growth potential measure.	• Energy intensity. • Material consumption per unit of product. • Key pollutant emissions and emission reductions per unit of product or service. • LCA indicators (Mid-point, End-point).
Energy Security	**Thermodynamics**
• Supply factors and confidence intervals (to be defined in more detail). • Time-phased evolution of supply conditions.	• 1st Law efficiency. • 2nd Law efficiency.
Geographical	**Technical**
• Demand for H_2 and potential reservoirs for CO_2 as well as H_2 storage. • Extent of utilisation of the existing natural gas reserves as well as infrastructure. • Infrastructure and upgrade requirements based on the type of existing pipeline material (Cast iron, HDPE)	• Safety and operability. • Reliability and risk analysis. • Barriers to entry. • Technology readiness level (TRL).
Social	**Policy**
• Social costs of carbon pollution – discounted value of economic costs from additional unit of CO_2 or equivalent emissions. • Ability to fit with the current and future ecosystem of low – carbon alternatives.	• Regulations and incentives. • Carbon pricing.

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3.4 User interface and interaction

This section summarises how the user will interact with the tool-kit to specify input data and other scenario elements, review the results and store the data associated with a run. It is expected that the different levels of users discussed above will do this in different ways. ‘Basic users’ should be able to carry out all of the tasks they need to be able to do, using familiar software (e.g. Microsoft Excel). It is expected that ‘Expert Users’ are likely to have to interact with the environment in which the modelling tool-kit has been developed to carry out some activities while others are done from a similar interface as the ‘Basic Users’. The results of the modelling should be stored in a database, as discussed in the Outputs section above, for later interrogation.

Currently, Pyomo is the software that is assumed to be used for the design mode and it requires at least Python versions 2.6 or 3.2. Additionally, installation of a scientific Python distribution is recommended by the design team. Both Pyomo and OpenModelica will run on Windows, Linux and MacOS operating systems. The modelling tool-kit will be designed to be run on a high-performance desktop PC and if such resources are not available, a dedicated desktop PC could be accessed and used remotely by users.

3.5 Future extensions

Following the initial development of the modelling tool-kit, it will be placed in the public domain with accompanying user documentation and will be made available for future extensions.

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